

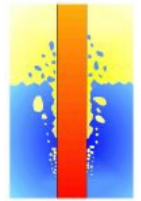


## **30<sup>th</sup> International QUENCH Workshop**

16-18 December 2025  
Karlsruhe Institute of Technology  
Karlsruhe, Germany

**Editor: Martin Steinbrück**

DOI: [10.5445/IR/1000189487](https://doi.org/10.5445/IR/1000189487)



## AGENDA

### 30<sup>th</sup> International QUENCH Workshop

Karlsruhe Institute of Technology, Campus North, H.-von-Helmholtz-Platz 1, 76344 Egg.-Leopoldshafen, Germany  
16-18 December 2025

**Meeting Location:** Fortbildungszentrum für Technik und Umwelt (FTU), Auditorium (Aula)

#### *Tuesday, 16 Dec 2025*

8:30	<b>Registration</b>	
9:00	Welcome	M. Steinbrück, W. Tromm, KIT
9:10	Update of the QUENCH Program	M. Steinbrück, KIT
	<b><u>JUBILEE SESSION 30 YEARS QWS</u></b> (Chair: F. Gabrielli, KIT)	
9:30	History of nuclear research in Karlsruhe (working title)	M. Popp, invited
10:00	Overview of the CODEX experimental programme	Z. Hozer, HUN-REN
10:30	<b>Coffee break (Group Photo)</b>	
11:00	Materials science for nuclear safety. From unexpected findings to improved severe accident codes	M. Steinbrück, KIT
11:30	The importance of taking into account the temperature gradient on the processes occurring in the cladding tube during high-temperature oxidation, melting and mechanical deformation	J. Stuckert, KIT
12:00	Neutron imaging investigations of hydrogen in cladding tube materials	M. Grosse, KIT
12:30	From QUENCH-01 to QUENCH-ATF-2: Three Decades of AC <sup>2</sup> /ATHLET-CD Validation using QUENCH Experiments	T. Hollands, GRS
13:00	<b>Lunch</b>	
	<b><u>LONG-TERM DRY STORAGE – SYSTEM ZR-H</u></b> (Chair: D. Schaefer, KIT)	
14:00	The SPIZWURZ project, overview and single effect tests	M. Grosse, KIT
14:20	Experimental results of the SPIZWURZ bundle test	J. Stuckert, KIT
14:50	Hydride Morphology in Zirconium Tubes After SPIZWURZ Bundle Tests: Experimental Data and Preliminary Simulation Results	M. Kolesnik, KIT
15:10	SPIZWURZ Benchmark	A. Rezchikova, GRS
15:30	<b>Coffee break</b>	

16:00	Hydrogen in Claddings - Investigations on Hydrogen Axial Mobility, Role of Liner and Creep	J. Bertsch, PSI
16:30	Dedicated investigation of secondary hydriding: Experimental insights and modelling	M. Kpemou, ASNR

**Wednesday, 17 Dec 2025**

**MODELLING AND CODE APPLICATION I** (Chair: M. Cazado, KIT))

9:00	Expanding the Capability of the ASTST VER3.5 System Thermal Hydraulic and SCDAPSIM Modeling Options to Support the Fukushima Daiichi Decommissioning R&D Analysis and Assessment	R. Pericas, ISS
9:20	Analysis of the COAL Reflooding Experiments: Recent Simulations with AC <sup>2</sup>	G. Stahlberg, RUB
9:40	Validation of AC2/ATHLET using QUENCH data	L. Lovasz, GRS
10:00	Modeling of QUENCH-06 and QUENCH-20 tests with RELAP/SCDAPSIM, Focus on Bundle Asymmetry	T. Kaliatka, LEI
10:20	<b>Coffee break</b>	

**MODELLING AND CODE APPLICATION II** ( Chair: L. Lovasz, GRS)

10:50	Infinite lattice depletion of accident-tolerant fuel pin-cells with OpenMC and cladding inventory analysis with FISPACT-II	P. Bochtler, BASE
11:20	Simulation of Cr-coated Zry-4 cladding tube ballooning and burst behavior using MERCURY	D. Lee, KAERI
11:40	Simulating Cr-Coating Behavior with AC <sup>2</sup> : From QUENCH Analysis towards Integral Plant Application	G. Stahlberg, RUB

**EXPERIMENTS** (Chair: L. Lovasz, GRS)

12:00	COSMOS-H first experiments at the new thermohydraulic facility	S. Gabriel, KIT
12:20	Synergistic influence of oxygen, hydrogen and microstructure on thermal shock behavior of PHWR cladding subjected to integral LOCA test	T. Sawarn, BARC
13:00	<b>Lunch</b>	
14:00	Technical tour to FR2 Nuclear Museum and KATRIN facility	
17:30	<b>Dinner (Restaurant Ritter, Büchenau)</b>	

**Thursday, 18 Dec 2025**

**ATF CLADDING I** (Chair: M. Grosse, KIT))

9:00	Results of the IAEA Coordinated Research Project (CRP) on 'Testing and Simulation of Advanced Technology and Accident Tolerant Fuels (ATF-TS)' (2020–2024) and Plans for the Next CRP"	A. Khaperskaia, IAEA
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9:30	Separate effects tests with ATF cladding materials within the IAEA ATF-TS CRP	M. Sevecek, CTU
9:55	Development Status of Accident-Tolerant Control Rods in Light Water Reactors at CRIEPI	K. Nakamura, CRIEPI
10:15	Post-test examination of the integral air ingress experiment CODEX-ATF-AIT	R. Farkas, HUN-REN
10:30	<b>Coffee break</b> <b><u>ATF CLADDING II</u></b> (Chair: M. Sevecek, CTU)	
11:00	Accident tolerant fuel: Cr coated cladding development at Westinghouse	K. Frederick, WEC
11:20	Oxidation and degradation of Cr-coated zirconium alloy: Effect of Cr thickness	M. Steinbrück, KIT
11:45	Effect of initial Cr-coating thickness on the high-temperature steam oxidation behavior of Cr-coated Zr-based alloys: Comparison between TGA experiments conducted at several institutes using “Equivalent Chromium Reacted” (ECrR) parameter	J.-C. Brachet, CEA
12:10	Steam Oxidation of Cr-Coated Zircaloy-4 Rods Across a Wide Range of Heating Rates	D. Bachurina, KIT
12:30	Multiscale Insights into Embrittling Mechanisms of Cr-Coated Zircaloy Cladding under Ultra-High Temperature Conditions	T. Liu, SJTU
12:50	<b>Lunch</b> <b><u>ATF CLADDING III</u></b> (Chair: D. Bachurina, KIT)	
14:00	Behaviour of Fuel Cladding with Cr Coating during LOCA and Study of Oxygen Diffusion into Zr-alloy using Different methods	V. Boucek, UJP
14:20	High-Temperature Oxidation of Cr Coated Claddings with Interdiffusion Barrier & Solute (Al, Si) Additions	B. Nowak, Queen’s University
14:40	Experimental Observations on the CHF Performance of Cr/ CrN-Coated Zircaloy-4 in Low-Pressure Flow Boiling	N. Wefers, KIT
15:00	Update of the KIT contributions to the SCORPION project	M. Grosse, KIT
15:30	<b>Closure of the Workshop</b>	M. Steinbrück, KIT

# 30th International QUENCH Workshop





**Martin Steinbrück**

**KIT**

## **Update of the QUENCH program**

The 30th International QUENCH Workshop, held at Karlsruhe Institute of Technology (KIT) from December 16–18, 2025, provided an update on the QUENCH program, which focuses on reactor safety research under severe accident (SA) and design-basis accident (DBA) conditions. Key topics included experimental investigations on Accident Tolerant Fuel (ATF) cladding concepts, long-term dry intermediate storage of spent fuel, and modeling for code validation. The talk highlighted recent advancements in bundle and separate-effects tests, including high-temperature oxidation and quench experiments on ATF materials such as Cr-coated ZIRLO, FeCrAl, and SiC composites. International collaborations under OECD-NEA, IAEA, and EC projects were emphasized, alongside progress in hydrogen behavior studies during extended storage and neutron radiography campaigns. Future directions involve Phase 2 of QUENCH-ATF, safety research for Small Modular Reactors (SMRs), and integration with fusion programs. These efforts aim to enhance accident management strategies and support the development of robust safety concepts for current and next-generation nuclear systems.

# Update of the QUENCH program

**M. Steinbrueck, J. Stuckert, M. Grosse, D. Bachurina, D. Schaefer**

*30th International QUENCH Workshop*

*Karlsruhe Institute of Technology, 16-18 Dec 2025*



# Outlook

- Current topics
- Experimental facilities
- ATF activities
- Long-term dry intermediate storage activities
- Modelling / Code validation
- Reporting
- Future planning

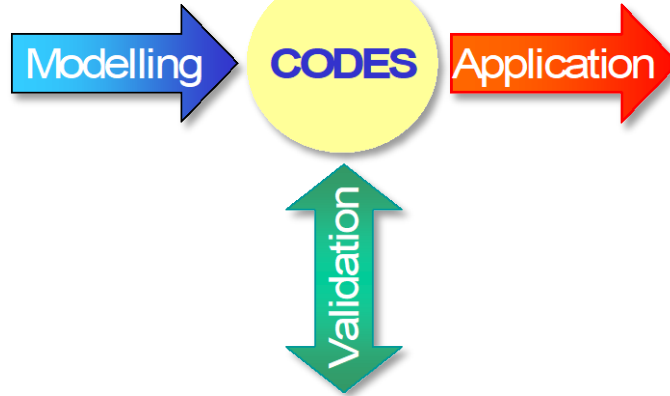




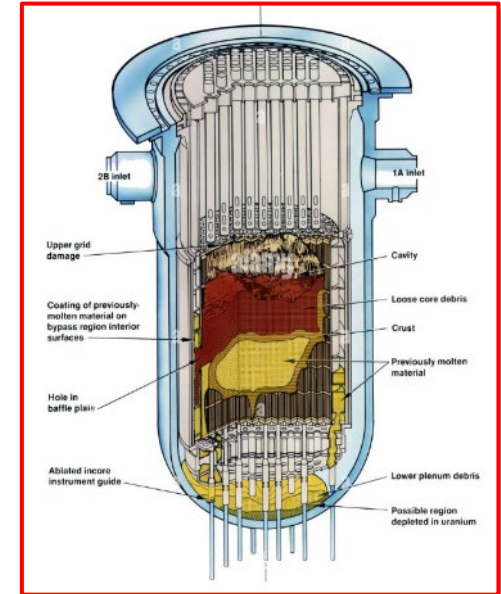
# QUENCH program



Separate-effects tests



Bundle experiments



Application for simulation of nuclear accident scenarios

# Current topics

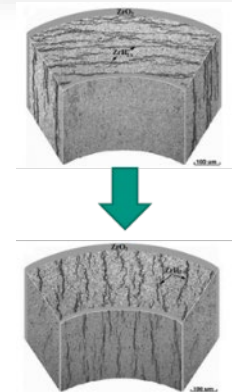
## ■ Accident tolerant fuel (ATF) cladding

- ATF research after Fukushima Daiichi accidents
- Characterization of promising ATF cladding concepts at (very) high temperatures
- Degradation mechanisms and kinetic data
- Max. temperature and coping time for AMMs



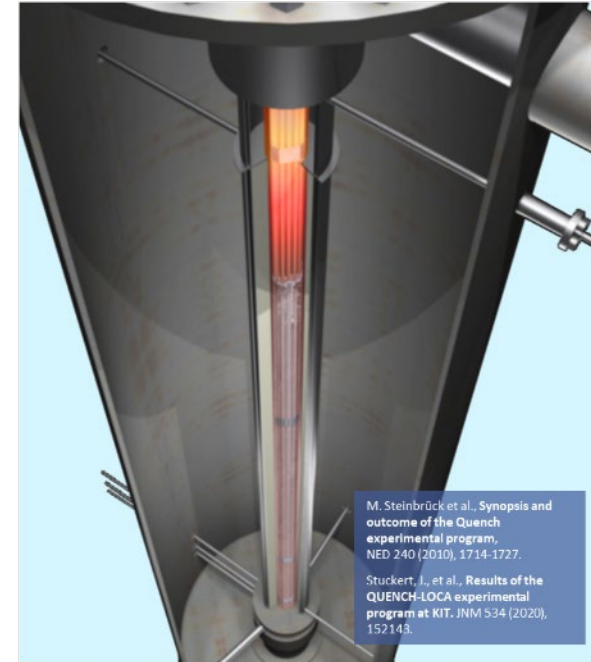
## ■ Long-term dry intermediate storage

- No final storage on the horizon in Germany and many other countries
- Hydrogen/hydride behavior in Zr cladding during 50-100 years storage e.g. in CASTOR casks
- Hydride reorientation and its effect on mechanical properties



# QUENCH/LICAS facility

- Unique out-of-pile bundle facility to investigate reflood of an overheated reactor core
- 21-31 electrically heated fuel rod simulators;  
T up to >2000°C
- Extensive instrumentation for T, p, flow rates, level, etc. + MS
- So far, 20+1 experiments on SA performed (1996-today)
  - Influence of pre-oxidation, initial temperature, flooding rate
  - B<sub>4</sub>C, Ag-In-Cd control rods
  - Air ingress; debris formation
  - Advanced cladding alloys & ATF
- 7+1 DBA LOCA experiments with separately pressurized fuel rods
- Upgrade of PC's and control software



# Experimental setup for ATF research (SET)



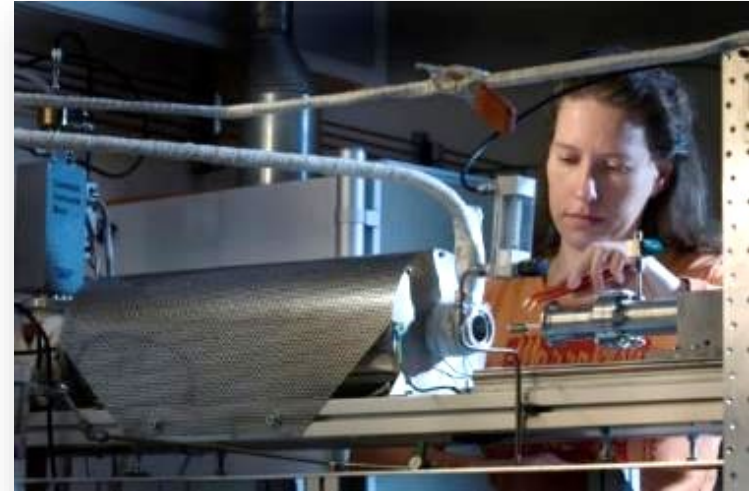
## QUENCH-SR

- 10-15 cm cladding tube segments
- Fast inductive heating up to 2000°C
- Water quench



## DTA-TG systems

- Max. temp. 1600°C (1250°C in steam)



## Tube furnaces

- Max. temp. 1600°C (all atmospheres)
- Sample airlock

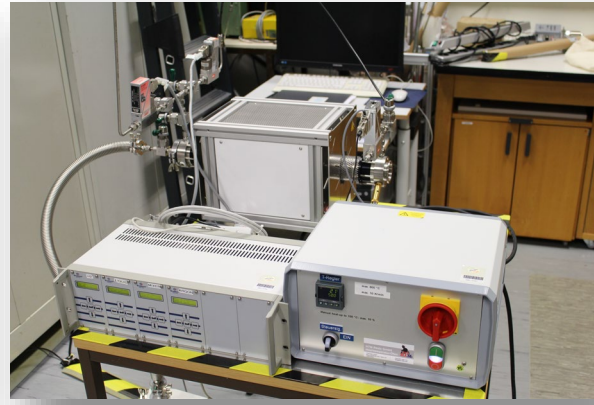
All systems with water steam supply and mass spectrometer coupling

# Test facilities for long-term storage research



## INCHAMEL

- Apparatus for in-situ neutron radiography experiments under defined mechanical load and temperature



## VAKO

- Sieverts chamber for hydrogen loading of small Zry samples



## HOKI

- 2.5 m long furnace for hydrogen pre-loading of cladding tubes for bundle tests

# QUENCH activities on ATF cladding materials

- Bundle tests in the framework of OECD-NEA QUENCH-ATF
- Single-rod oxidation and quench tests of ATF cladding segment samples
- HT furnace tests with small samples in various atmospheres for analysis of oxidation kinetics and degradation mechanisms
- Tests on all promising ATF cladding concepts, including Cr-coated Zry, FeCrAl, SiC-based composites
- Data for model development, code validation and code application

# International collaborations on ATF cladding

## ■ OECD-NEA Joint Undertaking QUENCH-ATF

- KIT is Operating Agent of the project
- Three bundle experiments with Cr-coated ZIRLO provided by Westinghouse (USA)
- Phase 2 under preparation

## ■ IAEA Coordinated Research Project ATF-TS

- Completed, TECDOC reports in 3 volumes to be published
- Final international meeting co-organized

## ■ EC Projects SCORPION and IL TROVATORE

- KIT coordinates WPs on fuel-cladding-coolant interaction

## ■ EC Project CONNECT-NM

- New project CROCODOX (CEA) accepted

## ■ OECD-NEA project SCIP-V

# QUENCH-ATF3 test preparation

- ZIRLO cladding tubes at NNL for Cr coating by PVD, ready to be shipped
- Spacer grids provided by WEC
- All other materials for bundle construction are available
- Test conduct planned for 2026 (as early as possible)
- Test scenario: slightly modified QUENCH-11 with boil-off phase, max. temperatures of 1600°C and 50 g/s flooding rate



# Separate-effects tests on ATF cladding

- Isothermal and transient tests with different coating types
  - Cr, Cr-Al, Cr-Si with and w/o Mo diffusion barrier
  - In the framework of an TCOFF-2/NEST internship (Brock Nowak, Queens University)
- Transient tests on Cr/Zry cladding failure
  - QUENCH-SR tests up to melt release
  - In cooperation with ASNR (Martial Kpemou)
- Experiments in different atmospheres (steam, O<sub>2</sub>, air) above eutectic temperature
- Experiments with porous SiC in various atmospheres (SCORPION)

# Activities on long-term intermediate storage

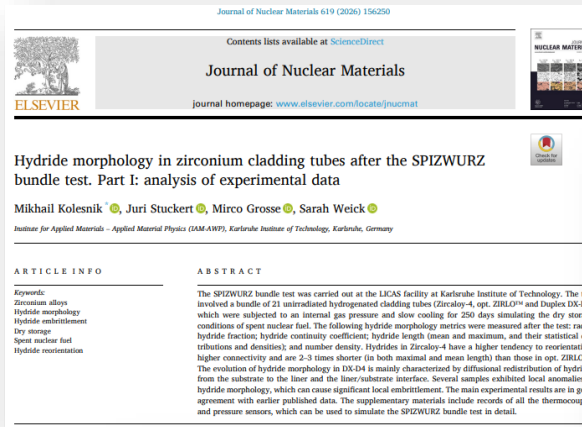
- Work was embedded in the German project SPIZWURZ (GRS, KIT) and the HGF HOVER infrastructure program
  - Completed in 2025
  - 8-month lasting bundle test
  - Post-test analyses and benchmark exercises well progressed
- Various SETs on hydrogen dissolution and precipitation in zirconium alloys
- Neutron radiography and tomography campaigns
- Follow-up project SPIZWURZ+ under preparation
  - Advice: Feasibility study showing capability of smoother cool-down phase

# Modelling and code validation

- QUENCH bundle tests are part of validation matrices of most SFD code systems
- Benchmark exercise (blind & open phase) on QUENCH-ATF2 test coordinated by GRS
- Benchmark exercise (blind & open phase) on SPIZWURZ bundle test coordinated by GRS
- Pre-test calculations for SPIZWURZ+
- Separate-effects test data are available for model development

# Reporting

- Several papers
- Invited lectures
  - MRS Spring Meeting, Seattle
  - Reactor Safety Commission (RSK)
  - Shanghai Jiao Tong University
  - INCT Warsaw
  - IAEA Technical Meeting
- Visit of journalists at QUENCH
- Two evaluations with outstanding results for NUSAFE program



Journal of Nuclear Materials 619 (2026) 156205

Contents lists available at ScienceDirect

ELSEVIER

Journal homepage: [www.elsevier.com/locate/jnucmat](http://www.elsevier.com/locate/jnucmat)

Hydride morphology in zirconium cladding tubes after the SPIZWURZ bundle test. Part I: analysis of experimental data

Mikhail Kolesnik<sup>\*</sup>, Juri Stuckert<sup>\*</sup>, Mirco Grosse<sup>\*</sup>, Sarah Weick<sup>\*</sup>

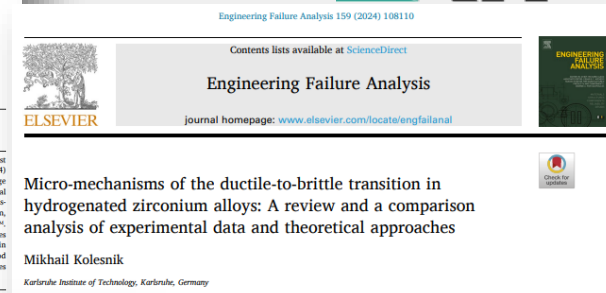
*Institute for Applied Materials - Applied Materials Physics (IAM-AWP), Karlsruhe Institute of Technology, Karlsruhe, Germany*

ARTICLE INFO

ABSTRACT

**Keywords:**  
Zirconium alloys  
Hydride morphology  
Hydride embrittlement  
Dry storage  
Spent nuclear fuel  
Hydride reorientation

The SPIZWURZ bundle test was carried out at the LICAS facility at Karlsruhe Institute of Technology. The test involved a bundle of 21 unirradiated hydrogenated cladding tubes (Zircaloy-4, opt. ZIRLO<sup>®</sup> and Duplex DX-D4) which were subjected to an internal gas pressure and slow cooling for 250 days simulating the dry storage conditions of spent nuclear fuel. The following hydride morphology metrics were measured after the test: radial hydride fraction; hydride continuity coefficient; hydride length (mean and maximum, and their statistical distributions and density); and number density. Hydrides in Zircaloy-4 have a higher tendency to reorientation, higher connectivity and are 2-3 times shorter (in both maximal and mean length) than those in opt. ZIRLO<sup>®</sup>. The evolution of hydride morphology in DX-D4 is mainly characterized by diffusional redistribution of hydrides from the substrate to the louver and louver/substrate interface. Several samples exhibited local anomalies in hydride morphology, which can cause significant local embrittlement. The main experimental results are in good agreement with earlier published data. The supplementary materials include records of all the thermocouples and pressure sensors, which can be used to simulate the SPIZWURZ bundle test in detail.



Engineering Failure Analysis 159 (2024) 108110

Contents lists available at ScienceDirect

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Journal homepage: [www.elsevier.com/locate/engfailanal](http://www.elsevier.com/locate/engfailanal)

Engineering Failure Analysis

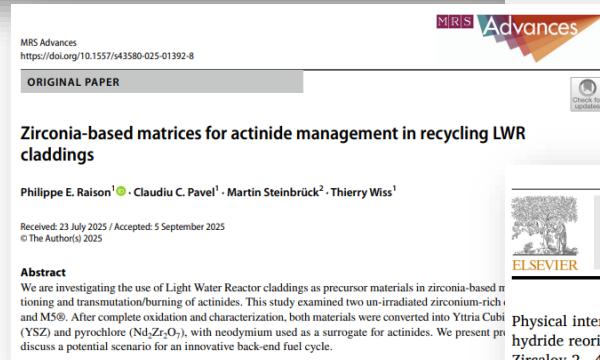
Micro-mechanisms of the ductile-to-brittle transition in hydrogenated zirconium alloys: A review and a comparison analysis of experimental data and theoretical approaches

Mikhail Kolesnik

*Karlsruhe Institute of Technology, Karlsruhe, Germany*

ABSTRACT

The primary objective of this article is to gather comprehensive experimental and theoretical data on the fracture process of hydrogenated zirconium alloys at micro- and nano- levels and conduct an extensive analysis to identify consensus statements and any potential contradictions. The article focuses on the physical mechanisms that contribute to the ductile-to-brittle transition in fracture mode and examines published hypothesis that explain these mechanisms. The manuscript contains a comprehensive list of published experimental studies on the mechanical properties of hydrogenated zirconium alloys. This study will be useful for developing and verifying models and for planning of experimental studies and analyzing their results.



MRS Advances  
<https://doi.org/10.1557/43580-025-01392-8>

ORIGINAL PAPER

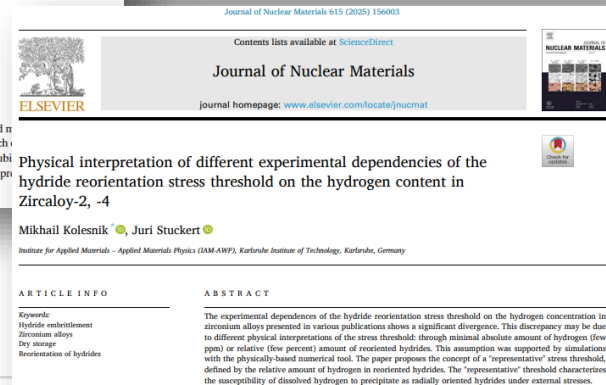
Zirconia-based matrices for actinide management in recycling LWR claddings

Philippe E. Raison<sup>\*</sup>, Claudiu C. Pavel<sup>1</sup>, Martin Steinbrück<sup>2</sup>, Thierry Wiss<sup>1</sup>

Received: 23 July 2025 / Accepted: 5 September 2025  
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ABSTRACT

We are investigating the use of Light Water Reactor claddings as precursor materials in zirconia-based re-irradiation and transmutation/burning of actinides. This study examined two un-irradiated zirconium-rich and MSO. After complete oxidation and characterization, both materials were converted into Ytria Cubi (YSZ) and pyrochlore (Nd<sub>2</sub>Zr<sub>2</sub>O<sub>7</sub>), with neodymium used as a surrogate for actinides. We present and discuss a potential scenario for an innovative back-end fuel cycle.



Journal of Nuclear Materials 615 (2025) 156003

Contents lists available at ScienceDirect

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Journal homepage: [www.elsevier.com/locate/jnucmat](http://www.elsevier.com/locate/jnucmat)

Physical interpretation of different experimental dependencies of the hydride reorientation stress threshold on the hydrogen content in Zircaloy-2, -4

Mikhail Kolesnik<sup>\*</sup>, Juri Stuckert<sup>\*</sup>

*Institute for Applied Materials - Applied Materials Physics (IAM-AWP), Karlsruhe Institute of Technology, Karlsruhe, Germany*

ARTICLE INFO

ABSTRACT

**Keywords:**  
Hydride embrittlement  
Zirconium alloys  
Dry storage  
Reorientation of hydrides

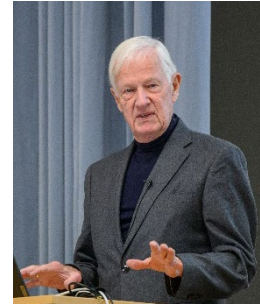
The experimental dependencies of the hydride reorientation stress threshold on the hydrogen concentration in zirconium alloys presented in various publications shows a significant divergence. This discrepancy may be due to different physical interpretations of the stress threshold: through minimal absolute amount of hydrogen (few ppm) or relative (few percent) amount of reoriented hydrides. This assumption was supported by simulations with the physically-based numerical tool. The paper proposes the concept of a "representative" stress threshold, defined by the relative amount of hydrogen in reoriented hydrides. The "representative" threshold characterizes the susceptibility of dissolved hydrogen to precipitate as radially oriented hydrides under external stresses.

# Perspectives

- Reactor safety research confirmed for the current and next HGF funding periods until 2035
- Three new positions for the QUENCH team to fill retirement gaps
- Future topics
  - Behavior of ATF materials under DBA and SA conditions (QUENCH-ATF Phase 2)
  - Safety research for long-term intermediate storage (Zr-H, SPIZWURZ+)
  - Safety research for SMRs (LWR- and GFR-type)
  - Joint projects with FUSION program

# Acknowledgement

- Helmholtz Association for funding program NUSAFE at KIT
- Program NUSAFE and IAM institute's management for broad support of our activities
- EC for funding the projects SEAKNOT, IL TROVATORE and SCORPION
- OECD-NEA and partners for support of QUENCH-ATF
  
- And last but not least the QUENCH team:  
M. Kolesnik, ~~J. Laier~~, J. Moch, U. Peters, C. Roessger, U. Stegmaier,  
~~S. Weick~~



## **Manfred Popp**

### **The history of nuclear research in Karlsruhe**

The presentation provides a comprehensive historical overview of nuclear research in Karlsruhe, tracing its development from the discovery of nuclear fission in 1938 to the establishment and current role of the Karlsruhe Institute of Technology (KIT). It begins with the German Uranium Project (1939–1945), which, unlike the highly industrialized Manhattan Project, was primarily a scientific exploration. Although extensive work was carried out on reactor physics, isotope separation, and nuclear data, Germany did not develop an atomic bomb. Evidence from the Farm Hall transcripts and later assessments by international physicists indicates that key technical knowledge and a focused weapons program were lacking.

After 1945, nuclear activities in Germany gradually resumed with an emphasis on theoretical studies and peaceful applications. The founding of the Gesellschaft für Kernforschung (KfK) in 1956 marked the start of large-scale nuclear research in Karlsruhe. Over the following decades, KfK built major experimental facilities, including research reactors, reprocessing plants, and extensive reactor safety programs. During the 1960s and 1970s, Karlsruhe became a central hub of German and European nuclear technology, with research covering reactor technology, fast breeder reactors, the nuclear fuel cycle, materials under irradiation, safeguards, and later fusion reactor technology.

From the late 1970s onward, energy policy shifts, major nuclear accidents (Three Mile Island and Chernobyl), and declining public acceptance led to the termination of key projects such as the Wackersdorf reprocessing plant and the fast breeder reactor SNR-300. This triggered a profound restructuring of the research center. Nuclear activities were reduced and refocused, while new programs emerged in environmental research, nanotechnology, astroparticle physics, medical technology, and synchrotron-based methods.

The merger of the Karlsruhe Research Center with the University of Karlsruhe to form KIT represents the culmination of this transformation. Today, KIT integrates strong basic research with large-scale applied science. Core nuclear competencies remain, particularly in reactor safety, radioactive waste management, and fusion research, and continue to shape KIT's guiding principle: new technologies must be thoroughly understood and rigorously tested before being deployed.



30th International QUENCH-Workshop  
Nuclear Research at Karlsruhe

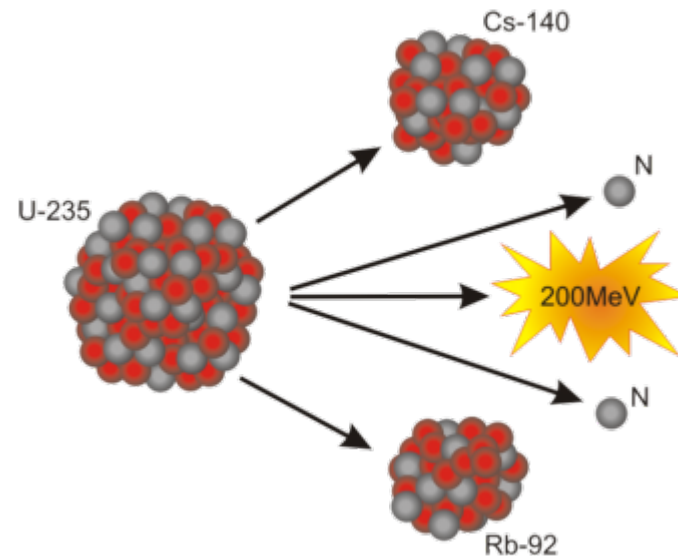
Prof. Dr. Manfred Popp  
16. December 2025



# Discovery of Fission on 16./17.Dezember 1938

## Energiequellen

1. Gravitation  
Wasserkraft
2. Elektromagnetismus  
Sonne, Wind, Holz  
Kohle, Öl, Erdgas
3. Kernkraft

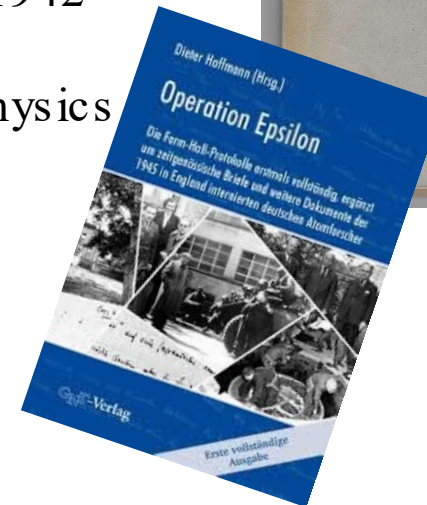
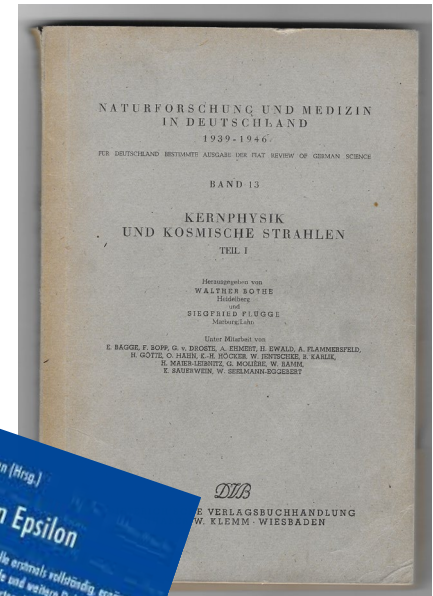
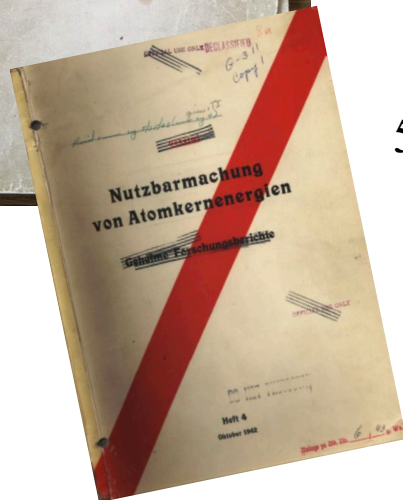
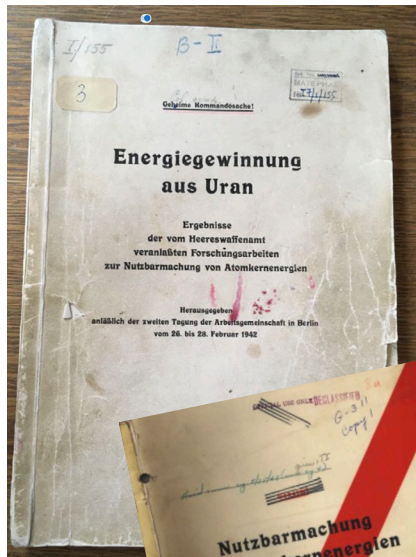


# The Pre-History

—

## The German Uranium Project 1939-1945

400 Secret Reports  
Report of Army Ordnance 2/1942  
FIAT-Reports 1948  
500 publications in Nuclear Physics  
Farm Hall transcripts



# Pre-History 2

Manhattan Project

versus

Uranium Project

1942-1945

1939-1945

2 billion \$

1 \$ = 5 RM  
140 000

Personal

10 Mio RM = 2 million \$

100

1000 : 1

Huge industrial project

Scientific exploration

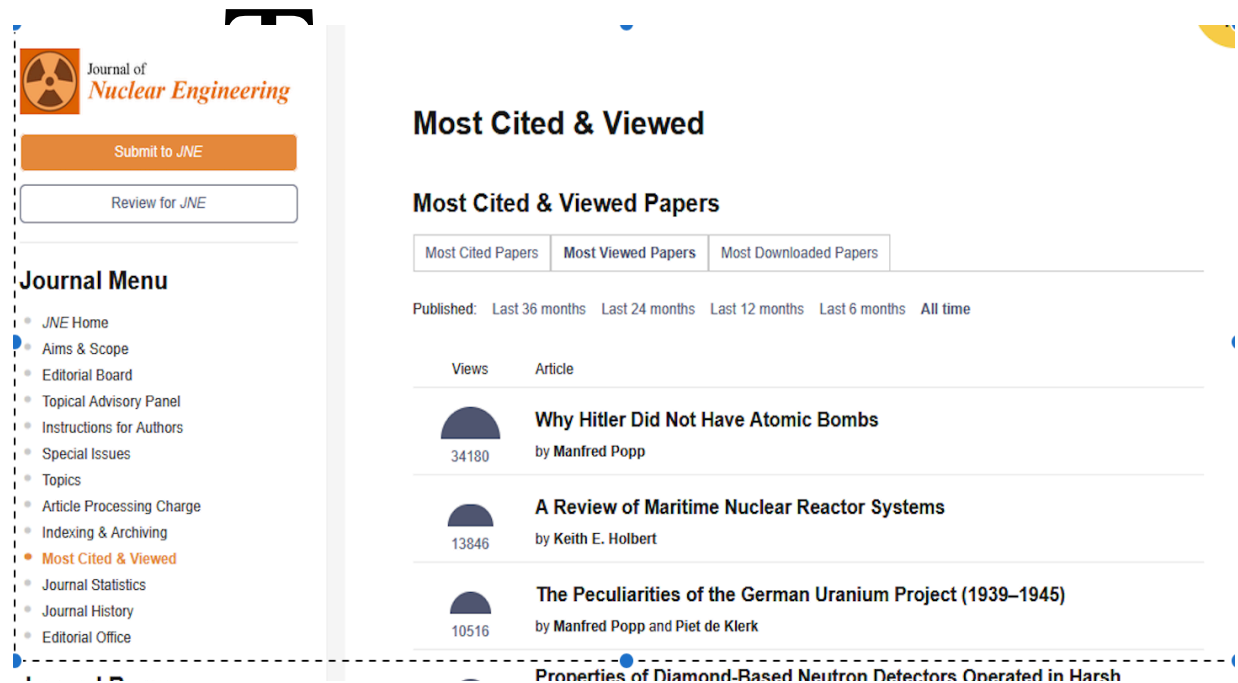
# Results of the Uranium Project

400 Reports on

- Reactor physics (Heisenberg, Wirtz, Höcker, Döpel, Diebner)
- Isotope separation (Harteck, Groth, Clusius, Bagge)
- Nuclear Data (Bothe, Gentner, Kopfermann, Stetter, Jentschke, Maier-Leibnitz, Otto Haxel)

No reports after may 1940:

- Explosive (Heisenberg)
- Plutonium (v. Weizsäcker)
- )



The screenshot shows the website for the Journal of Nuclear Engineering. On the left is a 'Journal Menu' with links to JNE Home, Aims & Scope, Editorial Board, Topical Advisory Panel, Instructions for Authors, Special Issues, Topics, Article Processing Charge, Indexing & Archiving, Most Cited & Viewed (highlighted), Journal Statistics, Journal History, and Editorial Office. The main content area is titled 'Most Cited & Viewed' and 'Most Cited & Viewed Papers'. It features three tabs: 'Most Cited Papers', 'Most Viewed Papers', and 'Most Downloaded Papers'. Below the tabs, there are filters for 'Published:' with options: 'Last 36 months', 'Last 24 months', 'Last 12 months', 'Last 6 months', and 'All time'. A table lists the top papers:

Views	Article
34180	<b>Why Hitler Did Not Have Atomic Bombs</b> by Manfred Popp
13846	<b>A Review of Maritime Nuclear Reactor Systems</b> by Keith E. Holbert
10516	<b>The Peculiarities of the German Uranium Project (1939–1945)</b> by Manfred Popp and Piet de Klerk

Below the table, the title of the next paper is partially visible: 'Properties of Diamond-Based Neutron Detectors Operated in Harsh'.

# Pre-History 2

Manhattan Project          versus          Uranium Project

1942-1945

1939-1945

2 billion \$

1 \$ = 5 RM

10 Mio RM = 2 million \$

140 000

Personal

100

1000 : 1

Huge industrial project

Scientific exploration

# Uranium Project: Reactor Physics



MONSANTO CHEMICAL COMPANY  
Clinton Laboratories

To: A. H. Compton Date: November 8, 1945  
From: A. K. Weinberg and L. W. Nordheim

We have just had an opportunity to read a few of the German Kernphysikalische Forschungsberichte. We are writing in order to correct what we believe to be a very prevalent misconception concerning the state of the art as known to the Germans in 1945. We will proceed by posing a number of relevant questions and then answering them insofar as we can from the few reports we have been allowed to see. Presumably when more reports are made available we will be able to document our statements more fully.

I. Did the Germans know the correct lattice dimensions for a P-9 system?  
(Via the progress we had heard earlier that the Germans were experimenting with plate lattices far too rich in U. Apparently those reports were based on very early reports which are not yet available to us. At present, however, the answer to the above question is an unequivocal yes. The March 1944 'Forschungsberichte' contains a description of experiments on various lattice arrangements performed by Bothe and Fünfer. The experiments are integral ones in which the strength of a source is measured with and without the lattice in place. The main conclusion drawn from these experiments is "eine Kombination von 20 cm U<sup>235</sup> und 1 cm Bismut als der richtige 18 (wird) etwa die kritische sein . . . Bismut hat man wohl mit einem PFR vom U-Behälter geschnitten." This conclusion is exactly the same as that reached by us, on the basis of calculations in August 1943 (CP-923). The German work apparently was done at the same time as ours.

Plates seem to have been preferred because they were most convenient for experiments. The advantage of cubes was recognized as early as June 1943 (Hoeker), and the use of cylinders had been suggested on technical grounds.

II. Did the Germans know the critical dimensions of the P-9 machine?  
We have not had access to the reports in which critical size calculations are made. However, there are repeated references, in the reports available to us, of about 4 tons as the required amount of P-9. This figure is essentially correct.

Endnote (65) Schenker to Bielefeld 10/11/48

A. H. Compton - 2 - November 8, 1945

The Laplacians measured by the Germans are of the order  $1000 \times 10^{-6} \text{ cm}^{-2}$ . This value is in excellent agreement with ours. It indicates, and this is important, that the U metal used by them was about as pure as ours.

III. What was the state of German theory of the chain reaction?  
Here we are badly hampered by the unavailability of the reports. What we do have shows:

- (1) Calculation of optimal lattice dimensions was understood and followed pretty much the same lines as ours. The calculated results on P-9 spheres agree well with ours.
- (2) The group model for reflector calculations was introduced in early 1944. This was a little later than the time we began to use it extensively.
- (3) Generally we would say their approach was in no wise inferior to ours; in some respects it was superior.

IV. Why didn't the Germans succeed in establishing a chain reaction with P-9?  
The answer is simple; they did not have sufficient P-9. The latest reference is to a 1.5 ton P-9 experiment. According to our estimates, with the volume ratio they used (20:1), they would have needed somewhat less than 4 tons.

V. Are there any "scientific secrets" concerning the design of the chain reaction which the Germans do not seem to have understood?  
From the general state of the art as deduced from the few reports we have seen, we would say their understanding of the principles is comparable to ours. The only non-engineering "secrets" we can think of which might affect the design of a chain reaction is the poisoning by Xe<sup>135</sup>, and possibly, the properties of Pu<sup>239</sup>.

VI. What bearing does this have on publication of the parts of the PFR dealing with principles of the chain reaction?  
The Germans knew how to design a lattice which will work. From the practical standpoint this is all that matters. The details of elegant perturbation theory or transport theory (which would be contained in Vol. III) or the details of heat transfer calculations (Vol. IV) would tell the nothing essential to the determination of lattice dimensions. They already know how to calculate the optimum dimensions.

A question of ethics is raised by the existence of the German reports. In many cases useful information is contained therein. It is certainly extra-

A. H. Compton - 3 - November 8, 1945

ordinary, in a scientific treatise, to attribute a given result to an American author without at the same time giving due credit to his German counterpart who is known to have also done the work. Such a situation will arise for example, in Vol. III in the discussion of the multi-group methods where the Germans have duplicated our work.

VII. What bearing does this have on the general question of our "secrets"?  
On this we can presume to speak only as individuals.

The general impression from the German reports is that they were on the right track and that their thinking and developments paralleled ours to a surprising extent. The fact that they did not achieve the chain reaction is primarily due to their lack of sufficient amounts of heavy water.

In one of the reports a vivid description is given of the work on struts in this respect. The heavy water factories in Norway were designed for a capacity of 3 - 4 tons a year and were successfully operating during part of 1942 and 1943. This capacity would have been sufficient for the construction of a pile. However, the production was interrupted by sabotage and finally the main factory was destroyed by a bombing attack. Toward the end of 1944 plans were made to initiate production of heavy water in Germany and to use enriched uranium in order to raise the material requirements.

It is also fairly clear that the total German effort was on a very considerably smaller scale than the American effort. This may be due to the strained German economy or to the less favorable attitude of their government. The fact remains that an independent group of scientists, of much smaller size than ours, operating under such more adverse conditions achieved so much.

We must proceed therefore on the basis that anyone knowing what is in the German reports can establish a chain reaction, provided he has sufficient materials. The Smyth report will give additional very helpful hints. The time when others can establish a chain reaction is therefore no longer a matter of scientific research but solely a matter of procurement. The policies of our authorities must, it seems to us, be formulated with a clear realization of these facts.

Distribution: 1. A. H. Compton 9. S. P. Tignor  
2. A. V. Peterson 10. P. Vorreiter  
3. K. D. Whitaker 11. L. W. Nordheim  
4. J. R. Osw 12. A. K. Weinberg  
5. R. S. Mulliken 13-18 Central Files  
6. A. D. Nichols 19. Working Files  
7. T. A. Rogness  
8. F. Dennis

AKM:LAM:dk

A. M. Weinberg  
L. W. Nordheim

# The reactor experiments

Year

1940

Hamburg (Harteck)

185 kg U/ 15 t CO<sub>2</sub> ice

Berlin/Haigerloch

Leipzig

HWA (Gottow/Stadtilm)

Heisenberg/Wirtz

Heisenberg/Döpel

Diebner

1940

B1 uranium oxide/paraffin L1 uranium oxide/paraffin  
B2 uranium oxide/paraffin L2 142 kg U/ 164 kg D<sub>2</sub>O

G1 uranium oxide/Paraffin 1941 19419  
G2a 200 kg U, 220l D<sub>2</sub>O-

1942

B3 551 kg U/ 44 kg paraffin L3 uranium metal/150 l D<sub>2</sub>O  
B4 740 kg U/ 37 kg paraffin L4 755 kg U/164 kg D<sub>2</sub>O  
B5 864 kg U/ 8 kg paraffin

G2b 200 kg U, 220l D<sub>2</sub>O-ice

1943

B6a-d 0,9 -2,2 t U/1,5 t D<sub>2</sub>O

G3a 540 kg U/525 l D<sub>2</sub>O

1944

B7 2,2 t U/1,5 t D<sub>2</sub>O

G3b 540 kg U/525 l D<sub>2</sub>O

1945

B8 1,5 t U/1,5 t D<sub>2</sub>O/ 10 t graphite

G4 ?

# Uranium Project: Reactor Physics

## The German Reactor Experiments 1940-1945 in the Light of Modern Reactor Physics

Ron Dagan, Manfred Popp

Karlsruhe Institute of Technology, Hermann von Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen

[ron.dagan@kit.edu](mailto:ron.dagan@kit.edu); [popp@kit.edu](mailto:popp@kit.edu)



# Farm Hall (07/45 – 01/46)



Heisenberg v. Weizsäcker Hahn Diebner Gerlach Harteck von Laue Wirtz Bagge  
und Korsching

## 3.9 Heisenberg on the atomic bomb at Farm Hall

August 6 Heisenberg tries to calculate the critical mass of a bomb with 20 kt power. He got 1 t, but only by mistake. His result should have been 12,5 t.  
August 14, Heisenberg gives a lecture on the physics of the bomb,

Edward Teller:

Hans Bethe:

„ These two lectures prove to me that Heisenberg, the scientific leader of the German effort, did not work on a bomb. They show that he did not know critical information, and that he could have derived the information if he had tried.“

Bethe, Hans: The German Uranium Project, Physics Today (2000) 34-36



# Theoretical Nuclear Technology 1946-1955

## Göttingen

1946 No nuclear physicist invited to the USA

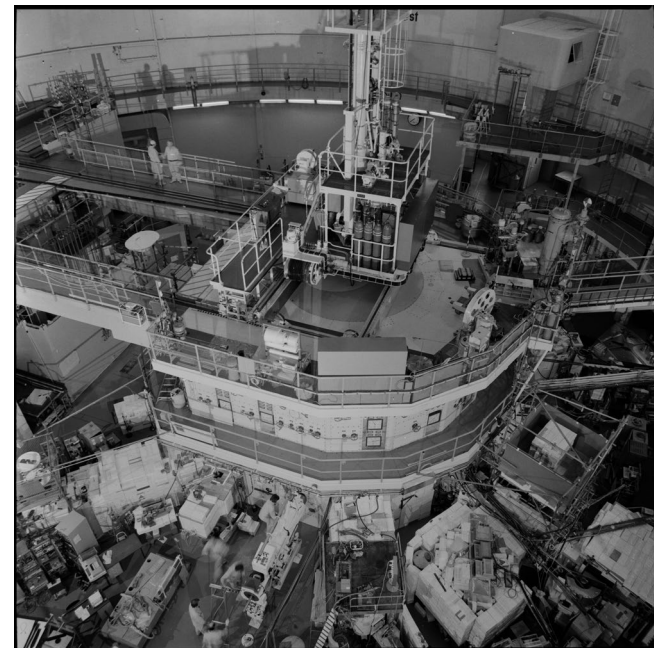
1948 Max-Planck-Institut für Physik in Göttingen

Physikalische Studien-Gesellschaft

1955 Geneva Conference: Atoms for Peace



Karl Wirtz and Otto Hahn



# Juli 1956 Company for Reactor-Construction and -Operation

Abschrift

Kurzprotokoll  
über

die konstituierende Sitzung der Deutschen Atomkommission  
am 26. Januar 1956 11 Uhr

Ort: Haus des Bundeskanzlers

send: Bundesminister Franz-Josef Strauß als Vorsitzender

Die Mitglieder der Deutschen Atomkommission  
mit Ausnahme der Herren Abs, Dr. Knott und  
Dr. Petersen

Vom Bundesministerium für Atomfragen:  
Ministerialdirigent Dr. Grau  
Regierungsdirektor Dr. Engelhardt  
Regierungsdirektor Dr. Pohlend  
Regierungsrat Spilker, persönlicher Referent  
des Bundesministers

Oberregierungsrat Costa  
Oberregierungsrat Dr. Pretsch  
Amtsgerichtsrat Dr. Scheidwimmer  
Dr. Hocker  
Dr. Weber  
Regierungsassessor Dr. May  
Dr. Lechmann, Geschäftsführer der  
Deutschen Atomkommission

Vertraulich

Birth of the  
Karlsruhe  
Research  
Center.

- 11 -

Professor Brandt wendet sich gegen den Plan eines deutschen Atomzentrums, da dies mit der Freizügigkeit und mit einer vernünftigen Konkurrenz unter den Wissenschaftlern nicht vereinbar sei. Man solle vielmehr die hierzu berufenen und bereits gebildeten Organisationen der deutschen Forschung und Wissenschaft, die Max-Planck-Gesellschaft, die Universitäten und Hochschulen, zu dieser Aufgabe heranziehen, also an mehreren Stellen Deutschlands zugleich arbeiten.

Professor Dr. Heisenberg ist der Ansicht, daß eine Zentralisation nicht notwendig sei, da es sehr verschiedene Aufgaben gebe: man müsse Physiker wie Techniker am Reaktor ausbilden, wissenschaftliche Messungen usw. anstellen und Materialprüfungen vornehmen. Diese Aufgaben könne man auf die einzelnen Reaktoren verteilen, so daß jeder Reaktor völlig ausgelastet sei. Ein wichtiges Gebiet sei auch die Forschung und Entwicklung auf dem Gebiet des Reaktorbaues. Hiermit befasse sich eine Arbeitsgruppe in seinem Institut. Für solche Forschungs- und Entwicklungsarbeiten mit dem Standort München interessiere er sich auch persönlich. Es sei erwünscht, daß die organisatorischen und personellen Voraussetzungen für den Karlsruher Reaktor bald geschaffen würden, damit die Vorarbeiten seines Instituts für den Bau dieses Reaktors zur Verfügung gestellt werden könnten.

Professor Dr. Hahn schlägt in der Frage des Standorts der ersten Reaktoren einen Kompromiß vor. Man sollte sowohl in Karlsruhe bauen als auch für Herrn Professor Heisenberg einen Reaktor in München vorsehen.

Bundesminister Strauß tritt der Meinung von Prof. Brandt bei, möglichst vielen Universitäten und Hochschulen die Möglichkeit der Kernenergieforschung zu geben. Er sei persönlich ein Gegner jeder Staateregulierung und Zentralisierung in der Forschung. Der Vorschlag von Prof. Hahn, eine Arbeitsteilung zu finden, die den Lebenswerk von Prof. Heisenberg Rechnung trage, stehe dieser seiner Auffassung nicht entgegen.

Die weitere Behandlung dieses Themas wird der entsprechenden Fachkommission zugewiesen.

Zu Punkt 7 der T.O. - Festsetzung des Zeitpunktes der nächsten Sitzung

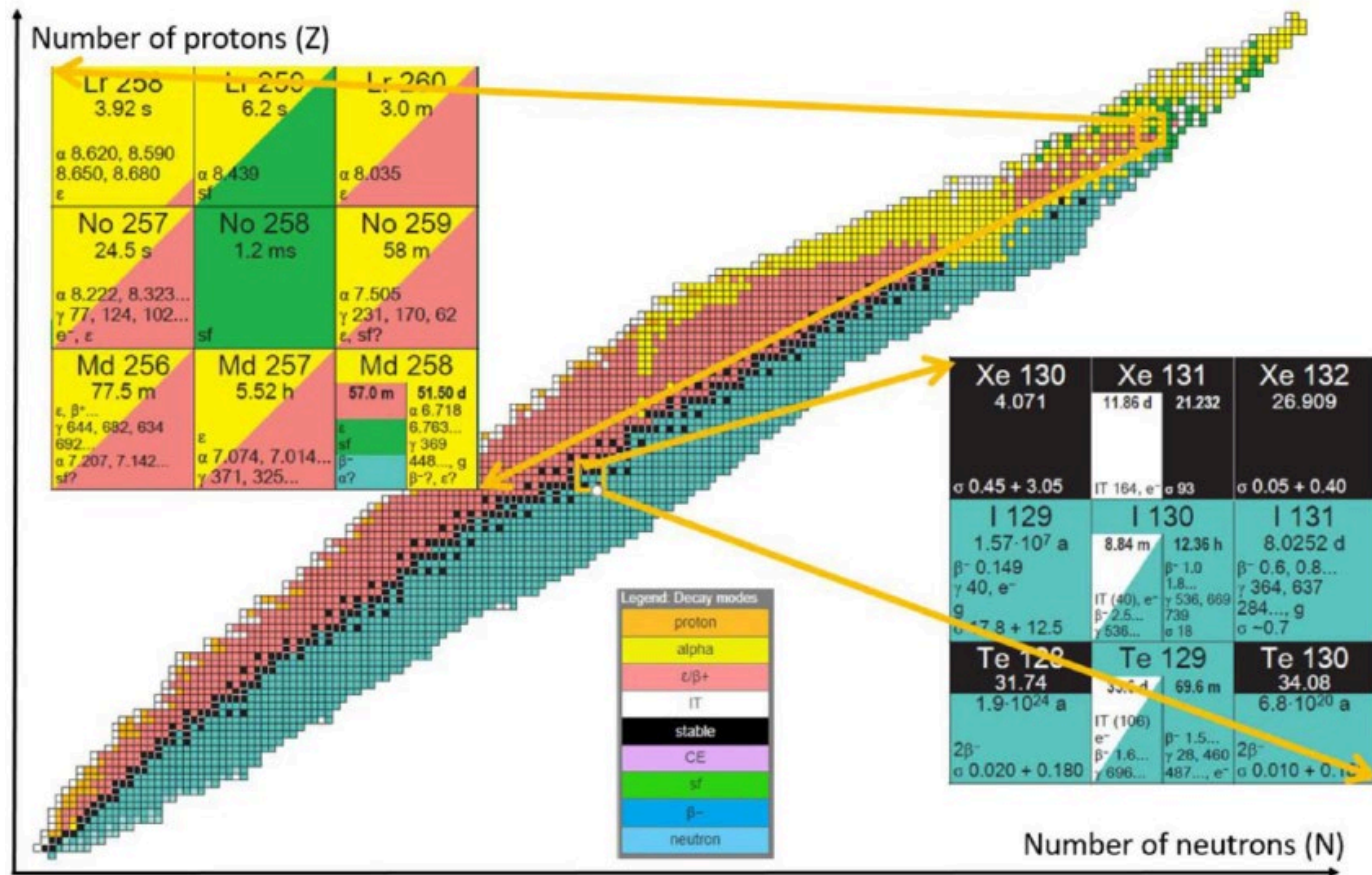
Als Termin für die nächste Sitzung der Deutschen Atomkommission wird der 2. März 1956, 11<sup>24</sup> Uhr, festgelegt.

Der Vorsitzende der  
Atomkommission:

Der Geschäftsführer der  
Atomkommission: gez. Strauß

gez. Dr. Lechmann

# Karlsruhe Nuclide Chart



1958: 1517 – 2022: 4017. W. Seelmann-Eggebert (1915-1988) until 1981  
 Gerda Pfennig (+2017) until 2015  
 Since 2006 JRC Karlsruhe, since 2012 Nucleonica

The reactor station grew.....

.....until end of 1958 in 5 steps:

A–C (70 Mio DM) Kernreaktor GmbH. - K1  
D–E (70 Mio DM) Bund und Land - K2

Main Project: FR-2

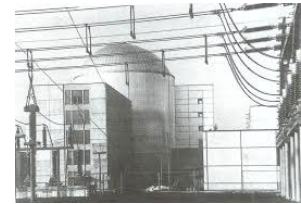
15 Institutes  
Administration Building  
Central Workshop  
Computer center  
Canteen

Architect: Erich Schelling



## 1961: Large experimental facilities

Multi-purpose research reactor MZFR  
Hot-Steam-Reactor Großwelzheim /Main  
Compact Ba-cooled nuclear reactor  
Nuclear Power Station  
Niederaichbach/Isar ( $D_2O - CO_2$ )  
Pilot-Reprocessing plant Karlsruhe



## The project-structure of KfK

- Institutes: Expert
- Projects: Finances
- Directors of institutes and projects on equal footing
- R&D-Commissions decide
- Internal reporting system



## KfK- Program in the 1970s.

- Reactortechnology
- Material research (radiation damage)
- Fast Breeder
- Instrumental fissile material flow control (Safeguards)
- Actinides
- Nuclear fuel cycle (reprocessing, waste management and final storage)
- First steps into environmental research

# Nuclear - and Computer-technology grow in parallel

counter

1957 Computing center

Reason: digital measurements in nuclear physics :



„Otto Hahn's table“

## 1960s: First joint ventures with the university

### Institut für Kernverfahrenstechnik (separation nozzle)

- 1958 TH Karlsruhe: Professorship for Erwin Willy Becker
- 196? Institute built by BMA
- 196? Extension and technology center by KfK

### 1964 Rektor as guest in supervisory committee

### Institute for nuclear physics

- 1964 new building, also for University
- University provides workshop (until 2009)
- No joint program

1967 University may use the KfK Computing center

1964 -1970 joint calls of professors with difficulties

# End of 1960s Jahre: 1 st ideas of phasing out nuclear research



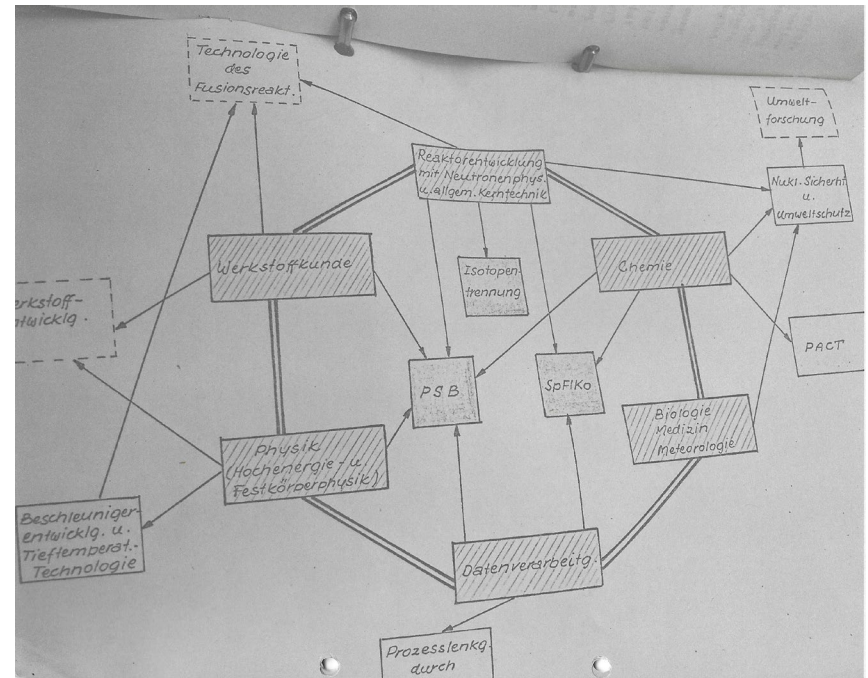
1969 Begin of Biblis A (1300 MWe)



1968 Landing on the Moon



1969 KfK-Kommission "Future tasks of kfk"  
1971 Presentation by Prof. Horst Böhm



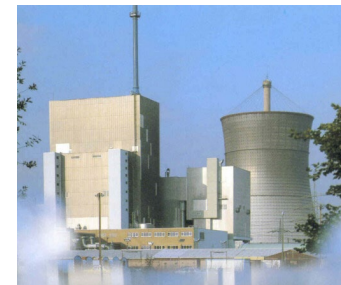
## Early 1970s: The planned progress by big science



ICE und TRANSRAPID



AIRBUS und ARIANE



THTR 300 und SNR 300



# 1972 : Diversification of nuclear research centers

1. März 1972: Quickborner Team:  
„Mobility and Diversification of nuclear research centers

New structure:

Federal Government 90 %, Land 10%  
Industrial Organization

New activities:

Environmental research and technology  
Biology and Medicine

## 1974 : New Energy Policy

- 1973 4th „Atomprogramm“ 1973-1976
- 1973 1st Energy crises
- 1974 1. Energy-Program “Away from oil!”
  - 45 GWe Kernenergie
  - Stabilisation of domestic coal production
- 1974 1st non-nuclear energy research Energieforschung
  - 1st Energy research program

New tasks for KfK: back to nuclear

Nuclear Safety, Reprocessing, Waste Management and Storage, Fast Breeder.

# The international sodium fast breeder cooperation

International consensus: Breeders necessary because of Limitations of the world's uranium reserves

Breeder development

in Europe: F, NL, B, F, D

World: USA, UdSSR, Japan, Indien

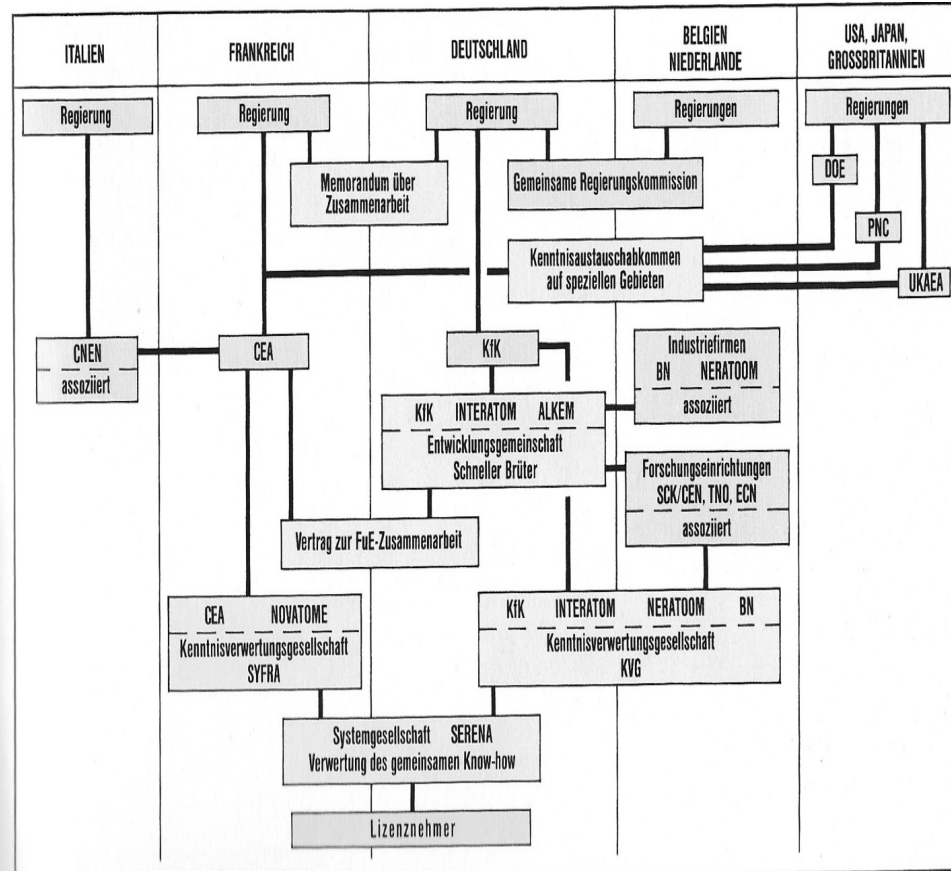
All (!) for Na-cooled breeder

Int. Exchange of know how

1970 Phenix, SNR 300, Phenix (F), BN350(UdSSR), Monju (J), Kalpakkam,

1980 Superphenix (F) , planning SNR2 (D, B, NL) by utilities

44. Meeting KfK-AR in May 1986 in Creys-Malville





# Project Reprocessing (1st civil plant)

1974 DWK founded

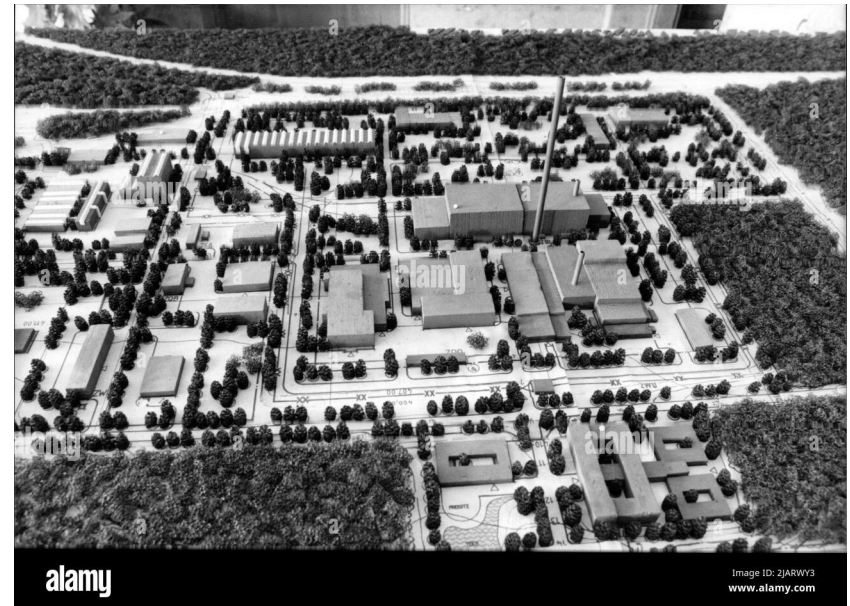
1978. Test facility MILLI (35 kg Pu)

1979 KfK as industrial partner for DWK  
for the construction of Wackersdorf plant

1979 TEKO (Test facility for components)

Annually 12,5 Mio DM Licences from DWK

Development of MOX-fuel



# Project Nuclear Safety

1972 Project Nuclear Safety

1975-1991 HDR-Safety research program

1979 Three mile Island

Contributions to German risk study for NPPs

1987-1992 BETA for core melt-concrete interaction

1986 Chernobyl

1987 Begin of „hypothetical accidents“

1991 Begin of design work for EPR

1991 Begin of cooperation with Russia, later in EU-Japan-USA-program

:

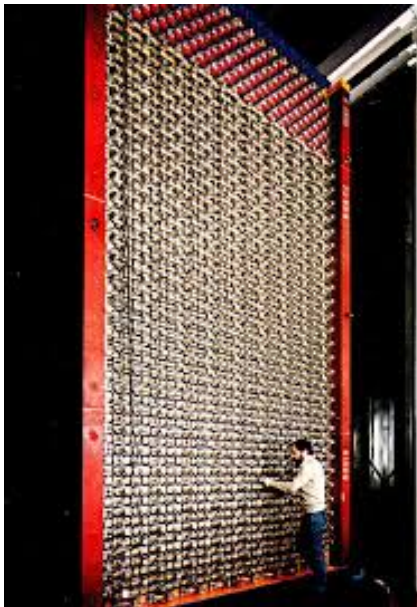
- Superconducting magnets
- 1976 Tokamak coil  
for international competition at Oak Ridge (USA),  
1987: highest ranking
- Blanket (more dpa than breeder)
- Tritium-Laboratory



# Kernphysik

Keine Gemeinsamkeit mit Uni-Kernphysik, da BMFT eine weitere Verstärkung der Elementarteilchenphysik ablehnte.

GALLEX-Experiment im Gran Sasso



KARMEN: Neutrino-Experiment at SNS Rutherford (GB)

KASKADE: Cosmic



# 1986 Decline of public and political acceptance of nuclear power and big science

Large accidents:

- Challenger
- Chernobyl

Depression in industry in general

## 1989/1991 two abrupt project terminations

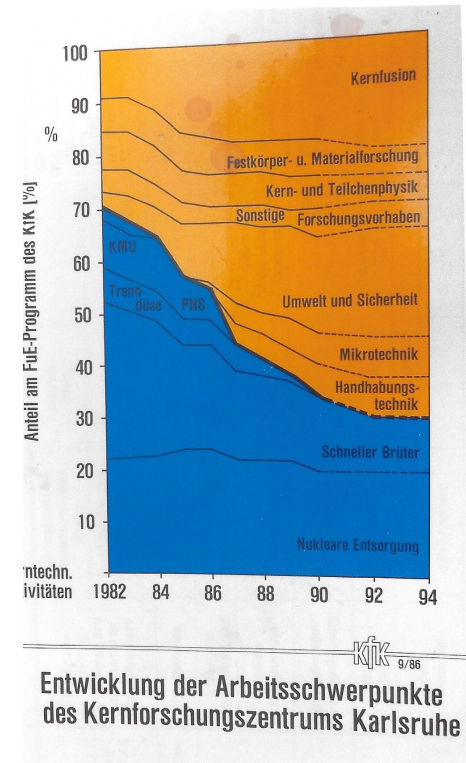
KfK-planning for reduction of nuclear power program

May 1989 Stop of the almost completed reprocessing facility at Wackersdorf by the utilities because of dumping offers from France.

March 1991, decision not to start hot operation of SNR 300.

My turn as CEO started exactly on that day

KfK-planning for faster reduction of nuclear program



# Framework for programatic change

- Budgetary strains because of re-unification
- Poor proposals by external advisory committee
- Loss of 750 positions
- + High Quality and Motivation of staff
- + More publications by stopping internal reporting system
- + reserves in personnel and finance in the oversized infrastructure

## Principles for changing more than 50% of the program

- No cancellation of contracts, only early retirements
- No termination of institutes except when staff had left to new jobs.
- Convincing staff members for new challenges
- New program based on special competences from nuclear
- Closure of old and opening of new institutes (25)
- Less infrastructure more science





After 40 years: „Research center Karlsruhe“

New program based on excellent nuclear know how:

- Use of synchrotron radiation in manufacture of micro-structures
- Nanotechnology: single atoms identification by decay, cloud chamber, radiochemistry (Gallex: few Ge atoms out of 10<sup>11</sup> t Ga Cl)
- Minimal invasive surgery (remote handling)
- Astroparticle physics

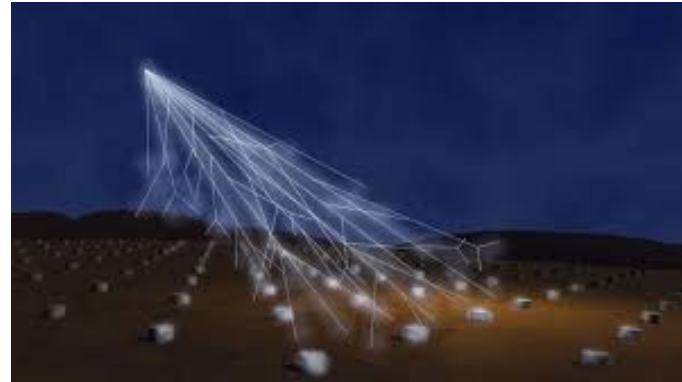
Continued nuclear R&D:

- Experiments for EPR
- Waste management and final stoprage
- Fusion reactor technology

## 2000: New large projects in Nuclear Physics



KATRIN-Neutrinoexperiment



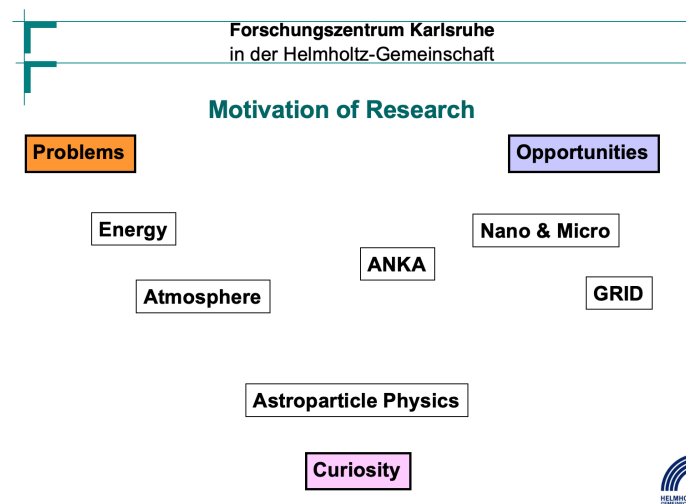
Pierre Auger Observatory

## 1996 -2006 from FZK to KIT

Change in research policy: less applied more excellent basic science

Program-oriented funding: less administrative steering, more evaluations

Change in FZK: less problem-oriented, more opportunity oriented program

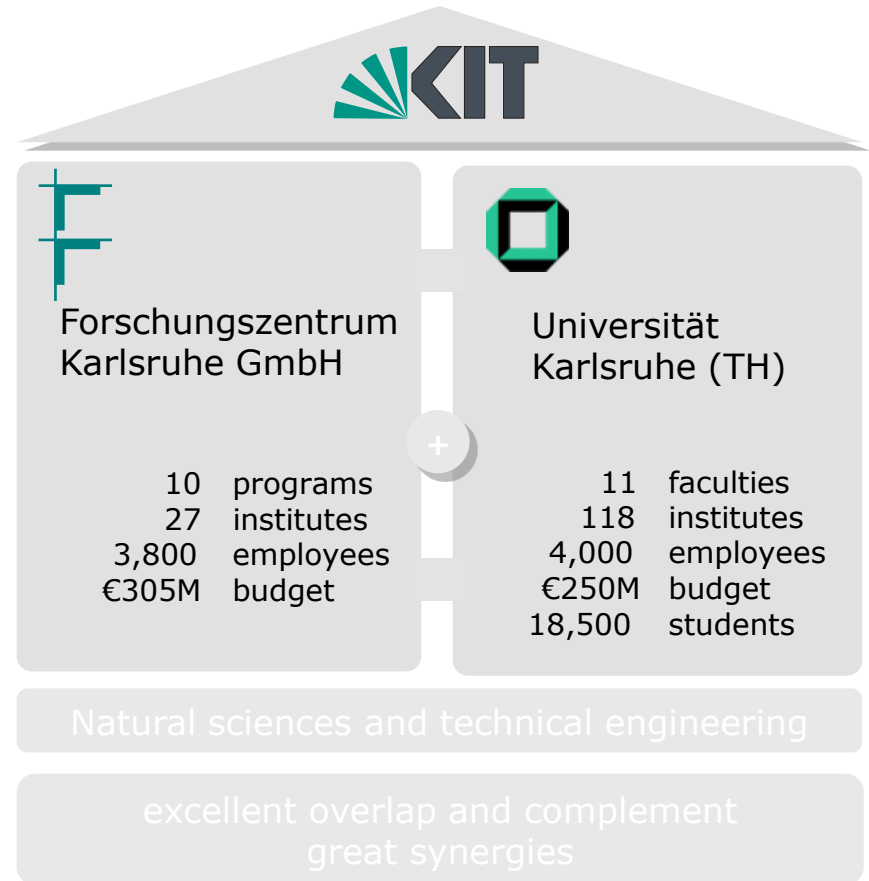


# KIT represents a unique opportunity

## Forschungszentrum Karlsruhe GmbH



**Universität Karlsruhe**



## Synergies by KIT

Research center

University

Strong basic funding

poor basic funding

Demand for young scientists

Education of young scientists

Students participation in research – expert participation in lecturing

Better chances for third party financing

Broader basis for participation in Helmholtz-programs

# Phases of reactor safety research

1956 : Industry can take over in 1960

1958: Begin of materials research

1965-75: HDR Safety Program (Components, pressure Vessel

1970s. German Risk study

1979: Three Miles Island.

1980s: Mitigation of accidents: BETA, CORA

1986: Chernobyl

1990s: Control of accidents: Basics for EPR, Hydrogen control

1990s: Cooperation with Russia: Hydrogen, Synchrotron,  
Conversion of Russian war heads to MOXfuel

# What lives on from nuclear power research in KIT?

- Directly:
  - a base load in nuclear safety research
  - Participation in European programs
  - Research for safe disposal of radioactive waste
  - Fusion reactor technology
  - Application of nuclear safety know how in other areas.
- Indirectly:
  - The principle: What we do, we do thoroughly.
  - For us nothing is impossible.
  - New technologies need to be thoroughly investigated before used.



## 2006: Die KIT-Idee siegt





**Zoltan Hozer**

HUN-REN EK

## **Overview of the CODEX Experimental Programme**

At the CODEX (COre Degradation EXperiment) facility, a total of 20 experiments were conducted between 1995 and 2024 to simulate fuel behavior during the early phase of core degradation. The first experiments focused on comparing VVER and PWR cladding materials. These were followed by investigations of the consequences of air ingress and control rod degradation processes. The fuel degradation event that occurred in a cleaning tank at the Paks Nuclear Power Plant (NPP) was also simulated in two dedicated experiments. Detailed analyses of loss-of-coolant accident (LOCA) scenarios in both the reactor and the spent fuel pool were performed. Specific design extension condition (DEC) scenarios were also investigated, based on NPP reference cases such as station blackout (SBO) and nitrogen injection from hydroaccumulators. The two most recent experiments were dedicated to the testing of Accident Tolerant Fuel (ATF) designs.

The experimental program included both seven-rod hexagonal (VVER-type) and 3×3 rod square-lattice (PWR-type) bundles, with heated lengths ranging from 600 mm to 1000 mm. In the early tests, UO<sub>2</sub> pellets were used as fuel simulants; these were later replaced with Al<sub>2</sub>O<sub>3</sub> and ZrO<sub>2</sub> ceramics. A wide variety of cladding materials were employed, including traditional E110, sponge-based E110, thin-walled E110, Zircaloy-4, optZIRLO™ and Cr-coated optZIRLO™. The heating methods applied to the fuel rods were gradually refined over the years. By enabling internal pressurization of the rods, additional phenomena such as ballooning, burst, and secondary hydriding could be investigated. Temperature measurements were supported by a large number of thermocouples, which formed the core of the data acquisition system. Pressures and flow rates were also measured at several positions in the facility. The composition of the outlet gas was analyzed using thermal conductivity detectors, and later by mass spectrometry. In several specific experiments, the main parameters of the released aerosols were characterized, while in another test, on-line X-ray imaging was performed.

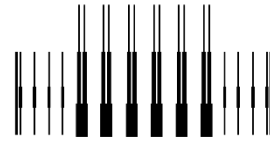
The maximum cladding temperatures ranged from 874 °C to 2300 °C, and the total hydrogen production reached up to 33 g. Depending on the simulated scenario, the tests were terminated either by water quenching or by slow cool-down in an argon atmosphere. Following each test, various post-test examinations were conducted to characterize the condition of the bundle. In most cases, the bundles were fixed in epoxy, and cross-sections were prepared for analysis using light optical microscopy and scanning electron microscopy. In cases where the fuel rods were not embedded, additional mechanical tests (four-point bending, ring compression), computed tomography, or prompt-gamma activation imaging were performed. Selected bundle fragments were also examined in hot vacuum extraction facilities to determine the amount of absorbed hydrogen.

Over the three decades of operation, a close collaboration developed between the CODEX and QUENCH teams. Several parallel and complementary experiments were conducted, and the CODEX program received very valuable technical support from KIT experts. Some memorable moments of this long-standing collaboration will be highlighted in the presentation.

HUN  
REN



Centre for  
Energy Research



MTA  
Centre  
of Excellence

HUN-REN  
Hungarian Research Network

# HUN-REN Centre for Energy Research

## Overview of the CODEX Experimental Programme

Zoltán Hózer, Róbert Farkas, Nóra Vér

*30th International QUENCH Workshop  
Karlsruhe, 16-18 December 2025*

Research. Innovation. Impact.

## CODEX experiments 1995-2025

- Core degradation experiments: scenarios, fuel design, post-test examinations
- Coolability experiments

## Necessary conditions for successful execution of tests

- Materials, team, projects and financing

## How was CODEX created?

- Some history, NIELS

## Examples of QUENCH-CODEX co-operation

- Air ingress phenomena
- Control rod degradation

## Conclusions

# CODEX experiments 1995-2025

Test	Bundle type	Pellet	Cladding material	Max. temp.	Hydrogen production	Cool-down	Test type	Year
CODEX-1	7-rod VVER	Al <sub>2</sub> O <sub>3</sub>	E110	>2000 °C	n.m.	slow	Scoping test	1995
CODEX-2	7-rod VVER	UO <sub>2</sub>	E110	2400 °C	26.6 g	slow	Escalation and slow cooling down	1995
CODEX-3/1	7-rod VVER	UO <sub>2</sub>	E110	1158 °C	0.05 g	bottom quench	Water quench at 1150 °C	1996
CODEX-3/2	7-rod VVER	UO <sub>2</sub>	E110	1643 °C	1 g	bottom quench	Water quench at 1500 °C	1997
CODEX-AIT-1	9-rod PWR	UO <sub>2</sub>	Zircaloy-4	2000 °C	0 g	slow	Air ingress	1998
CODEX-AIT-2	9-rod PWR	UO <sub>2</sub>	Zircaloy-4	1880 °C	n.m.	slow	Steam oxidation and air ingress	1999
CODEX-B4C	7-rod VVER	UO <sub>2</sub> ,B <sub>4</sub> C	E110, stainless steel	2300 °C	25 g	slow	Control rod degradation	2001
CODEX-CT-1	7-rod VVER	Al <sub>2</sub> O <sub>3</sub>	E110	1245 °C	33 g	bottom quench	Long term oxidation and quench	2006
CODEX-CT-2	7-rod VVER	Al <sub>2</sub> O <sub>3</sub>	E110	1384 °C	13 g	bottom quench	Treatment in hydrogen and quench	2006
CODEX-LOCA-200	7-rod VVER	Al <sub>2</sub> O <sub>3</sub>	E110, E110G	908 °C	n.a.	bottom quench	Large break LOCA	2015
CODEX-LOCA-E4	7-rod VVER	Al <sub>2</sub> O <sub>3</sub>	E110, E110G	874 °C	n.a.	bottom quench	Shutdown LOCA	2016
CODEX-LOCA-200B	7-rod VVER	Al <sub>2</sub> O <sub>3</sub>	E110, E110G	1089 °C	n.a.	bottom quench	Large break LOCA	2016
CODEX-LOCA-SFP1	7-rod VVER	Al <sub>2</sub> O <sub>3</sub>	E110, E110G	924 °C	n.a.	bottom quench	Spent fuel pool LOCA	2017
CODEX-LOCA-SFP2	7-rod VVER	Al <sub>2</sub> O <sub>3</sub>	E110, E110G	896 °C	n.a.	bottom quench	Spent fuel pool LOCA	2017
CODEX-AIT-3	7-rod VVER	ZrO <sub>2</sub>	E110G	1625 °C	5.2 g	slow	Air ingress with oxygen and steam starvation	2018
CODEX-NITRO	7-rod VVER	ZrO <sub>2</sub>	E110, E110G	1748 °C	11 g	slow	Nitrogen injection from hyroaccumulators	2018
CODEX-SBO	7-rod VVER	ZrO <sub>2</sub> , Al <sub>2</sub> O <sub>3</sub>	E110, E110G	1900 °C	32 g	bottom quench	Station blackout	2019
CODEX-SLIM	7-rod VVER	Al <sub>2</sub> O <sub>3</sub>	E110G	900 °C	0.69 g	bottom quench	LOCA with thin-walled cladding	2021
CODEX-ATF	7-rod VVER	ZrO <sub>2</sub> , Al <sub>2</sub> O <sub>3</sub>	optZIRLO™, Cr coated optZIRLO™	1655 °C	3 g	bottom quench	severe accident with ATF	2023
CODEX-ATF-AIT	7-rod VVER	ZrO <sub>2</sub> , Al <sub>2</sub> O <sub>3</sub>	Cr coated optZIRLO™	1544 °C	4.7 g	slow	Air ingress test with ATF	2024

Test
CODEX-1
CODEX-2
CODEX-3/1
CODEX-3/2
CODEX-AIT-1
CODEX-AIT-2
CODEX-B4C
CODEX-CT-1
CODEX-CT-2
CODEX-LOCA-200
CODEX-LOCA-E4
CODEX-LOCA-200B
CODEX-LOCA-SFP1
CODEX-LOCA-SFP2
CODEX-AIT-3
CODEX-NITRO
CODEX-SBO
CODEX-SLIM
CODEX-ATF
CODEX-ATF-AIT

## Reactor accidents

- LBLOCA
- Shut-down LOCA
- LOCA in spent fuel pool
- Station blackout
- Lower head failure
- Nitrogen from hydroaccumulators
- Cleaning tank incident

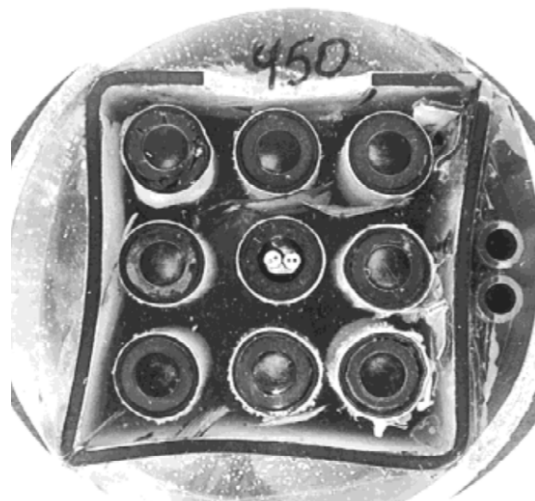
## Phenomena

- Escalation due to oxidation in steam and air
- Control rod degradation
- Steam starvation
- Oxygen starvation (air)
- ATF behavior in steam
- ATF behavior in steam+air

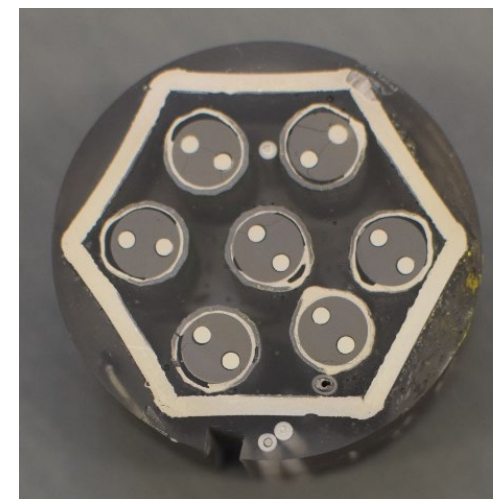
Test type	Year
Scoping test	1995
Escalation and slow cooling down	1995
Water quench at 1150 °C	1996
Water quench at 1500 °C	1997
Air ingress	1998
Steam oxidation and air ingress	1999
Control rod degradation	2001
Long term oxidation and quench	2006
Treatment in hydrogen and quench	2006
Large break LOCA	2015
Shutdown LOCA	2016
Large break LOCA	2016
Spent fuel pool LOCA	2017
Spent fuel pool LOCA	2017
Air ingress with oxygen and steam starvation	2018
Nitrogen injection from hydroaccumulators	2018
Station blackout	2019
LOCA with thin-walled cladding	2021
severe accident with ATF	2023
Air ingress test with ATF	5 2024

## PWR and VVER bundles

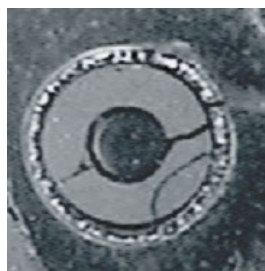
Test	Bundle type
CODEX-1	7-rod VVER
CODEX-2	7-rod VVER
CODEX-3/1	7-rod VVER
CODEX-3/2	7-rod VVER
CODEX-AIT-1	9-rod PWR
CODEX-AIT-2	9-rod PWR
CODEX-B4C	7-rod VVER
CODEX-CT-1	7-rod VVER
CODEX-CT-2	7-rod VVER
CODEX-LOCA-200	7-rod VVER
CODEX-LOCA-E4	7-rod VVER
CODEX-LOCA-200B	7-rod VVER
CODEX-LOCA-SFP1	7-rod VVER
CODEX-LOCA-SFP2	7-rod VVER
CODEX-AIT-3	7-rod VVER
CODEX-NITRO	7-rod VVER
CODEX-SBO	7-rod VVER
CODEX-SLIM	7-rod VVER
CODEX-ATF	7-rod VVER
CODEX-ATF-AIT	7-rod VVER



CODEX-AIT-1 450 mm



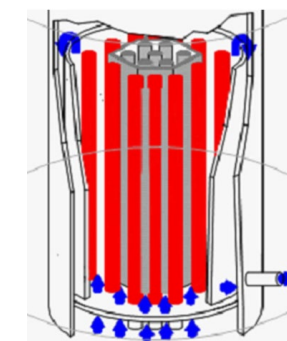
CODEX-ATF 200 mm



1 tungsten heater



2 tungsten heaters



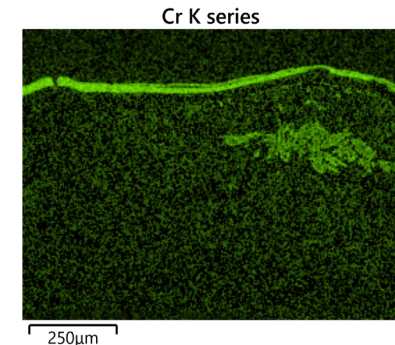
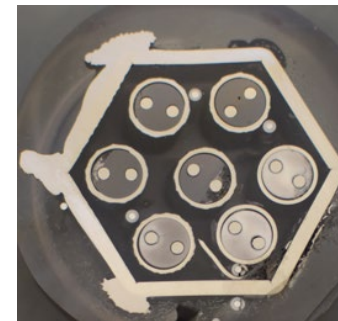
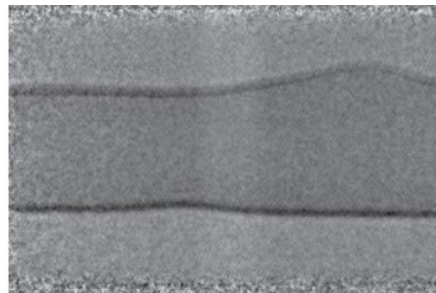
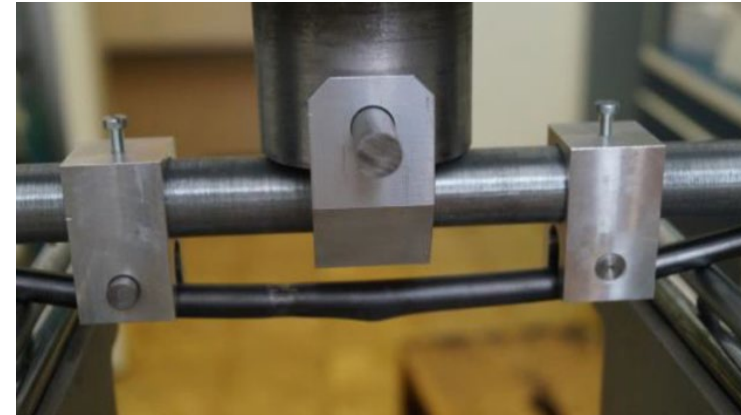
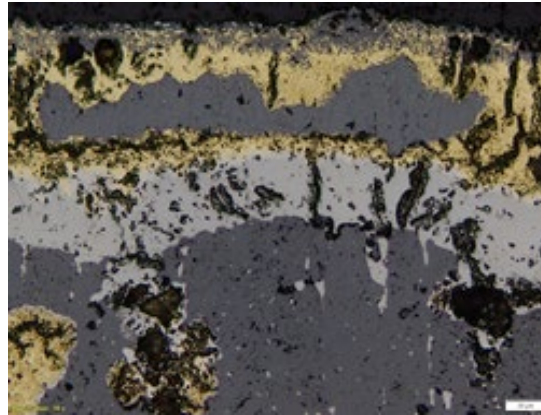
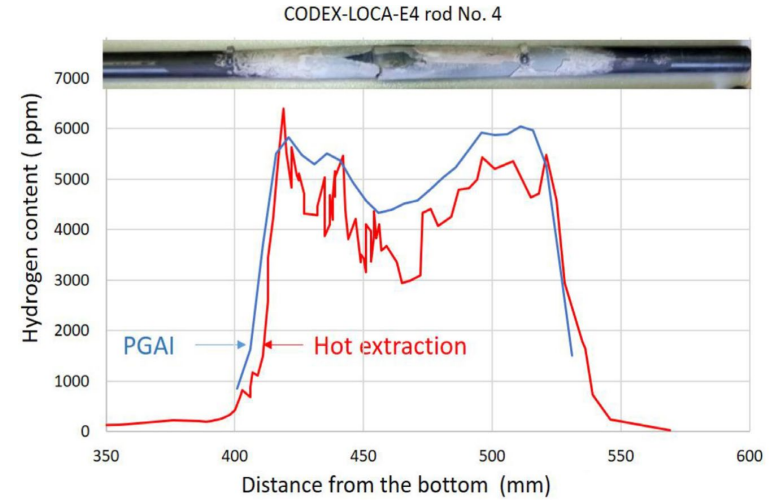
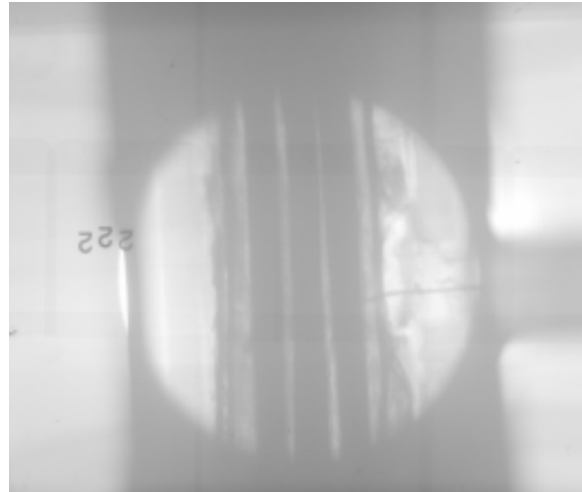
No internal heaters

- Closed top
- Internal pressurisation

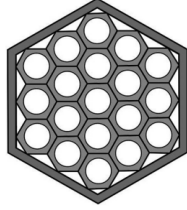
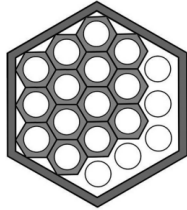
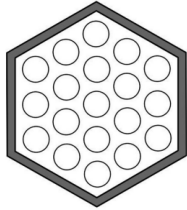
- Free movement of damaged fuel segments



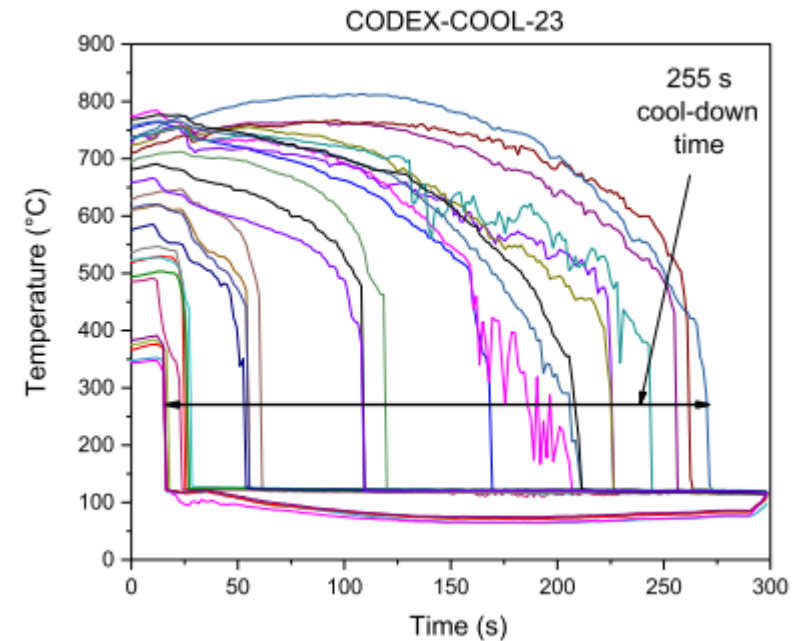
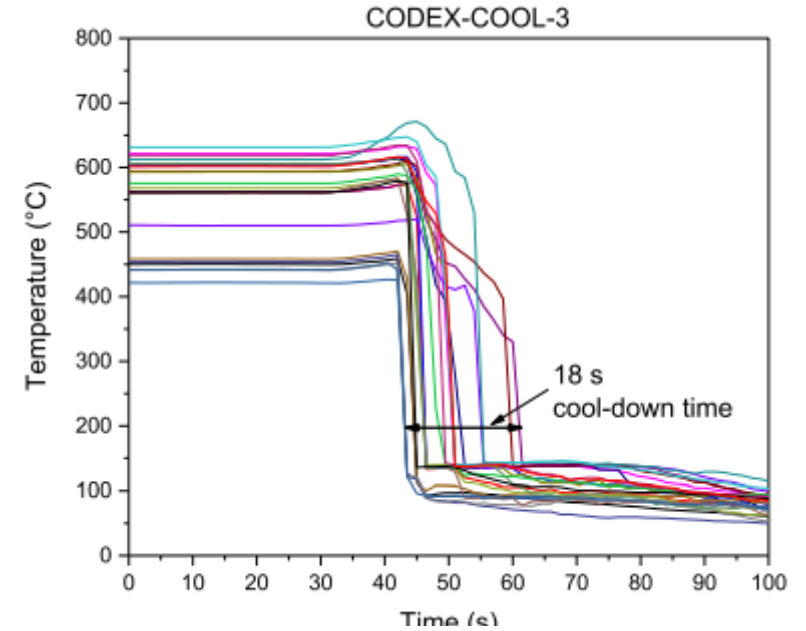
- Metallography
- SEM, EDX
- Endoscopy
- X-ray
- H content
- Mechanical tests
- CT
- PGAI-NR



Test	Number of rods with ballooning simulator sleeves	Power peak simulation	Bypass line
CODEX-COOL-1	0	No	No
CODEX-COOL-2	0	No	No
CODEX-COOL-3	0	No	No
CODEX-COOL-4	19	No	No
CODEX-COOL-5	19	No	No
CODEX-COOL-6	19	No	No
CODEX-COOL-7	19	Yes	No
CODEX-COOL-8	19	Yes	No
CODEX-COOL-9	19	Yes	No
CODEX-COOL-10	14	No	No
CODEX-COOL-11	14	No	No
CODEX-COOL-12	14	No	No
CODEX-COOL-13	14	No	No
CODEX-COOL-14	14	No	No
CODEX-COOL-15	14	No	No
CODEX-COOL-16	14	No	No
CODEX-COOL-17	14	Yes	No
CODEX-COOL-18	14	Yes	No
CODEX-COOL-19	14	Yes	No
CODEX-COOL-20	14	Yes	No
CODEX-COOL-21	14	Yes	No
CODEX-COOL-22	14	Yes	No
CODEX-COOL-23	14	Yes	No
CODEX-COOL-24	14	Yes	Fully open
CODEX-COOL-25	14	Yes	2 mm
CODEX-COOL-26	14	Yes	2 mm
CODEX-COOL-27	19	Yes	2 mm
CODEX-COOL-28	19	Yes	Closed
CODEX-COOL-29	19	Yes	Closed
CODEX-COOL-30	19	Yes	3 mm
CODEX-COOL-31	19	No	Fully open
CODEX-COOL-32	19	No	2 mm
CODEX-COOL-33	19	No	Closed
CODEX-COOL-34	19	No	Fully open



- 19 rod VVER bundles
- Simulation of ballooned section by artificial sleeves
- Thermal-hydraulic experiments
- Power peak (fuel relocation) and bypass line simulation





# Necessary conditions for success

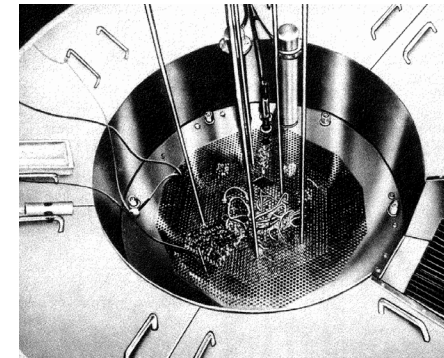
Test	Bundle type	Pellet	Cladding material
CODEX-1	7-rod VVER	Al <sub>2</sub> O <sub>3</sub>	E110
CODEX-2	7-rod VVER	UO <sub>2</sub>	E110
CODEX-3/1	7-rod VVER	UO <sub>2</sub>	E110
CODEX-3/2	7-rod VVER	UO <sub>2</sub>	E110
CODEX-AIT-1	9-rod PWR	UO <sub>2</sub>	Zircaloy-4
CODEX-AIT-2	9-rod PWR	UO <sub>2</sub>	Zircaloy-4
CODEX-B4C	7-rod VVER	UO <sub>2</sub> , B <sub>4</sub> C	E110, stainless steel
CODEX-CT-1	7-rod VVER	Al <sub>2</sub> O <sub>3</sub>	E110
CODEX-CT-2	7-rod VVER	Al <sub>2</sub> O <sub>3</sub>	E110
CODEX-LOCA-200	7-rod VVER	Al <sub>2</sub> O <sub>3</sub>	E110, E110G
CODEX-LOCA-E4	7-rod VVER	Al <sub>2</sub> O <sub>3</sub>	E110, E110G
CODEX-LOCA-200B	7-rod VVER	Al <sub>2</sub> O <sub>3</sub>	E110, E110G
CODEX-LOCA-SFP1	7-rod VVER	Al <sub>2</sub> O <sub>3</sub>	E110, E110G
CODEX-LOCA-SFP2	7-rod VVER	Al <sub>2</sub> O <sub>3</sub>	E110, E110G
CODEX-AIT-3	7-rod VVER	ZrO <sub>2</sub>	E110G
CODEX-NITRO	7-rod VVER	ZrO <sub>2</sub>	E110, E110G
CODEX-SBO	7-rod VVER	ZrO <sub>2</sub> , Al <sub>2</sub> O <sub>3</sub>	E110, E110G
CODEX-SLIM	7-rod VVER	Al <sub>2</sub> O <sub>3</sub>	E110G
CODEX-ATF	7-rod VVER	ZrO <sub>2</sub> , Al <sub>2</sub> O <sub>3</sub>	optZIRLO™, Cr coated optZIRLO™
CODEX-ATF-AIT	7-rod VVER	ZrO <sub>2</sub> , Al <sub>2</sub> O <sub>3</sub>	Cr coated optZIRLO™

## Pellets

- UO<sub>2</sub>
- B<sub>4</sub>C
- Al<sub>2</sub>O<sub>3</sub>
- ZrO<sub>2</sub>

## Claddings

- E110 (ZR-6)
- Zircaloy-4 (Karlsruhe)
- Stainless steel (ZR-6)
- E110, E110G (fuel factory)
- optZIRLO™ (CTU)
- Cr-coated optZIRLO™ (CTU)



## Spacer grids

- Stainless steel (manufactured)
- E110 (manufactured)
- PWR (Karlsruhe)
- VVER (fuel factory)
- Cr-coated (CTU)

## Shroud

- E125 (Zr2.5Nb)
- Cr coated E125



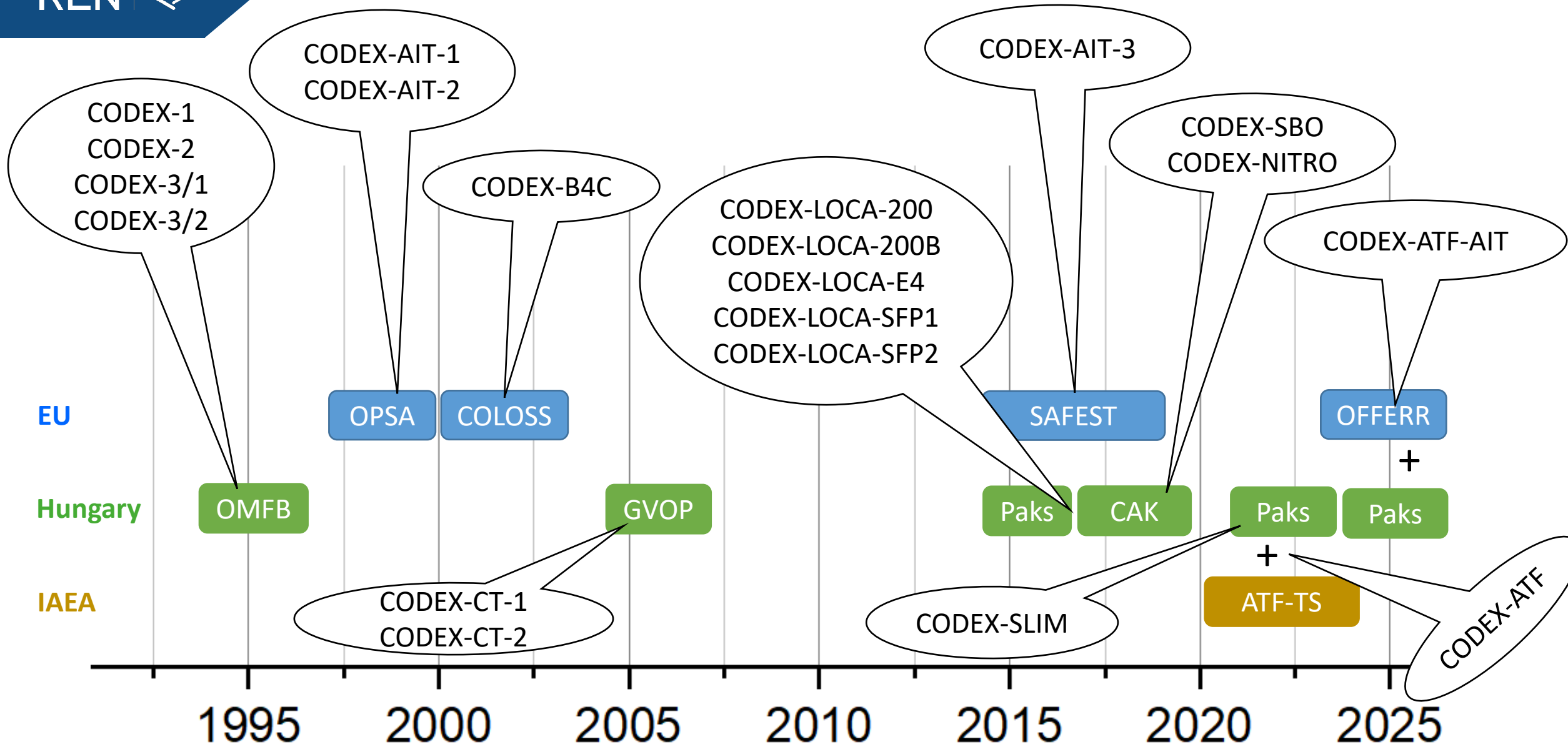
Péter Windberg



Imre Nagy



Róbert Farkas



# How was CODEX created?

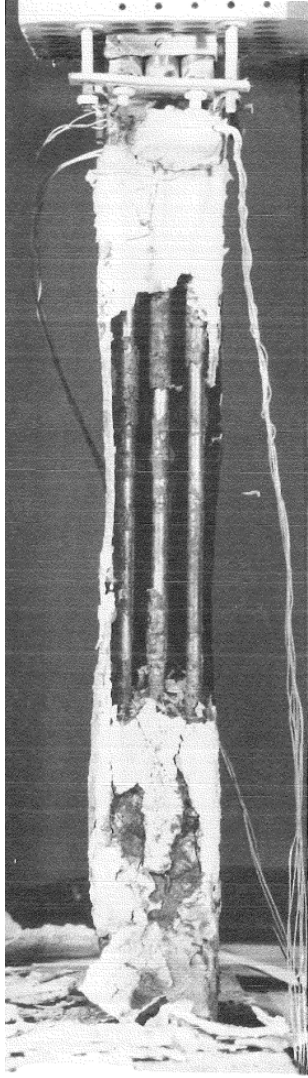
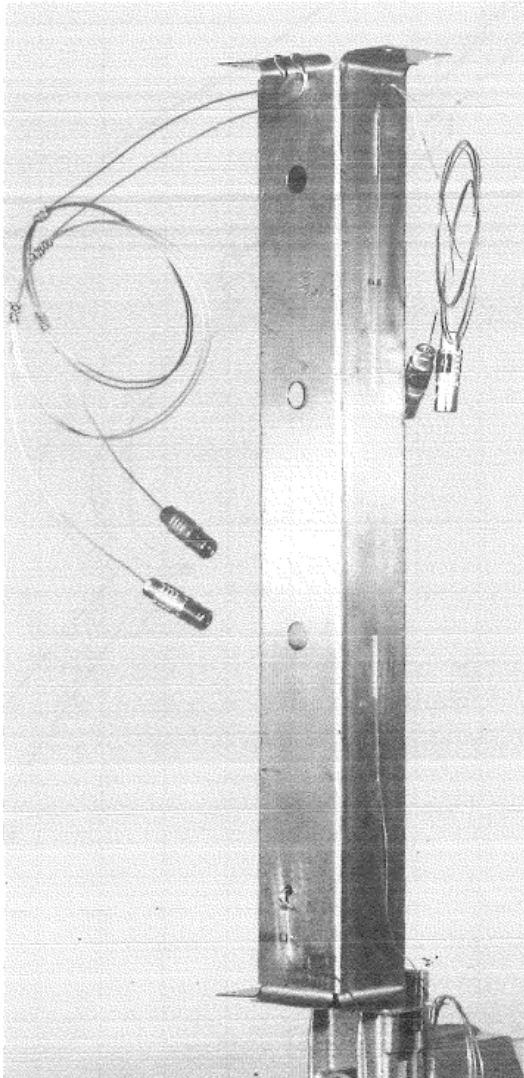
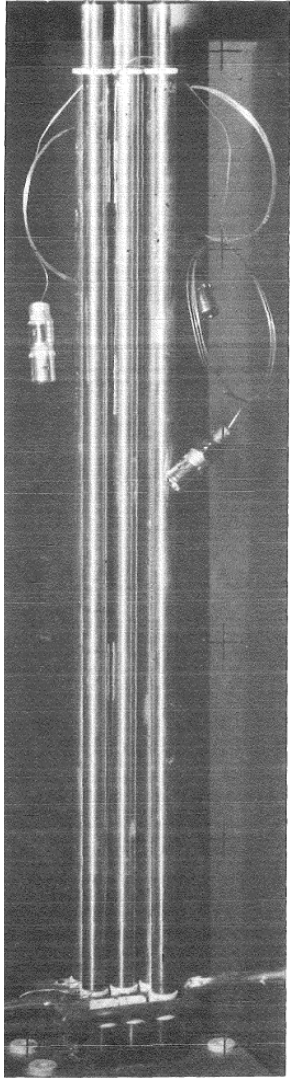
Early 1990s: beginning of fuel research in Hungary

Visits to Karlsruhe

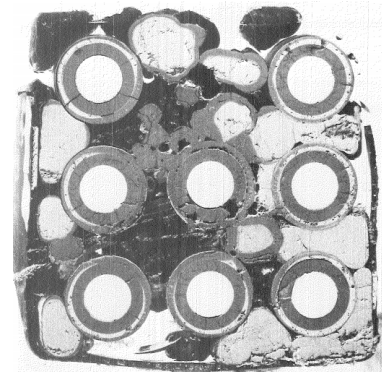
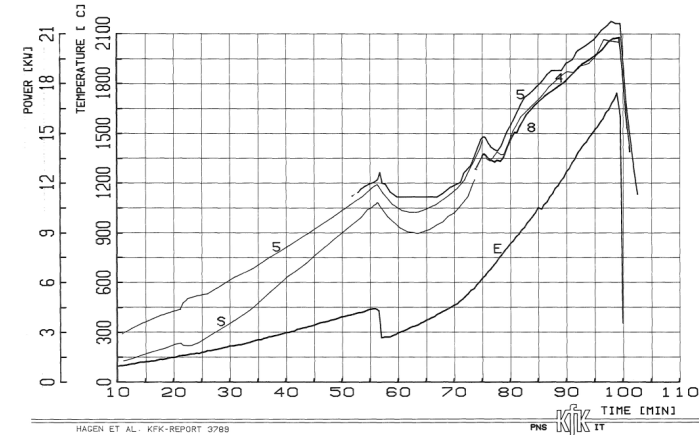
- László Maróti
- Lajos Matus
- Péter Windberg
- Peter Hofmann
- Gerhard Schanz
- Siegfried Hagen
- Review of severe accident experiments with Western fuel in Germany
- Potential for similar tests with VVER fuel in Hungary
  - Separate effect tests (oxidation, eutectic formation, burst,  $\text{UO}_2/\text{E110}$  interaction,  $\text{B}_4\text{C}/\text{E110}$  interaction, H uptake by E110)
  - Integral tests (CORA, NIELS) => CODEX



## CODEX – many similarities with NIELS



- 3x3 bundles
- 40 cm length
- Fuel rods with  $\text{UO}_2$  and control rods
- Electrical heating
- Up to 2250 °C (melting,  $\text{UO}_2$  dissolution by Zr)
- Experiments in 1982-1986
- Precursor of CORA (1987-1993)

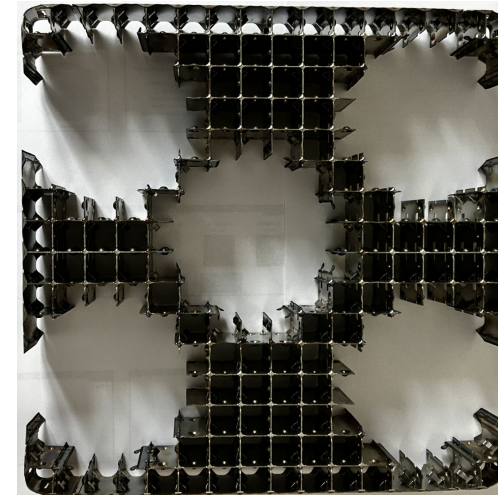
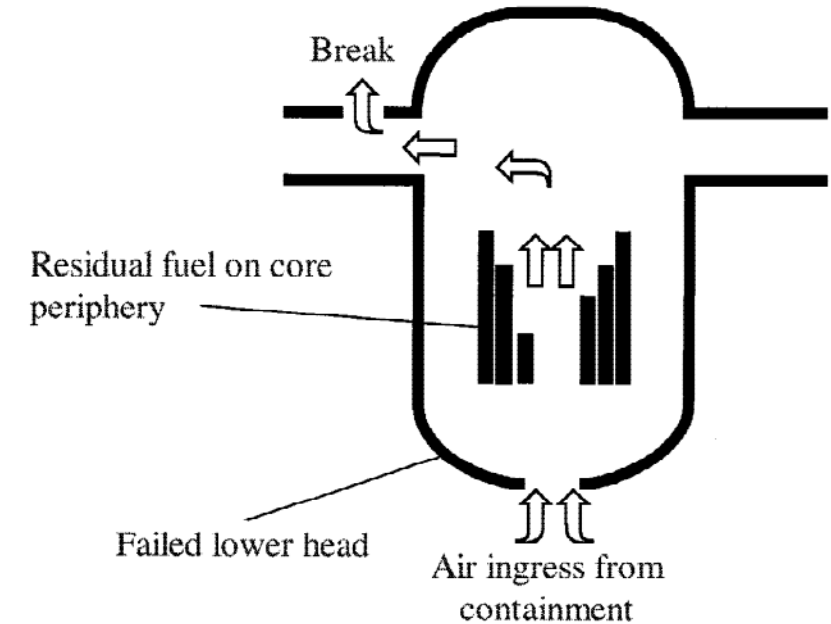


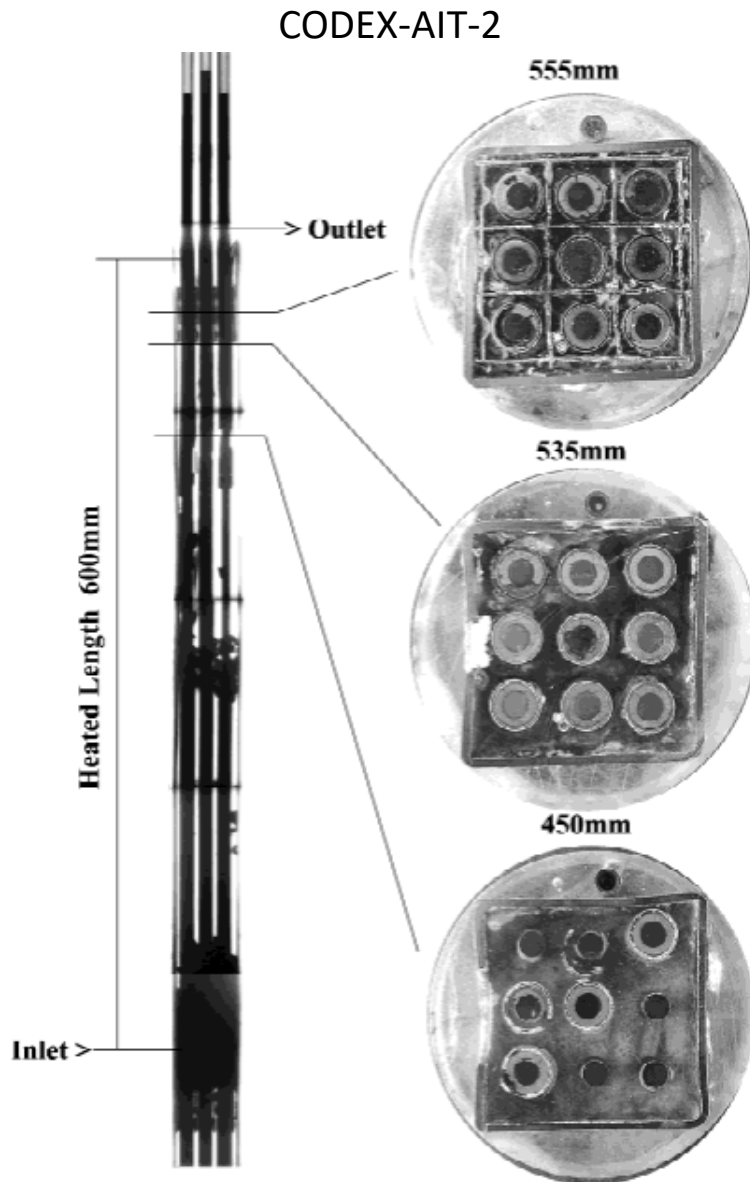
# Examples of QUENCH-CODEX co-operation

- EU OPSA project  
*(Oxidation Phenomena in Severe Accidents)*
- Oxidation of Zr alloys in air
- Oxidation of  $UO_2$  to higher oxides
- Proposal by Peter Hofmann:

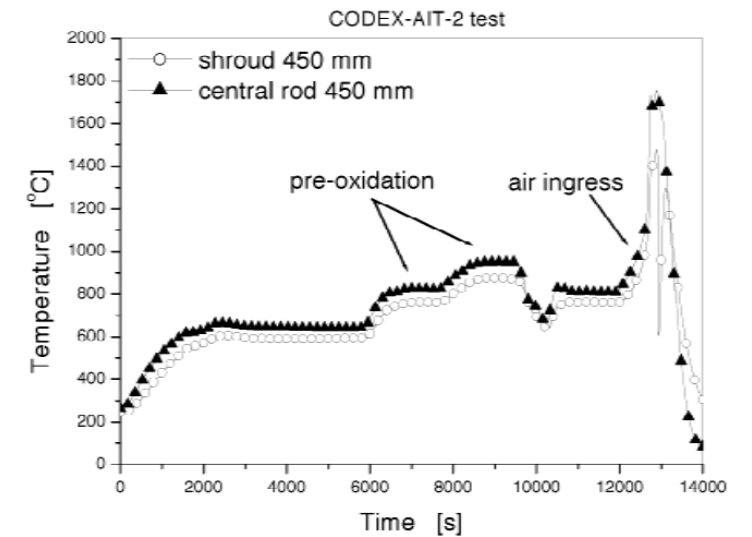
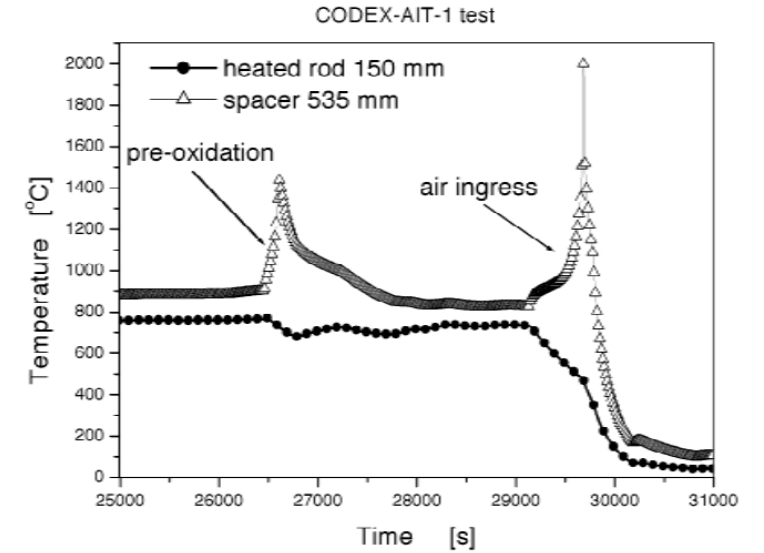
Air ingress CODEX tests with  $UO_2$  using remaining materials from CORA tests

- depleted uranium-dioxide pellets,
- Zircaloy-4 cladding tubes,
- PWR type spacer grid

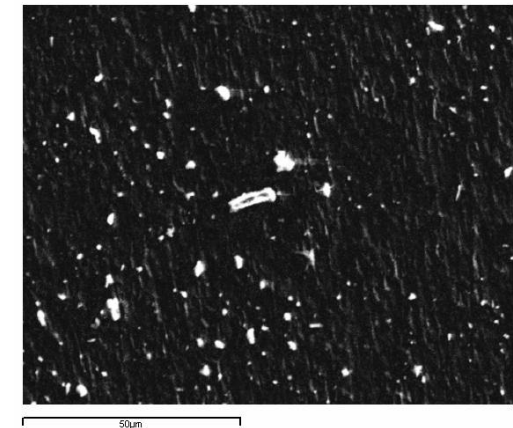
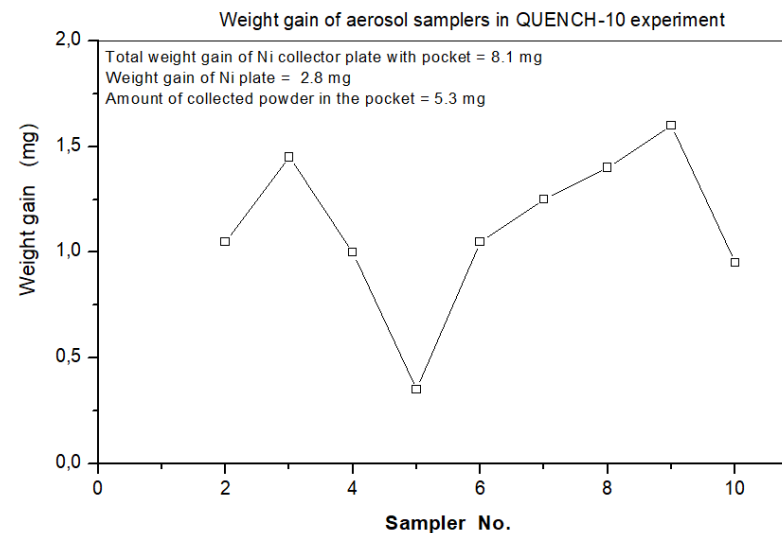
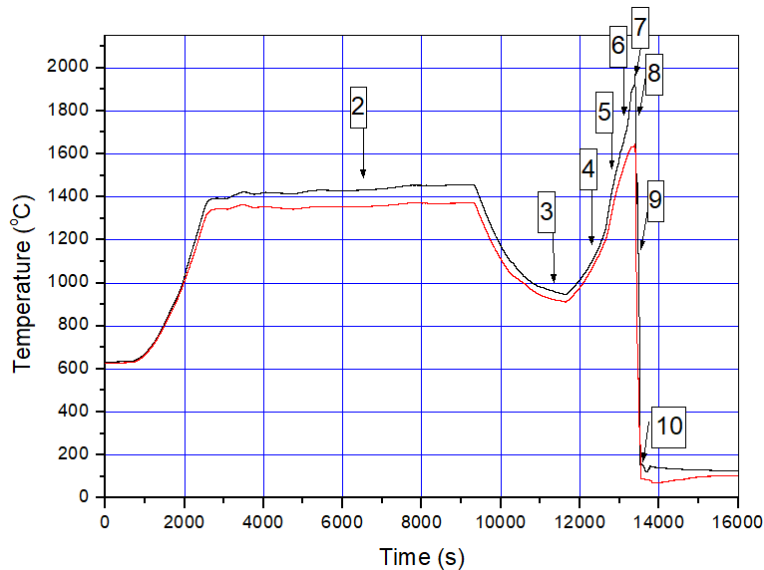
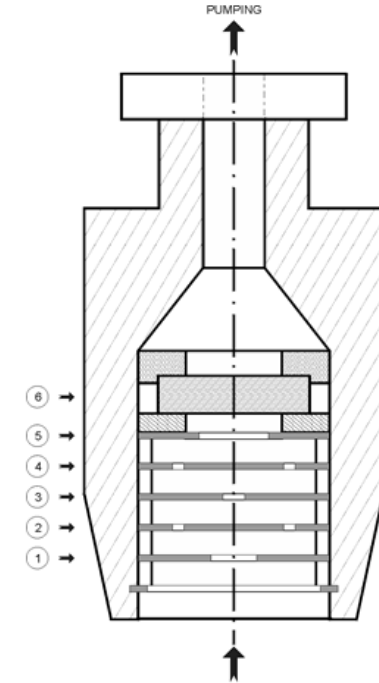
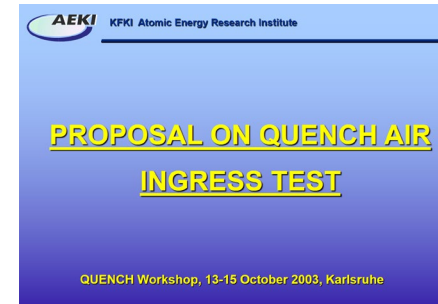




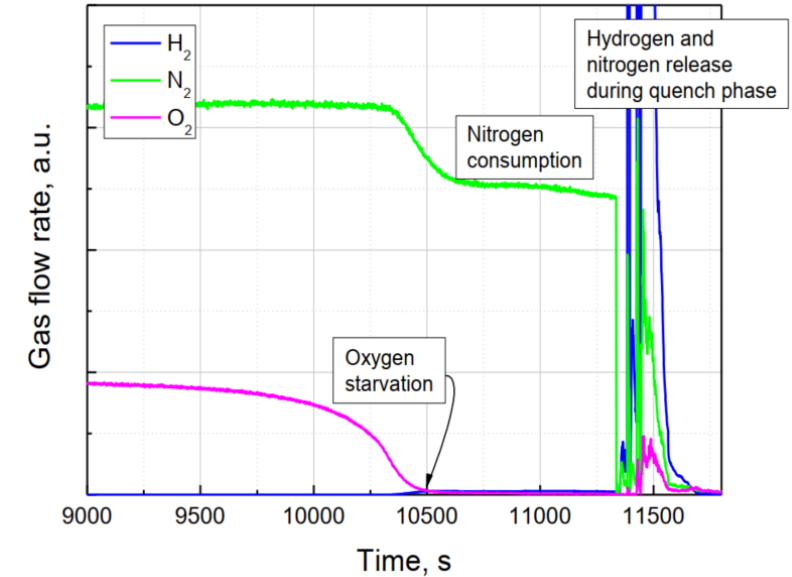
- Acceleration of oxidation and core degradation in air compared to steam
- Heavy oxidation and nitride formation on Zr surfaces
- Release of a large number of aerosol particles
- No signs of  $UO_2$  oxidation
- Slow cool-down



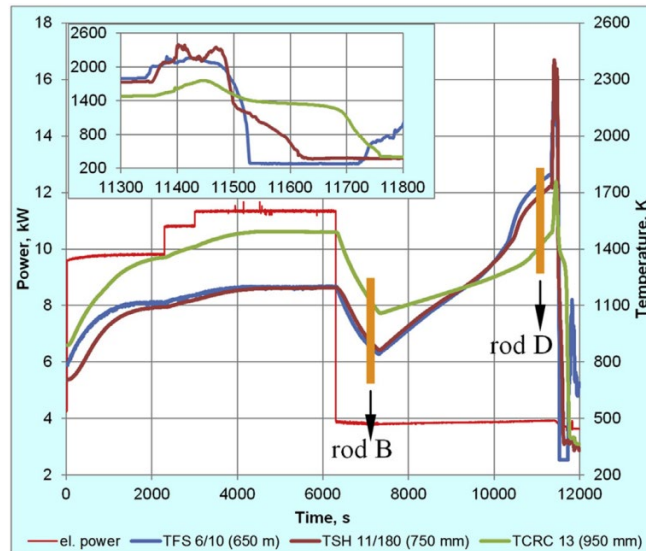
- EU LACOMERA project
- Test proposed by AEKI, Budapest:
  - Long pre-oxidation before air ingress
  - Final quench
- AEKI aerosol collection system
  - 10 impactors actuated at various times



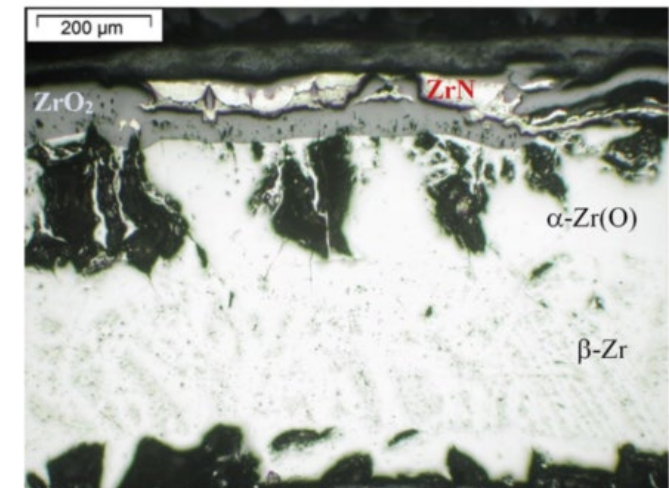
- EU LACOMECECO project
- AEKI proposal
  - Slow oxidation and nitriding of Zr in air
  - Final quench close to melting point
- Participation of Hungarian experts at the test



LACOMECECO Final Report, 2013

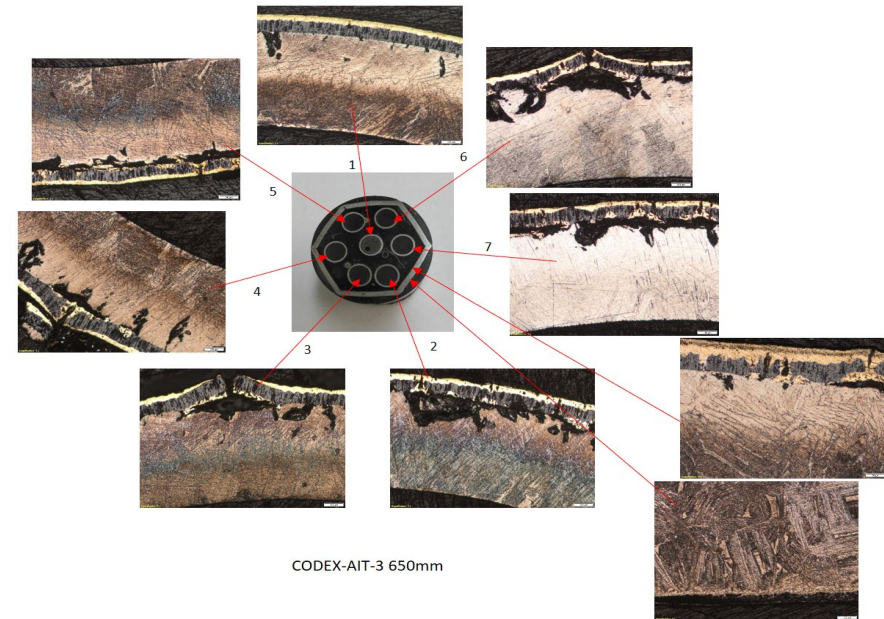
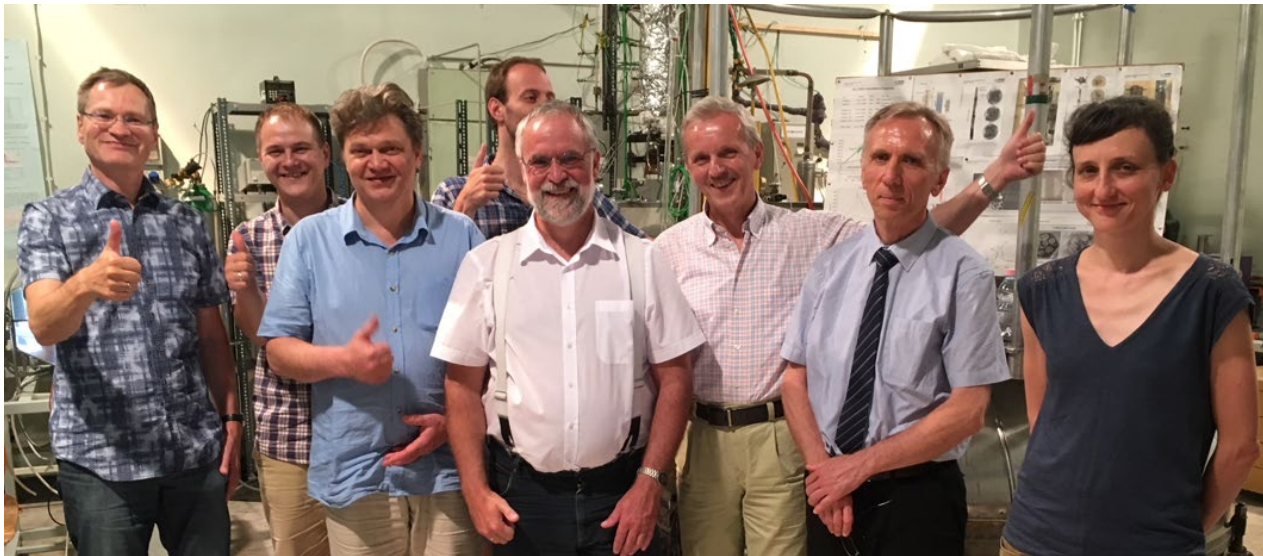
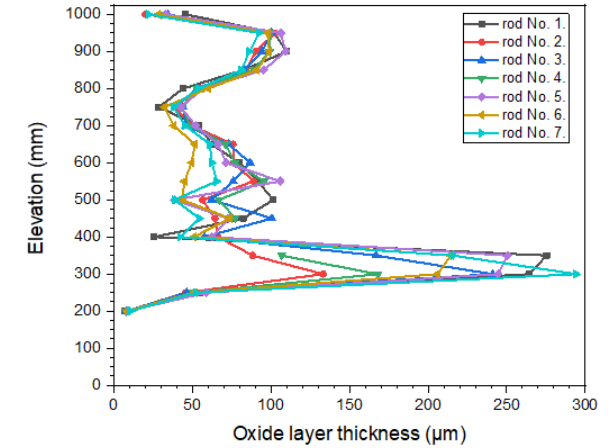
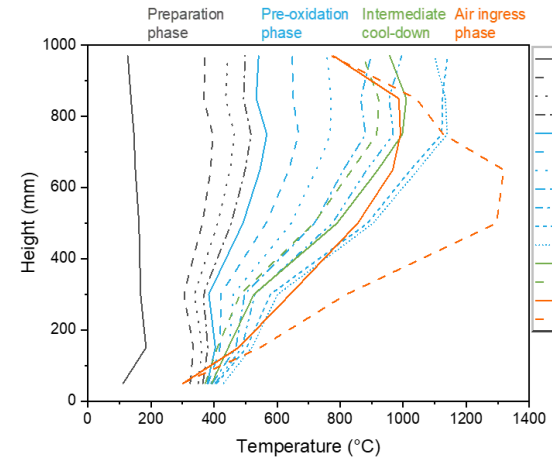


elevation: 430 mm

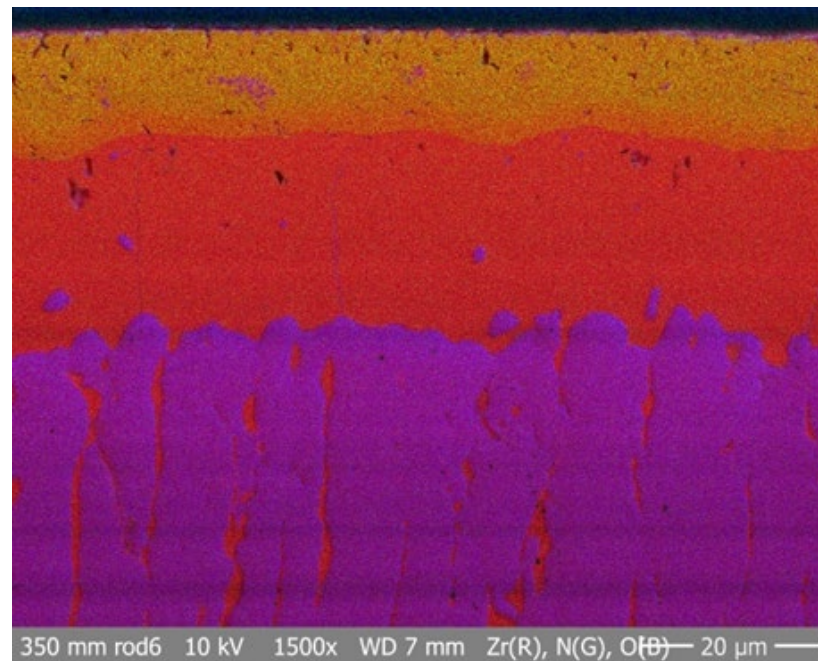
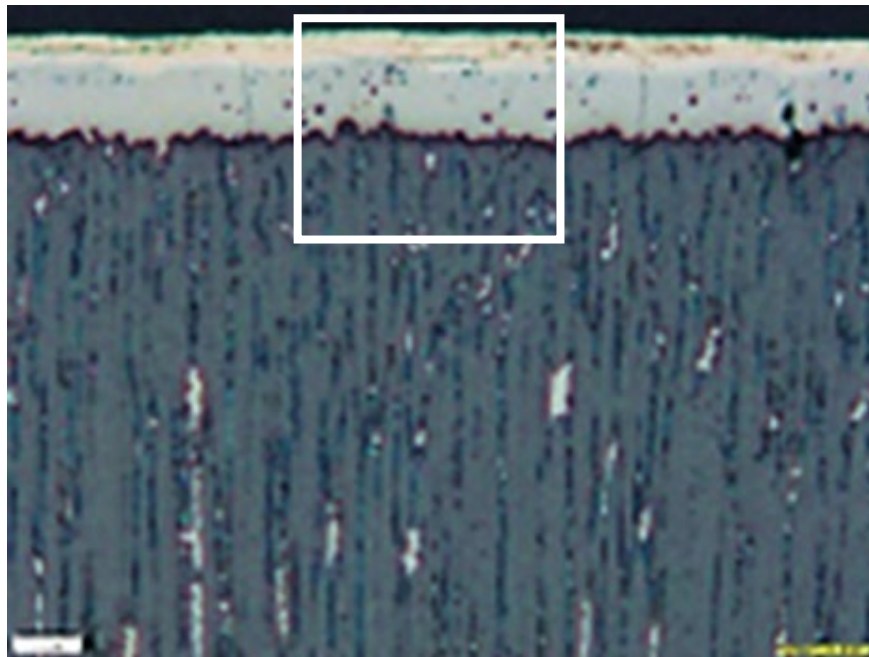
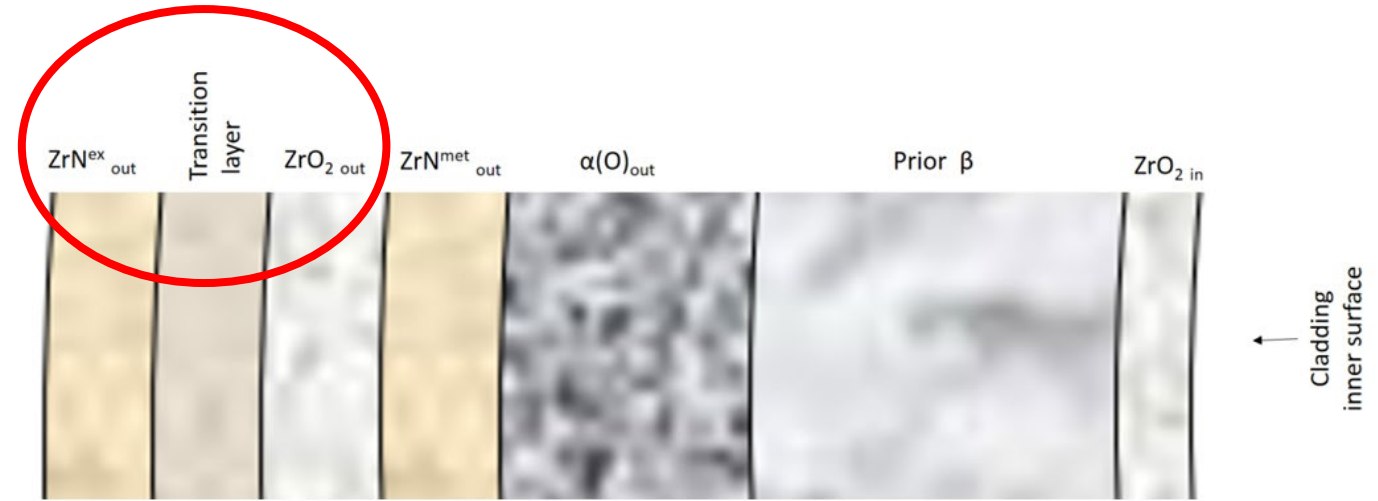


elevation: 350 mm; rod: 5

- EU SAFEST project
- Strong support from KIT
- Steam and oxygen starvation
- Shift of maximum temperature
- Slow cool-down – before quench conditions



- Transition layer between oxide and nitride
- SEM/EDS analyses by Ulrike Stegmaier



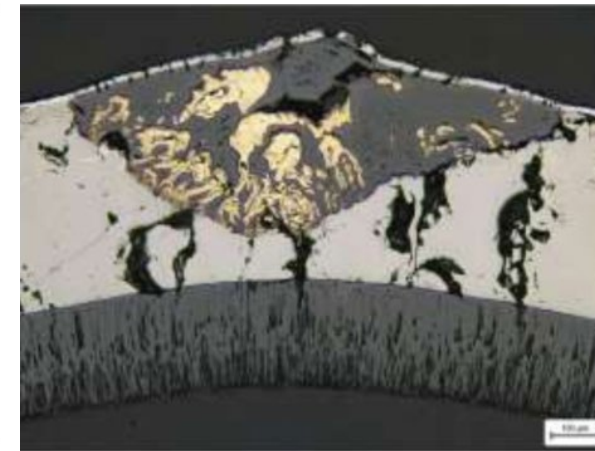
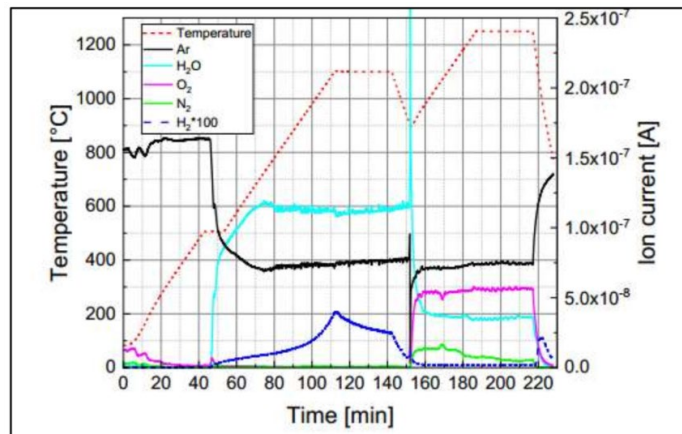
ZrN

Transition layer with Zr, O and N

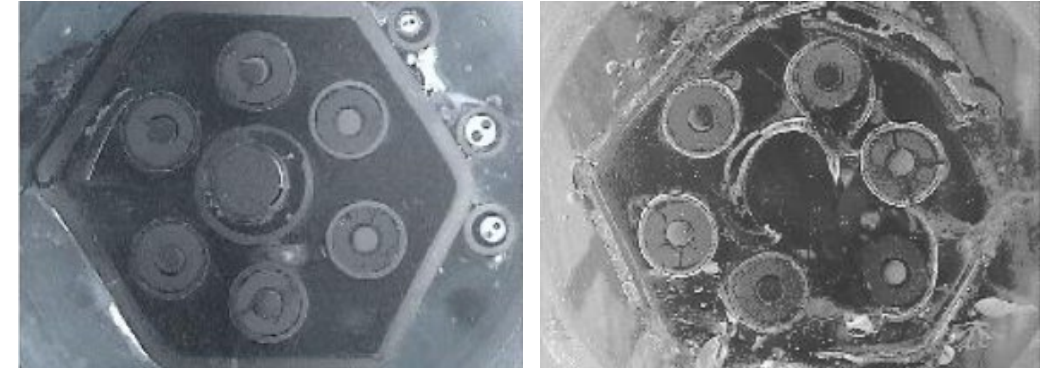
ZrO<sub>2</sub>



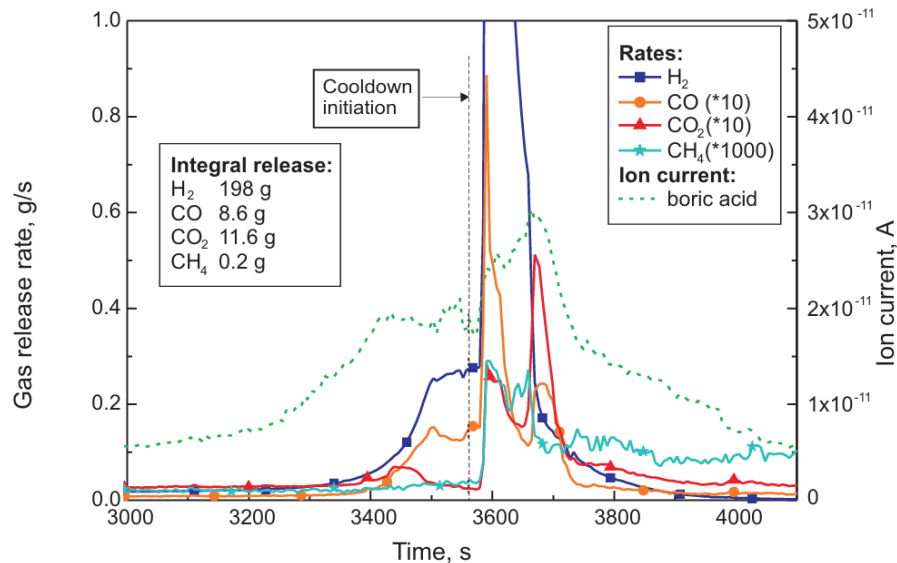
- EU OFFERR Project
- Principal researcher: Martin Steinbrück
- Visiting researchers: Juri Stuckert, Mirco Grosse
- Air ingress with Cr-coated bundle
- Thermogravimetric test at KIT with MS



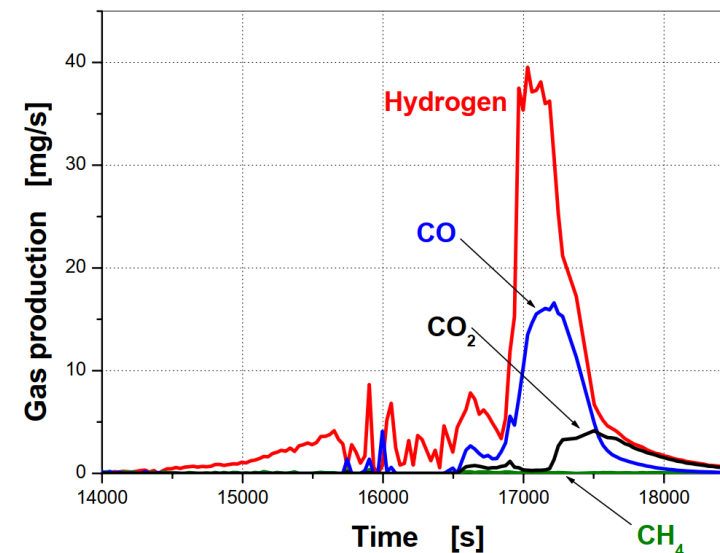
- B<sub>4</sub>C oxidation in steam – CH<sub>4</sub> production ?
- Integral tests with B<sub>4</sub>C control rods
- Very low methane production
- Confirmed by QUENCH-09, too



QUENCH-07 (2001) – reflow



CODEX-B4C (2001) – slow cool-down

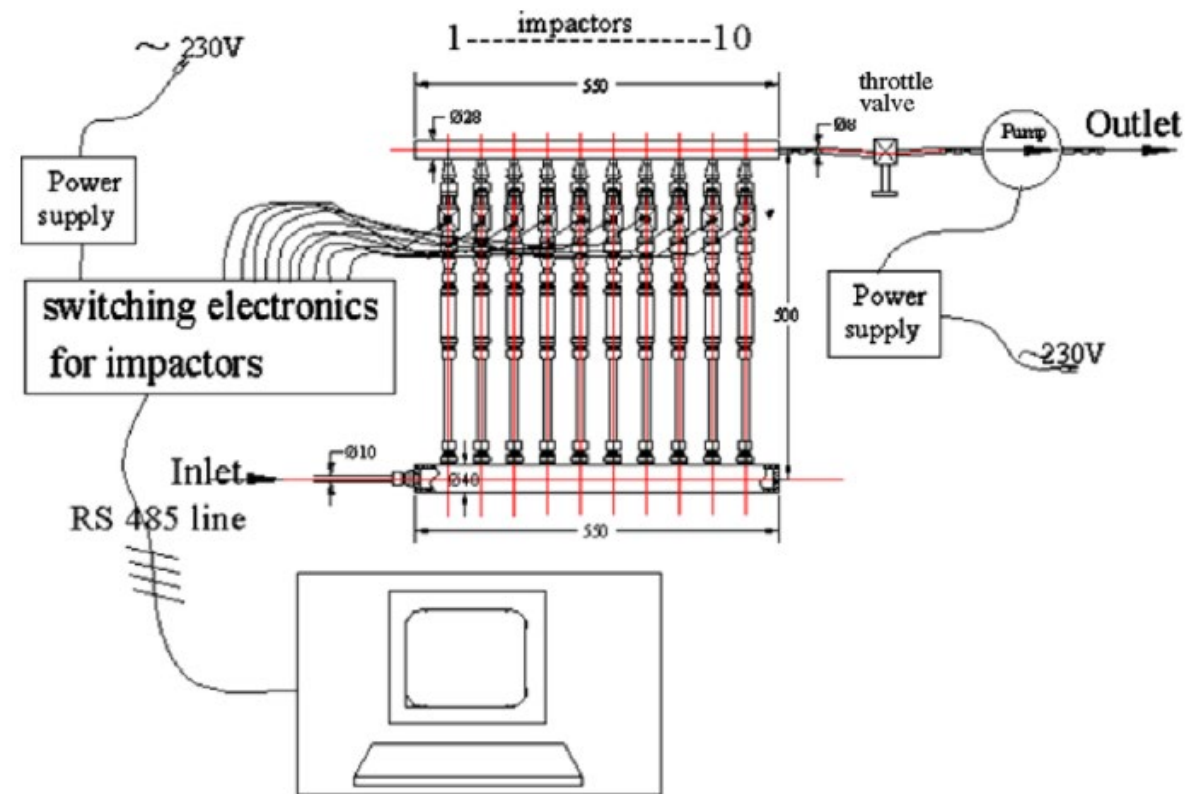


KFKI-2003-01/G

- QUENCH-13
- Silver-indium-cadmium control rod
- Aerosol measurements by AEKI
- Large burst of aerosols (Ag-In-Cd components)

Average composition of individual aerosol particles analyzed in samples collected with AEKI impactors, wt.%.

Sample	Time (s)	O	Cd	In	Ag	W	Fe
AEKI3	11,156	38	62	-	-	-	-
AEKI4	12,129	28	19	38	0	15	-
AEKI5	13,215	25	9	17	4	39	0.3
AEKI6	13,679	15	0	4	58	14	3
AEKI7	13,742	30	0	6	2	0	52





# Conclusions

- 30 years: 20 CODEX core degradation experiments
- VVER/PWR comparison
- VVER specific reactor scenarios
- Investigation of general severe accident phenomena
- Three decades of QUENCH-CODEX co-operation
  - Parallel tests
  - Supplementary tests
  - Outstanding results in air ingress phenomena

Thank you  
very much!

**Thank you for your  
attention!**



**Martin Steinbrück**

KIT

## **Materials science for nuclear safety. From unexpected findings to improved severe accident codes**

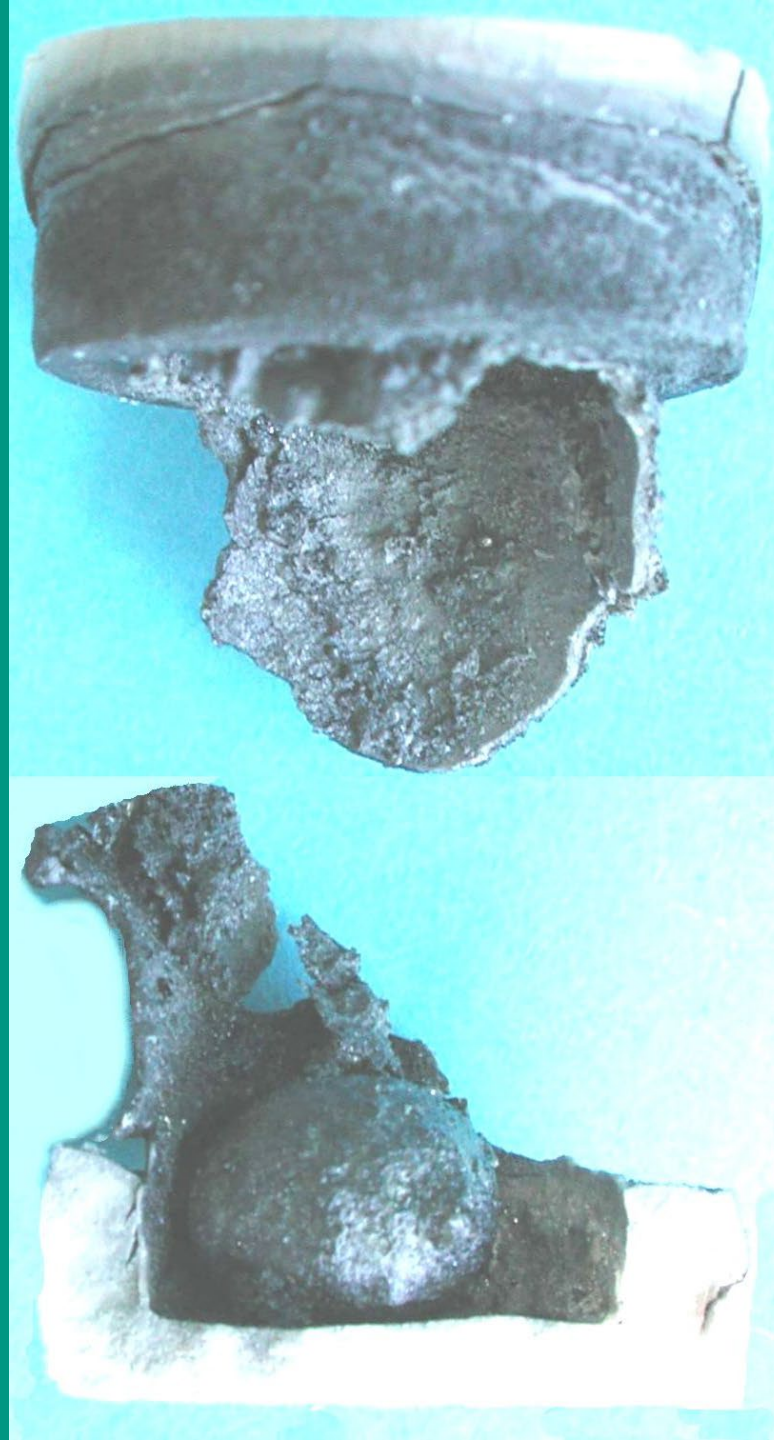
This presentation, delivered at the 30th International QUENCH Workshop, reviews three decades of materials science research for nuclear safety within the QUENCH program. Initially launched to quantify hydrogen generation during reflood of overheated reactor cores, the program has evolved from investigating the so-called “quench effect” to addressing complex phenomena influencing severe accident progression. Key findings include the role of water injection in triggering renewed oxidation of Zircaloy cladding, the impact of nitrogen ingress on cladding degradation and hydrogen release, and the critical influence of eutectic interactions between boron carbide and stainless steel on core melt behavior. Experimental campaigns combining large-scale bundle tests, separate-effects studies, and advanced imaging techniques have provided essential data for improving severe accident codes worldwide. The results underscore the importance of thermodynamic and kinetic considerations, as well as prototypical experimental design, in predicting accident scenarios. These insights have significantly enhanced accident management strategies and informed international safety standards for current and future reactor systems.

# Materials science for nuclear safety

From unexpected findings to  
improved severe accident  
codes

Martin Steinbrück, Mirco Große, Juri Stuckert

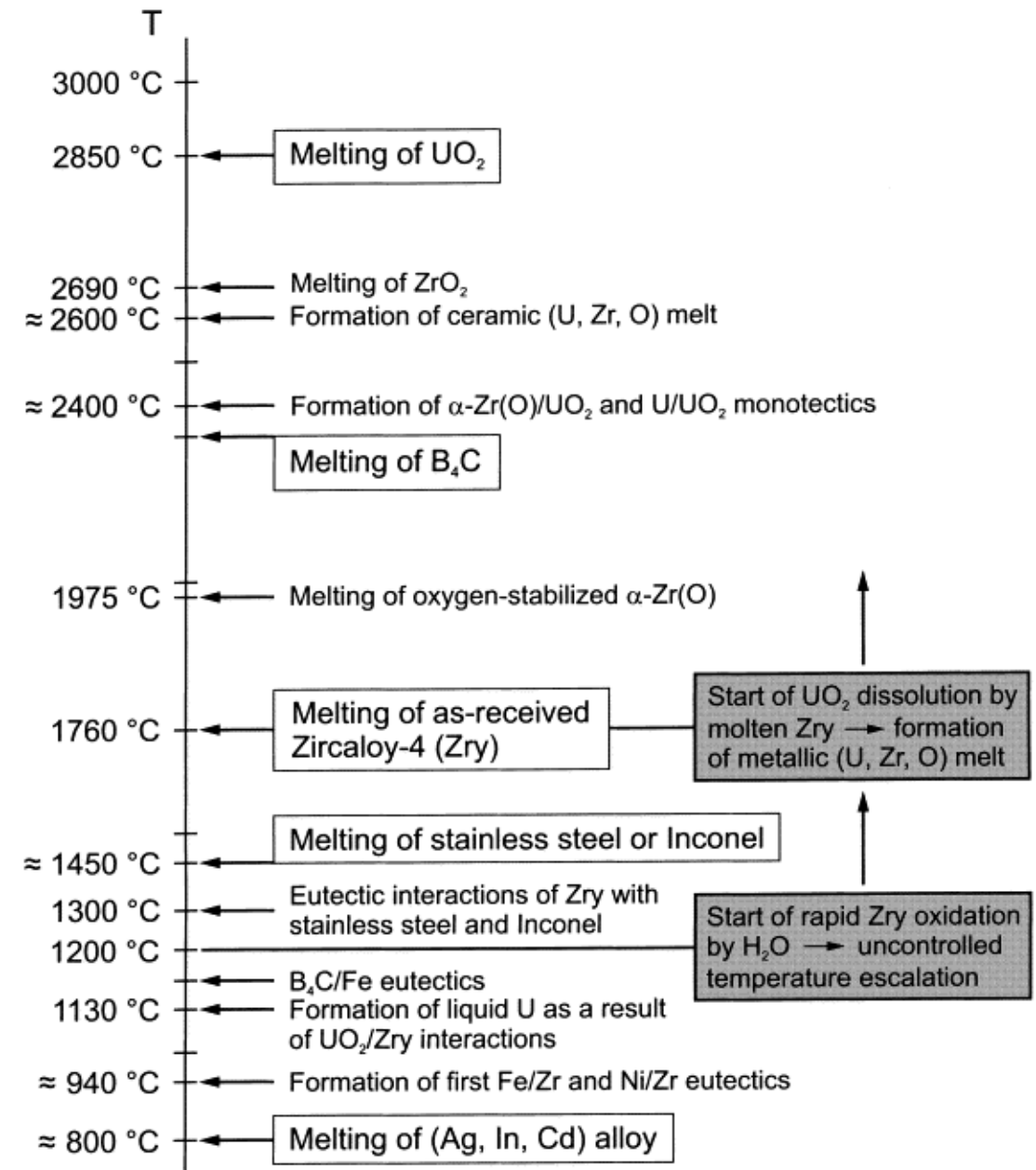
30<sup>th</sup> International QUENCH Workshop  
16-18 December 2025, Karlsruhe, Germany





# Background

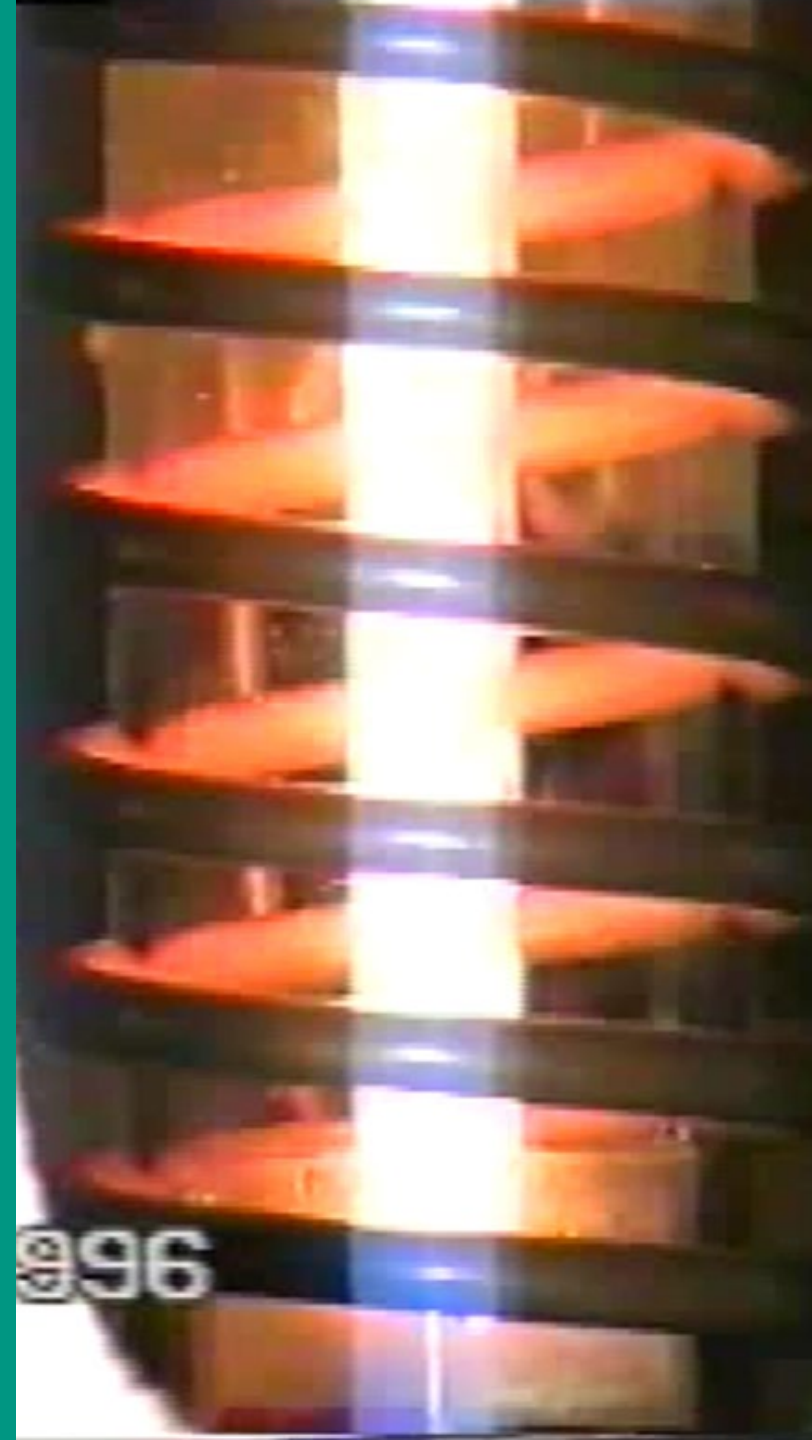
- QUENCH program initiated by Peter Hofmann after completion of the CORA program
  - Determination of the hydrogen source term during reflood of an overheated reactor core
- Overviews on separate-effects tests and bundle tests during 25<sup>th</sup> QWS  
(6 years ago, <https://publikationen.bibliothek.kit.edu/1000100298>)



## Content

1. Background
2. The “quench effect” on hydrogen source term
3. The effect of nitrogen on cladding oxidation and degradation
4. The effect of  $B_4C$ -SS eutectic interactions on accident progression
5. Takeaways

# The “quench effect” on hydrogen source term



# In search of the "quench effect"

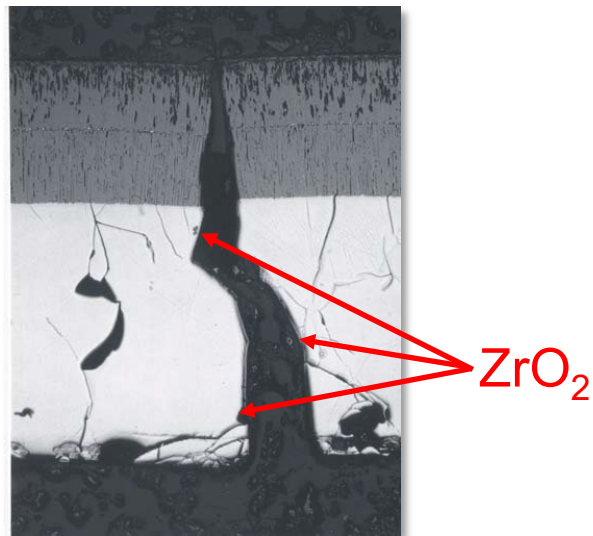
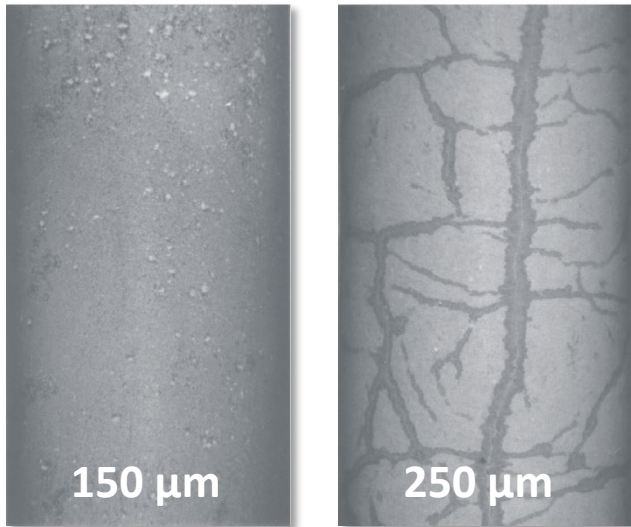
- Water injection is the primary AMM for cooling an uncovered core during a severe accident scenario
- Analysis of the TMI-2 accident as well as subsequent integral in-pile and out-of-pile experiments (PBF, LOFT, PHEBUS, CORA) has shown that water injection can result in temperature runaway, which is connected with intense hydrogen release
- The QUENCH program was designed to understand this phenomenon and to provide quantitative data on the hydrogen source term
- Initially we looked for a single “quench effect”

*Sepold et al., NED204 (2001) 205–220:*

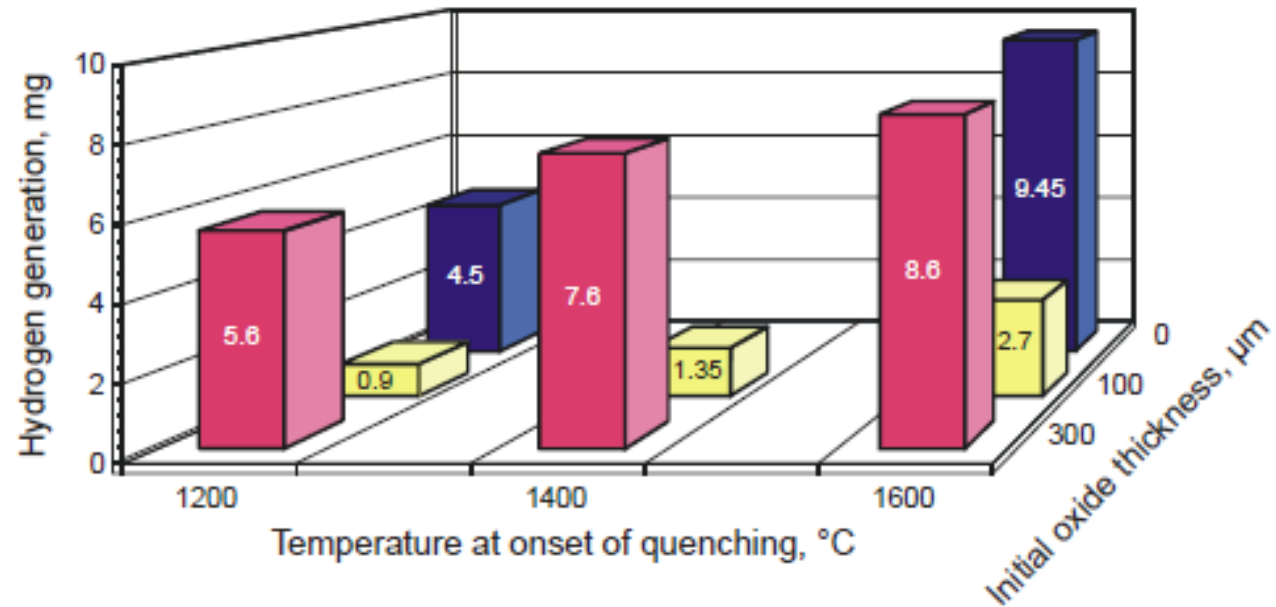
However, before the water succeeds in cooling the fuel elements, **water injection** can trigger a renewed enhanced oxidation of the Zircaloy cladding and, at the same time, cause a **rapid increase in temperature and hydrogen generation**.

This phenomenon was demonstrated by analyses of the TMI-2 accident and in results of out-of-pile (CORA) and in-pile LWR bundle experiments (LOFT, Phebus). **It was explained as being due to the generation of new metal surfaces by cracking and fragmentation of the oxygen-embrittled cladding tubes during flooding, and to enhanced exothermal oxidation of the newly formed metal surfaces** (Hofmann et al., Report FZKA 5846, 1997).

# Single-rod QUENCH tests – Main results

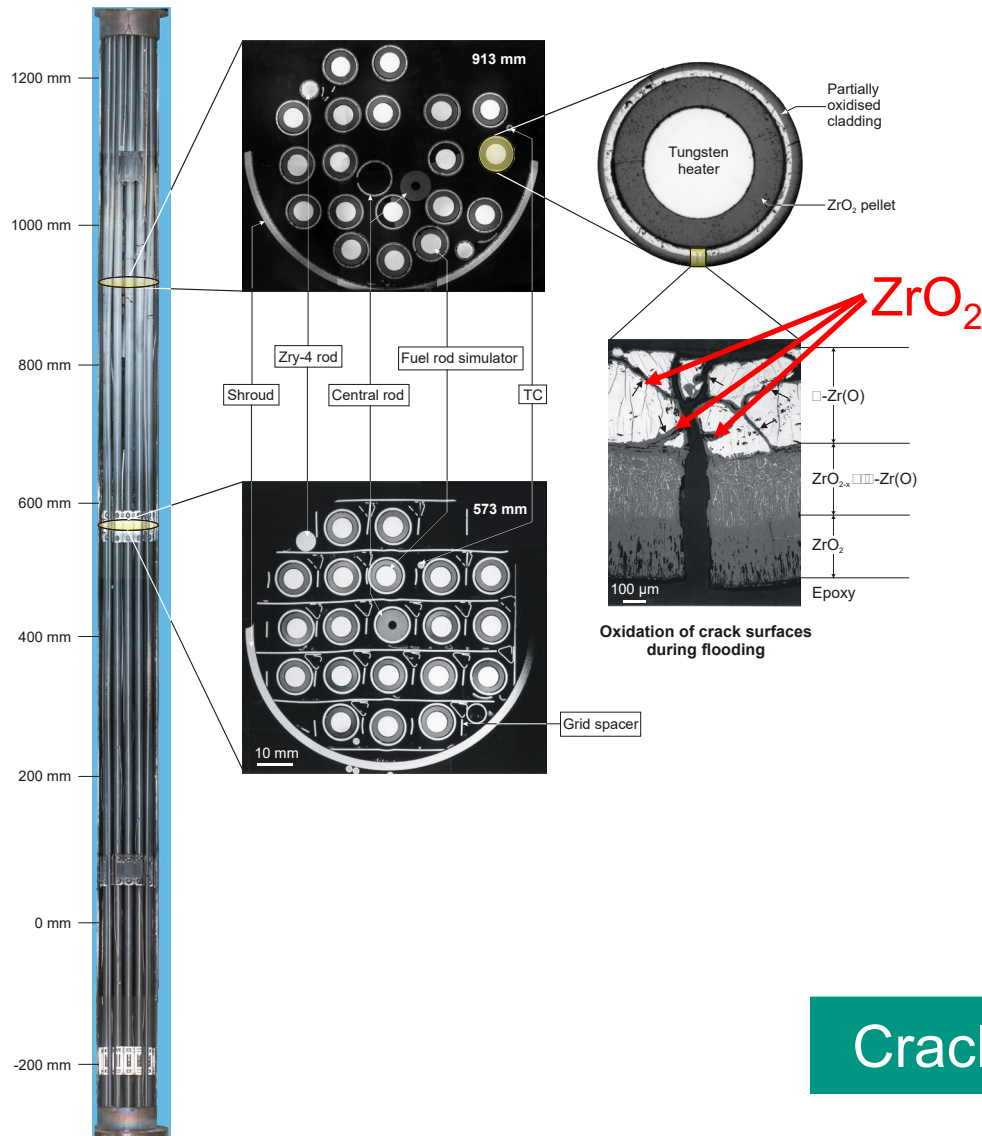


- Through-wall crack for pre-oxidation >200  $\mu\text{m}$  with a density of 0.5 mm/mm<sup>2</sup>
- Oxidation of crack surfaces connected with hydrogen generation and partly absorption by the metal



Hydrogen generation vs. oxide thickness

# Crack formation in QUENCH-01 bundle test



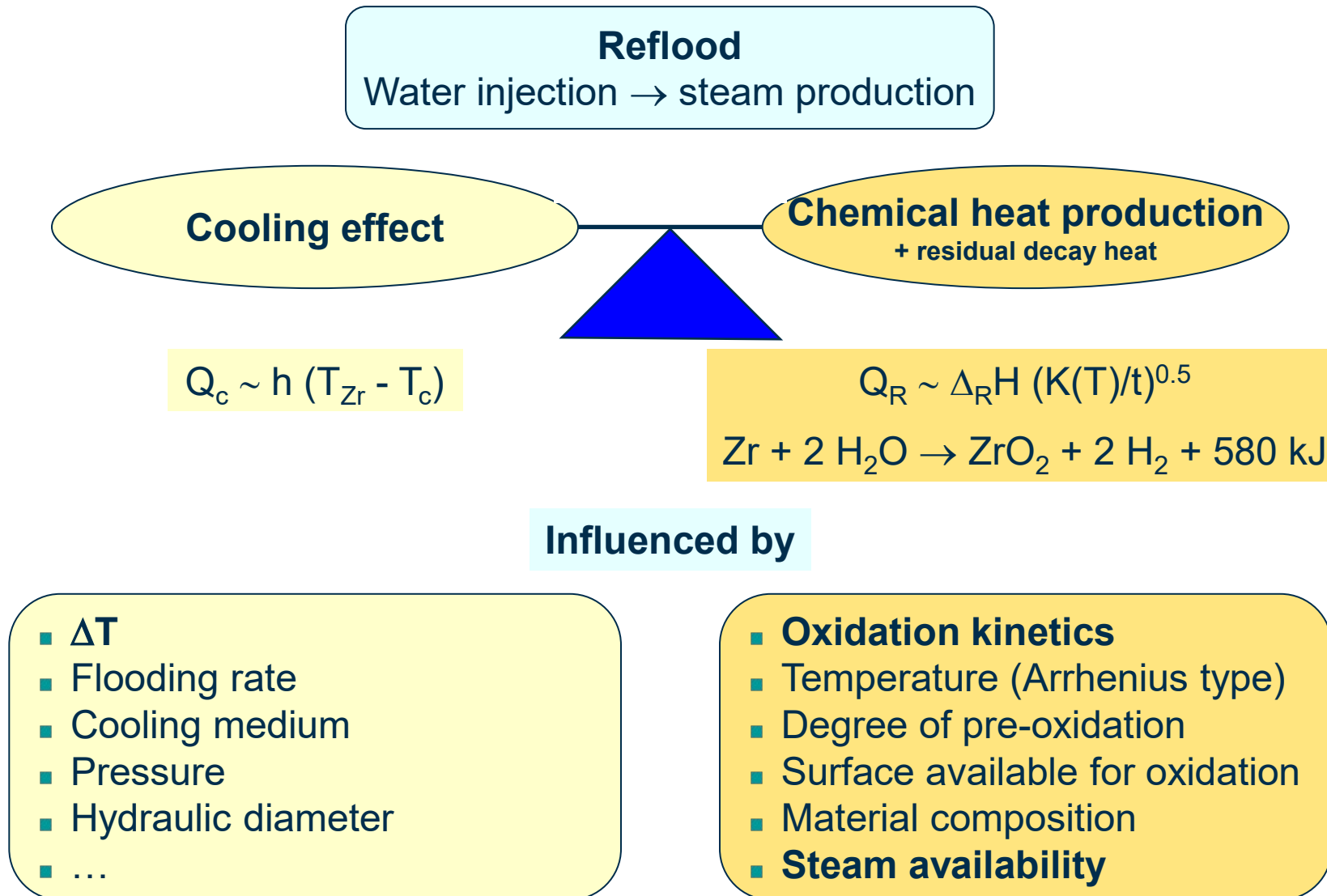
- Estimation of hydrogen production by crack oxidation gives only ca. 1-2 g for the whole bundle
- This could not explain temperature runaway during reflood

*However:*

- *Solution enthalpy of 1 g H<sub>2</sub> in 1 kg Zr increases temperature by 200 K*

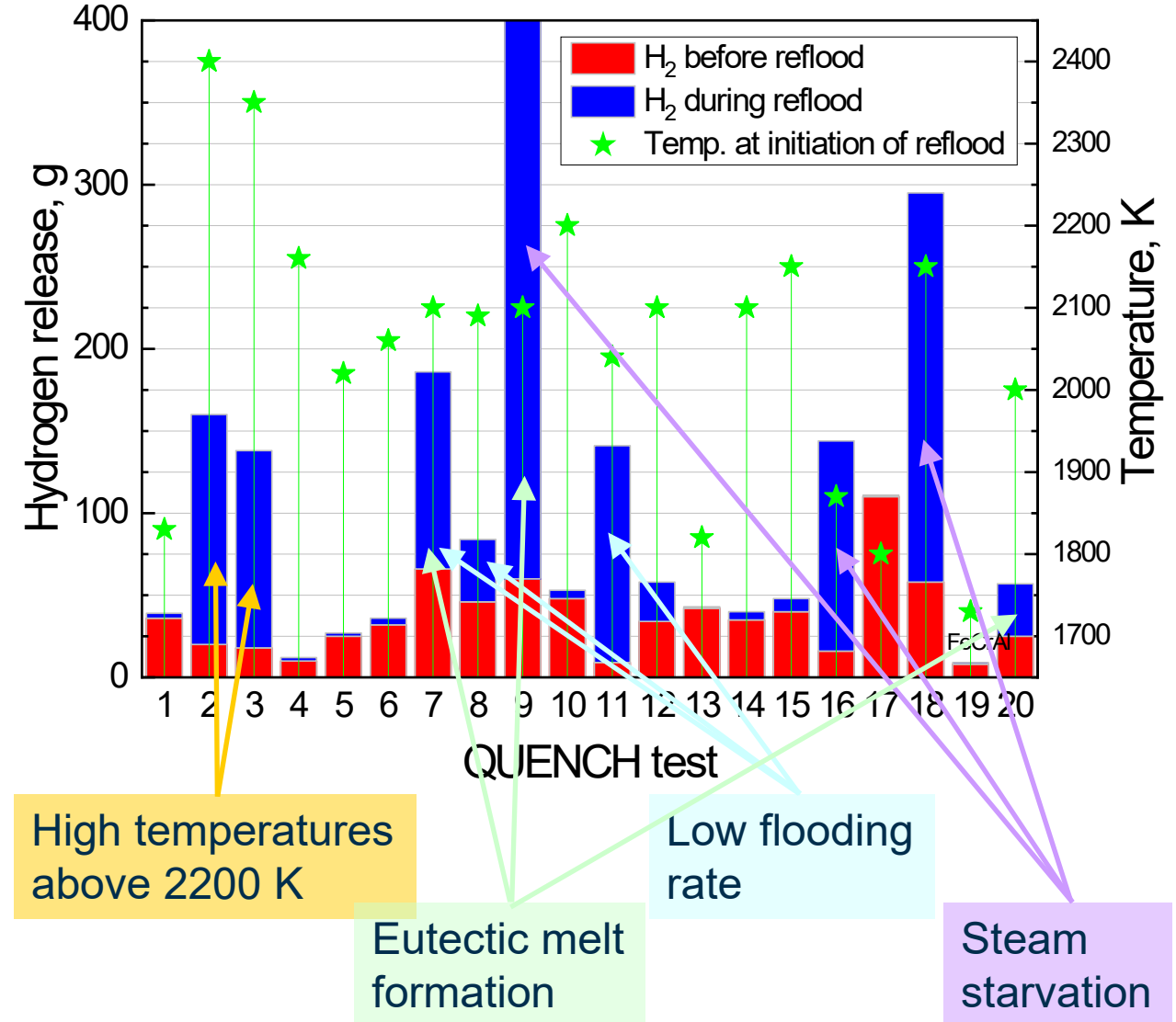
Crack formation and oxidation are only minor effects

# Successful reflood depends on many parameters

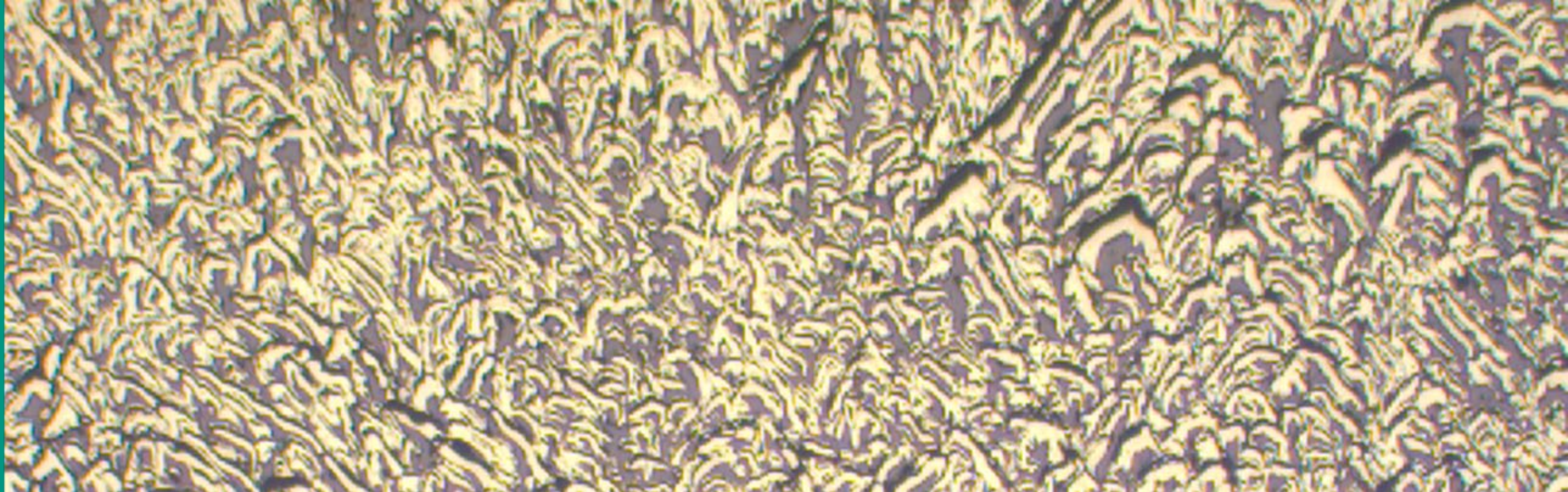


# Summary of QUENCH bundle tests

- Depending on the energy balance after reflood initiation, there will be a cooldown or temperature escalation
- Successful reflood if
  - Less chemical (and residual decay) energy is produced than can be eliminated by cooling
  - Cooling water rate is  $> 1$  g/s rod
  - No oxidizable melt in contact with steam
- Ultimately, we discovered that a variety of factors must be considered





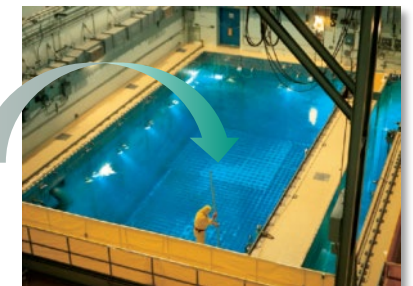
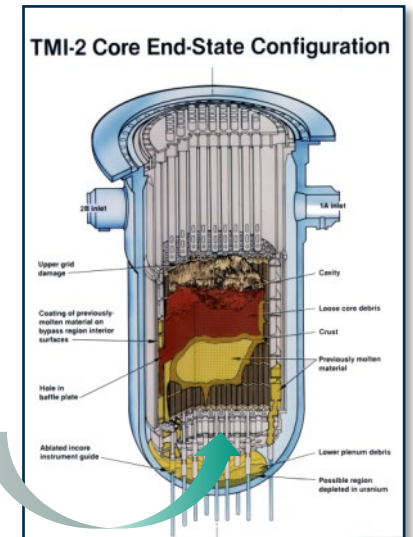


# The effect of nitrogen on cladding oxidation and degradation

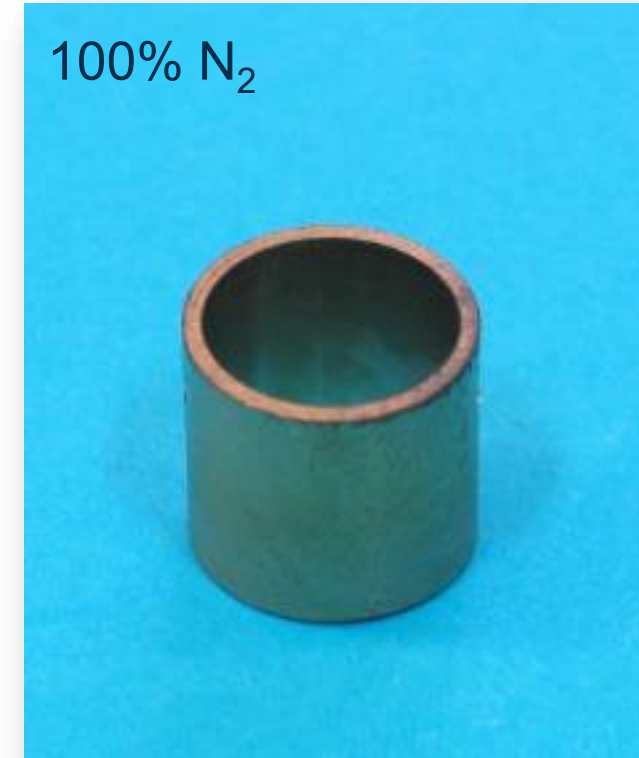
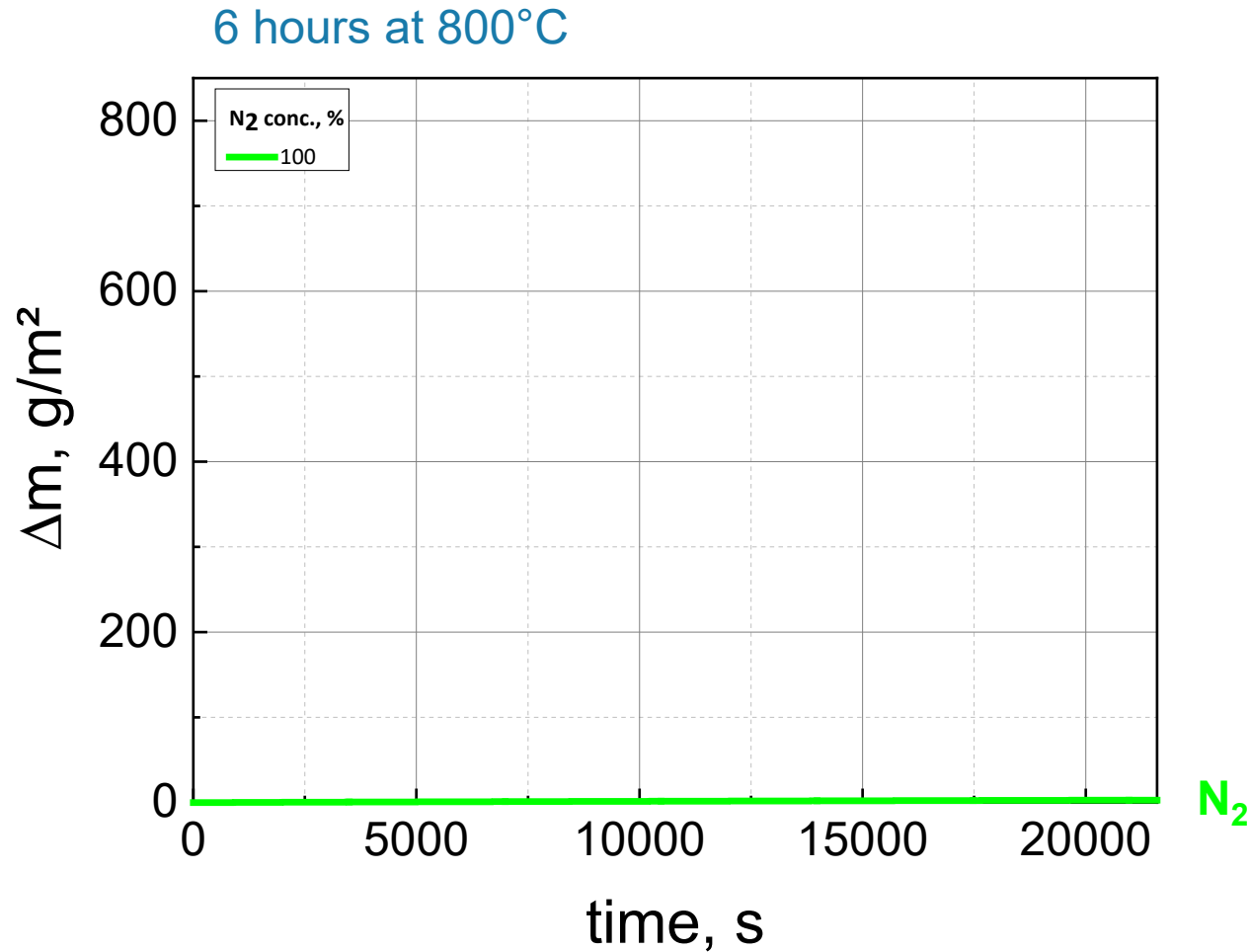
# Nitrogen in LWRs

- The “inert” gas nitrogen is used to inertize BWR containments and in ECCS pressurizers
- Air contains nitrogen and ingress may occur into reactor core, spent fuel pond, or transportation cask
- Typically, nitrogen comes into contact with the cladding after steam oxidation, mixing with the steam

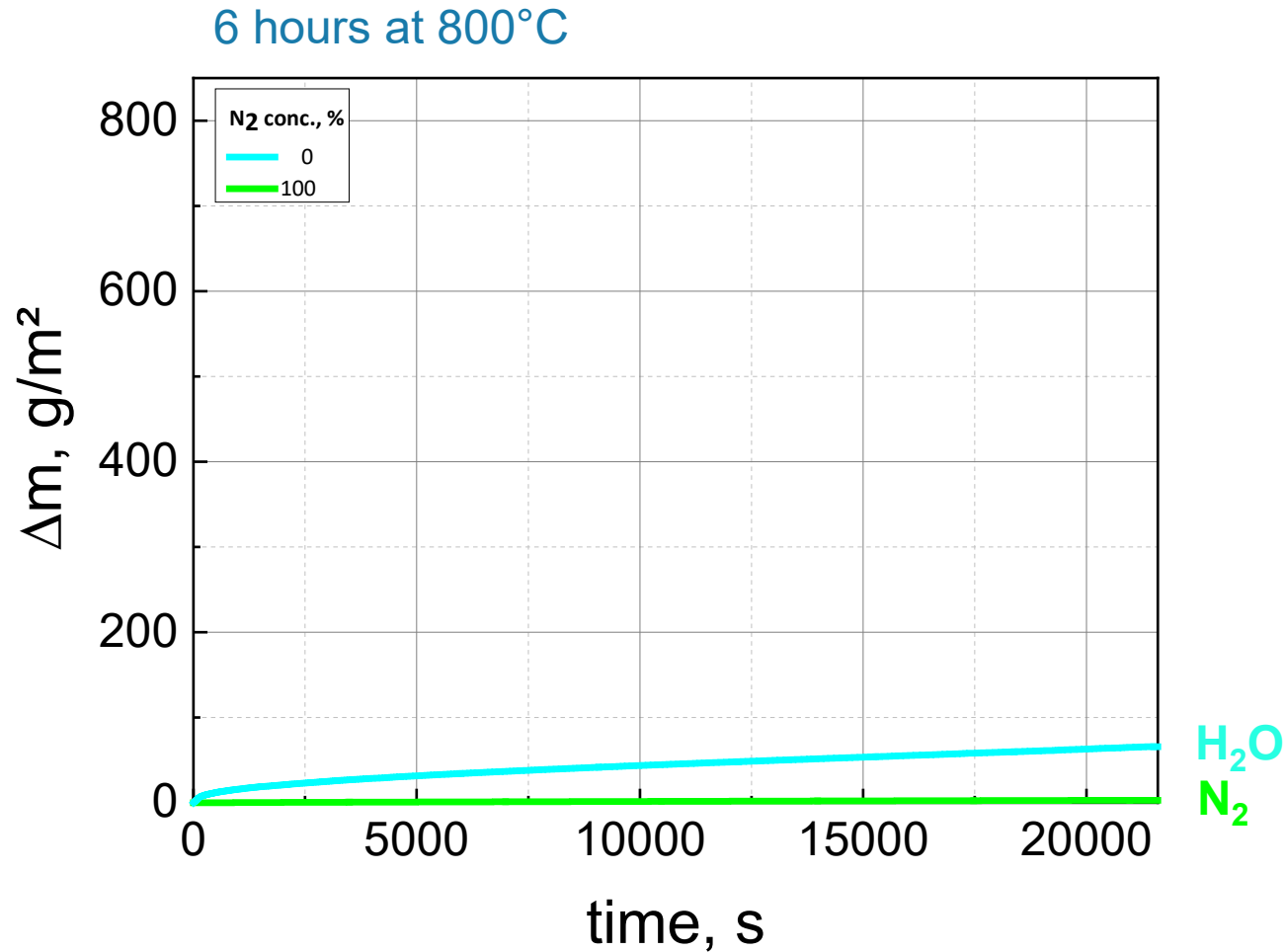
What are the consequences on hydrogen source term and cladding degradation?



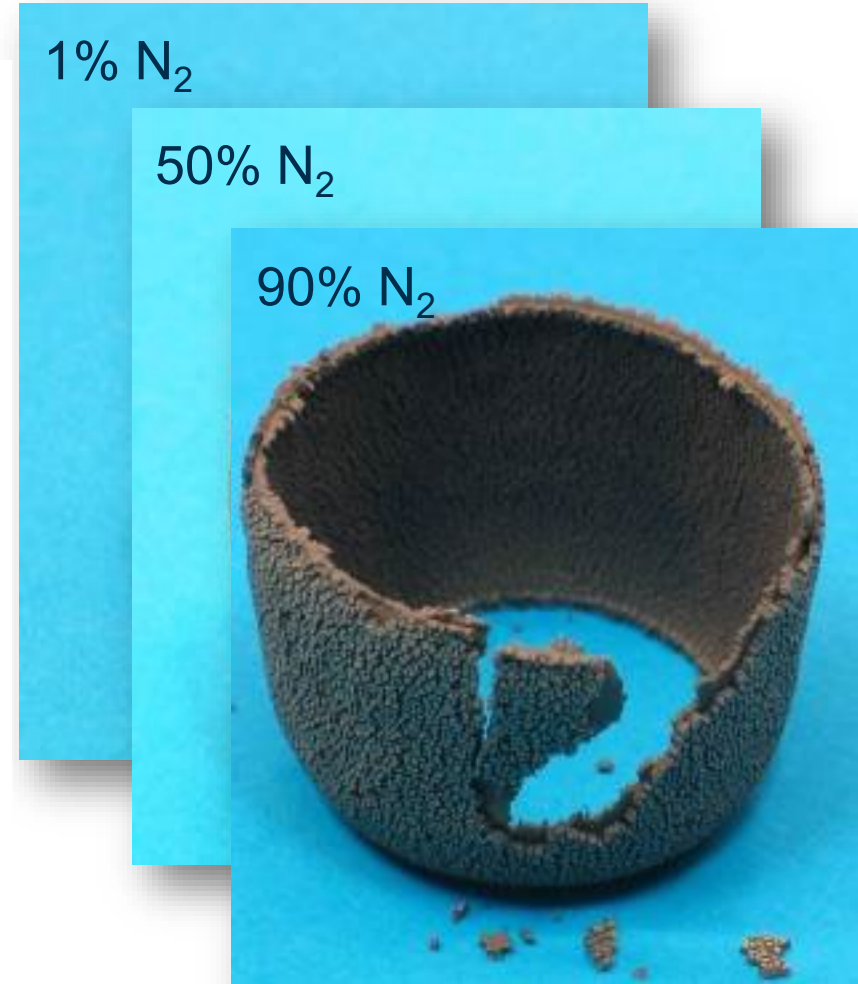
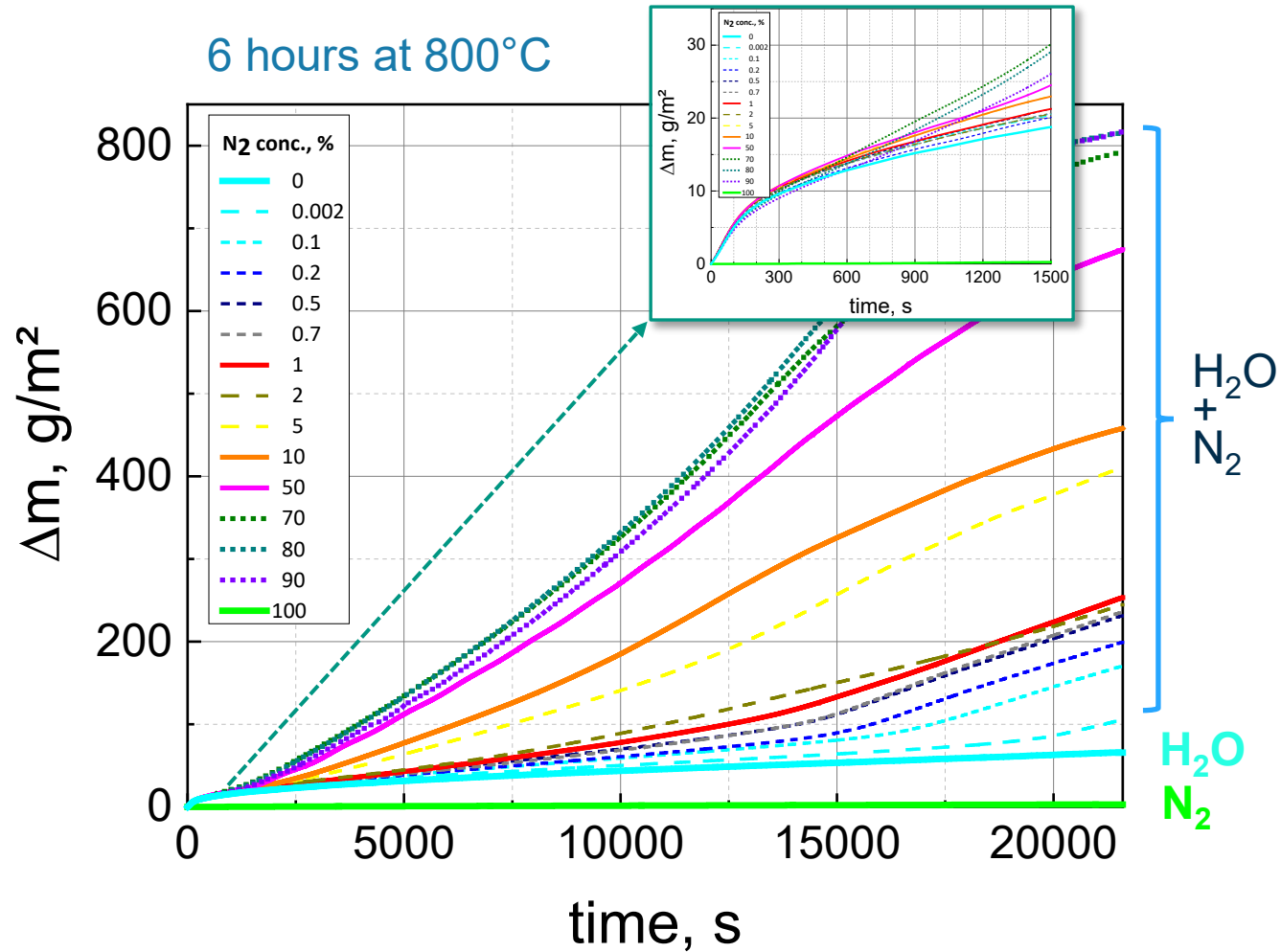
# The effect of nitrogen on the oxidation and degradation of Zr alloys



# The effect of nitrogen on the oxidation and degradation of Zr alloys

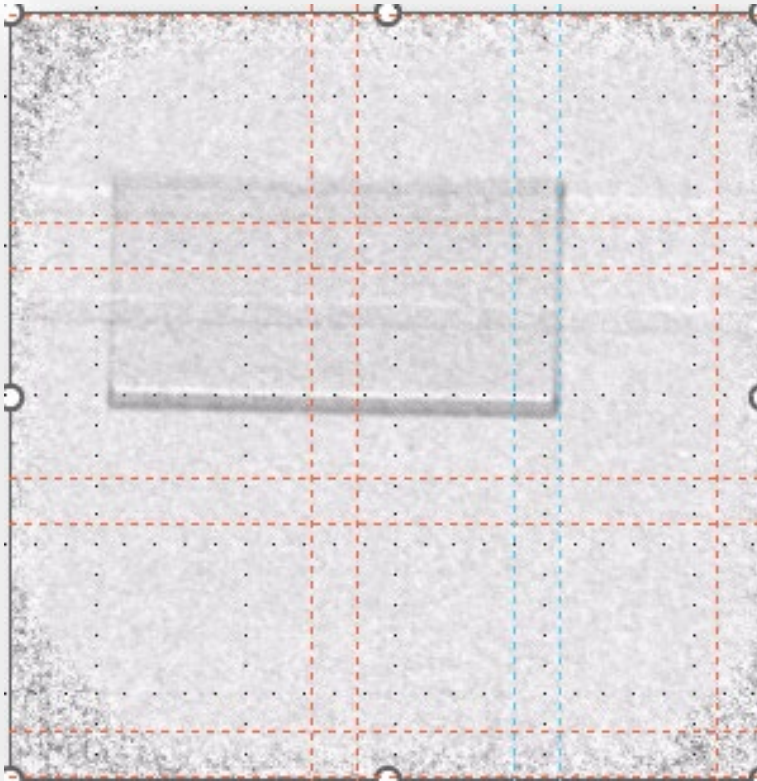


# The effect of nitrogen on the oxidation and degradation of Zr alloys

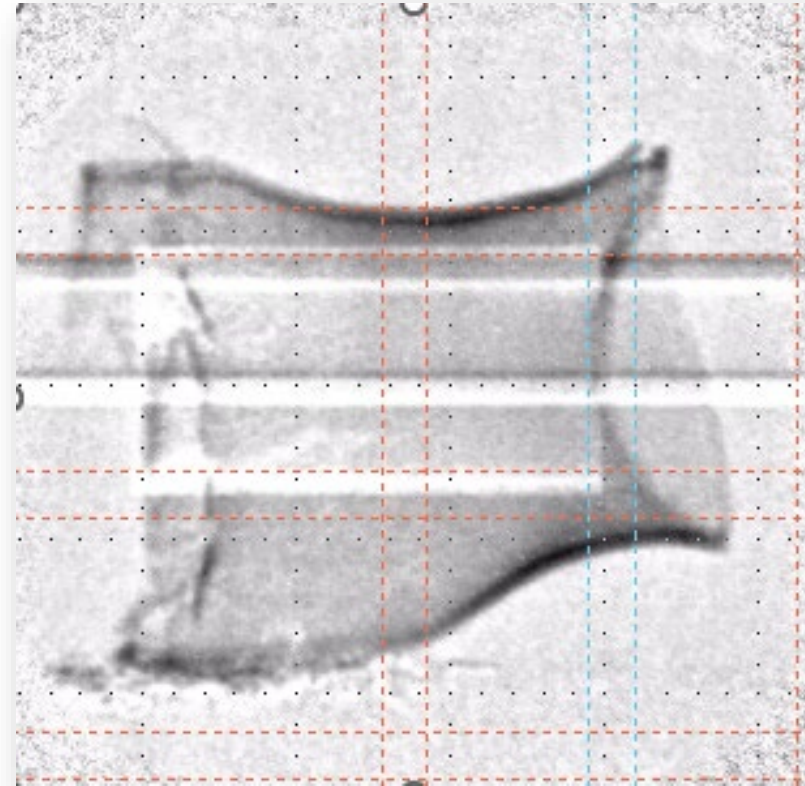


# In-situ Neutron imaging

Example: 2h oxidation of Zry-4 at 900 °C in steam and steam/N<sub>2</sub>



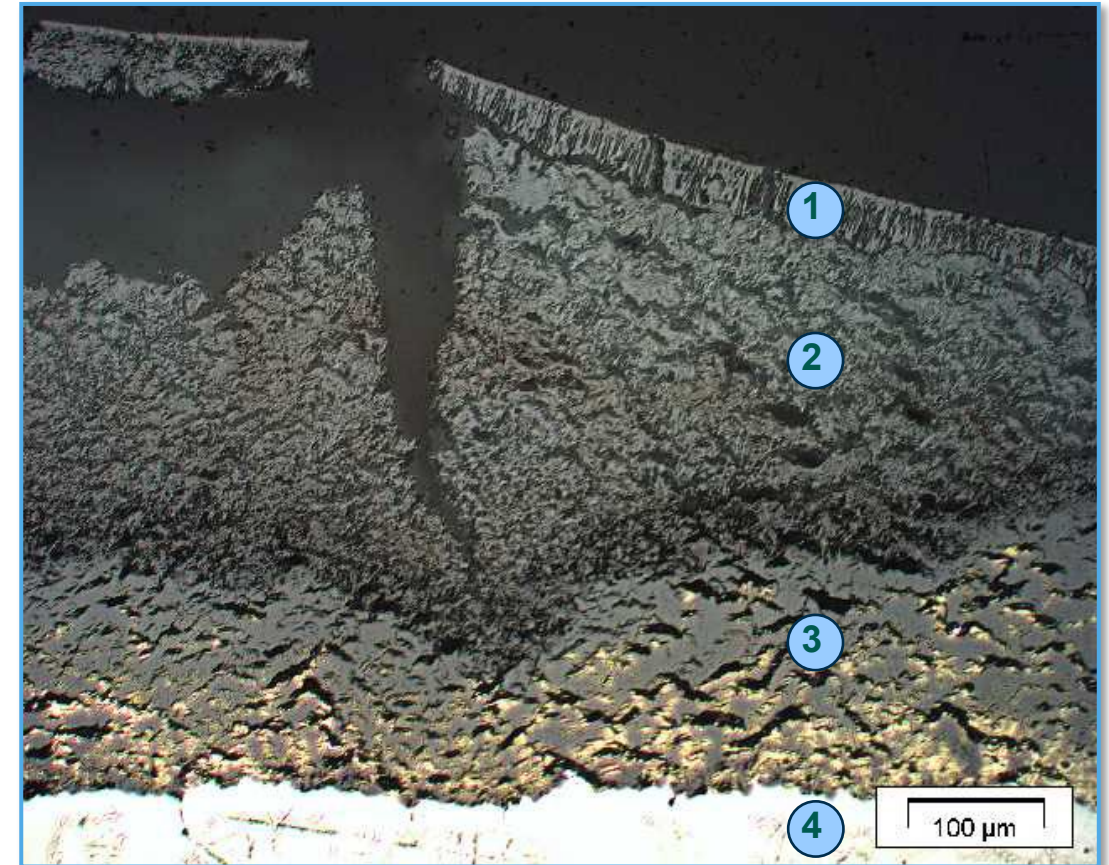
Steam



Steam + nitrogen

# Mechanism of air oxidation

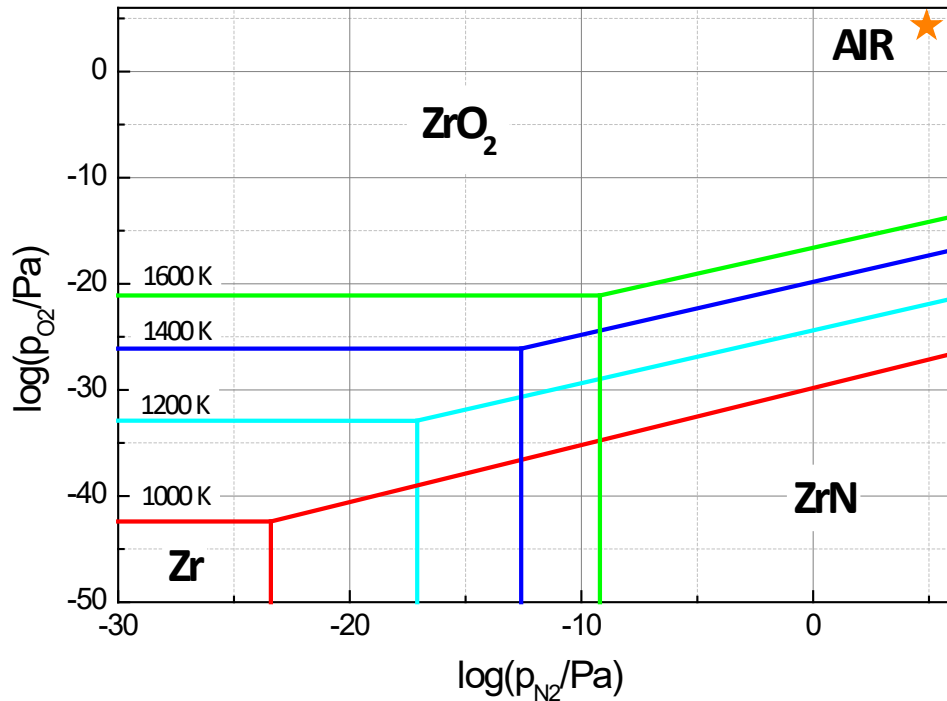
- Diffusion of the gas mixture through imperfections in the oxide scale to the metal/oxide interface
- Consumption of oxygen/steam
- Remaining nitrogen reacts with zirconium and forms ZrN
- ZrN is re-oxidized by fresh air with continuing reaction associated with a volume increase by 48%
- Formation of porous and non-protective oxide scales



- 1 – initially formed dense oxide  $ZrO_2$
- 2 – porous oxide after oxidation of ZrN
- 3 –  $ZrO_2$  / ZrN mixture
- 4 –  $\alpha$ -Zr(O)

# Mechanism of air oxidation

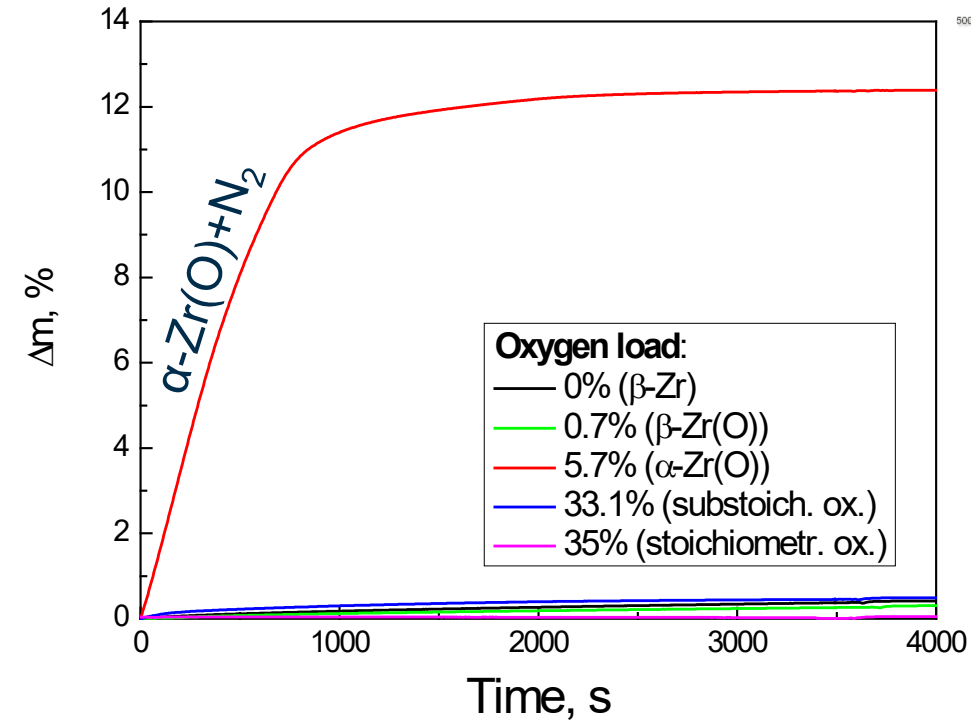
## Thermodynamic view



### Stability diagram Zr-O-N

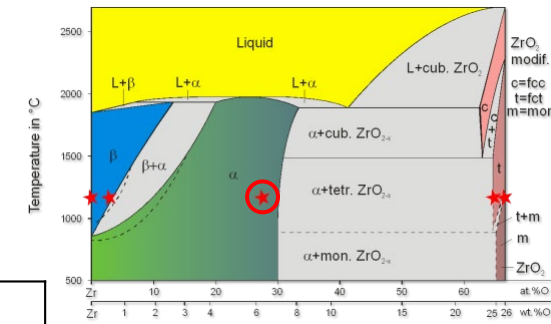
- ➔ ZrN only stable at very low oxygen partial pressure

## Kinetic view



### Reaction of $\text{ZrO}_x$ with nitrogen (1200°C)

- ➔ Fast reaction of oxygen-stabilized Zr with nitrogen



Both conditions are present locally at the metal-oxide interface

More information, see paper from Steinbrück  
<https://doi.org/10.1016/j.jnucmat.2009.04.018>  
<http://dx.doi.org/10.1016/j.jnucmat.2013.12.024>

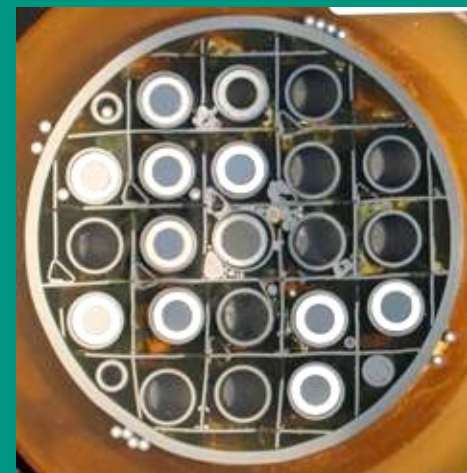
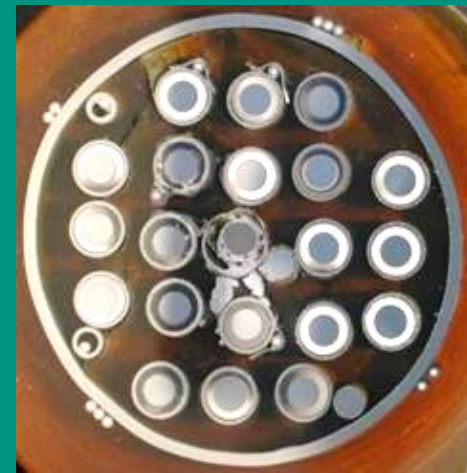


# Summary of oxidation in N<sub>2</sub> containing atmosphere

- Oxidation of zirconium alloys in atmospheres containing air or nitrogen is a very complex process, strongly dependent on experimental boundary conditions
- Nitrogen causes early loss of barrier effect against FP release and contributes to enhanced hydrogen source term
- The effect of nitrogen (“air ingress”) has been considered in the severe accident codes, using experimental data from KIT and other laboratories

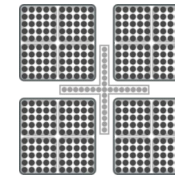
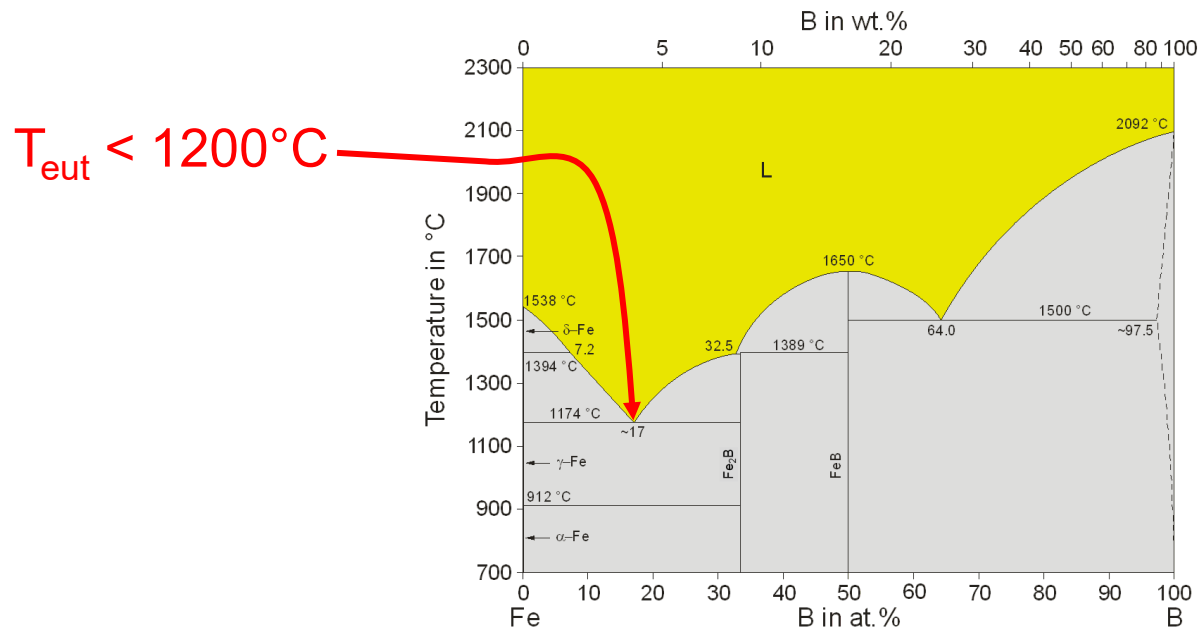
**Nitrogen is not an inert gas under the conditions of a nuclear accident!**

# The effect of $B_4C$ -Fe eutectic interaction on accident progression



# B<sub>4</sub>C control rods in LWRs

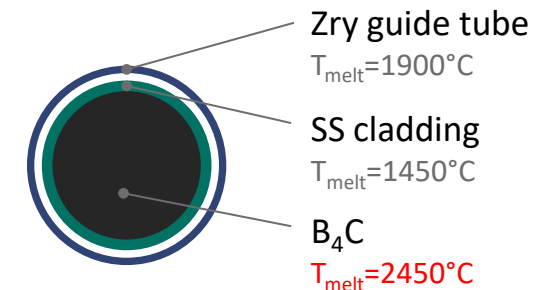
- Boron carbide is used in boiling water reactors (BWR), VVERs, some pressurized water reactors (PWR)
- Oxidation of B<sub>4</sub>C (containing melts) in steam produces large amounts of hydrogen, C+B containing gases, and heat
- Surrounded by stainless steel (cladding, blades) and Zry (guide tubes, canisters)



BWR control blade



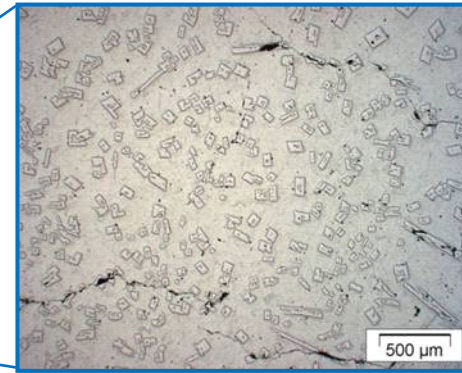
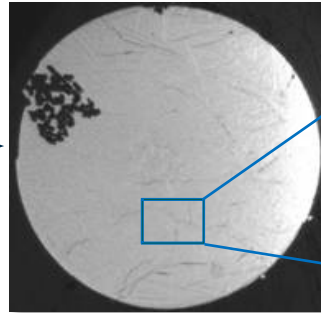
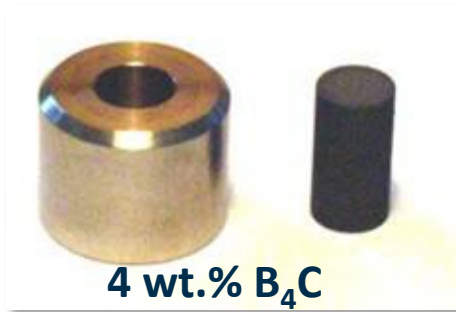
B<sub>4</sub>C pellet



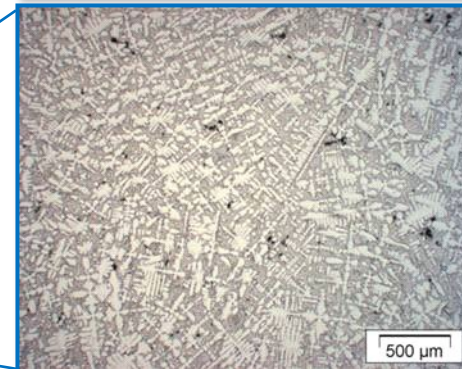
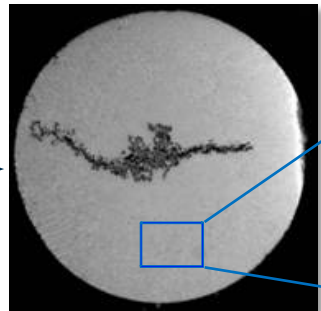
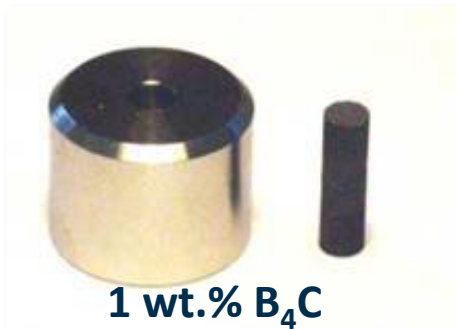
BWR control rod

# Eutectic interaction of stainless steel with B<sub>4</sub>C

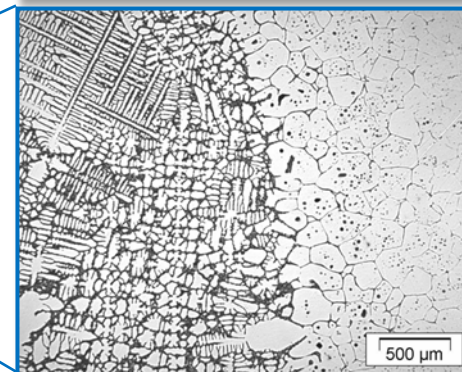
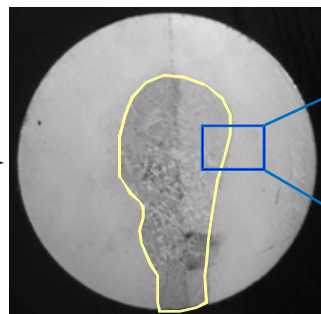
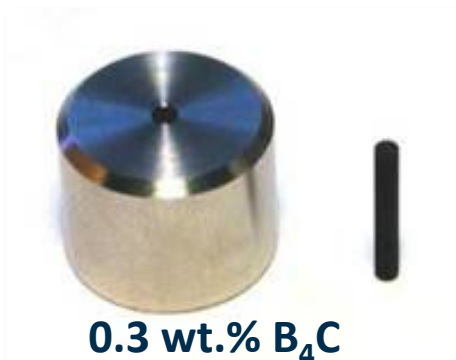
1 h at approx. 1250 °C



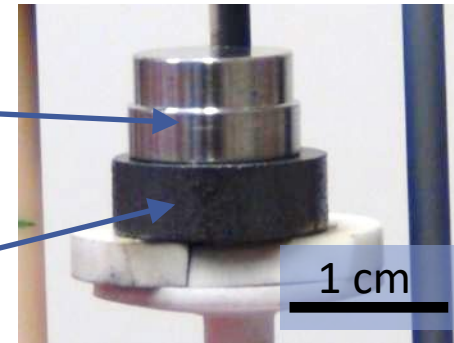
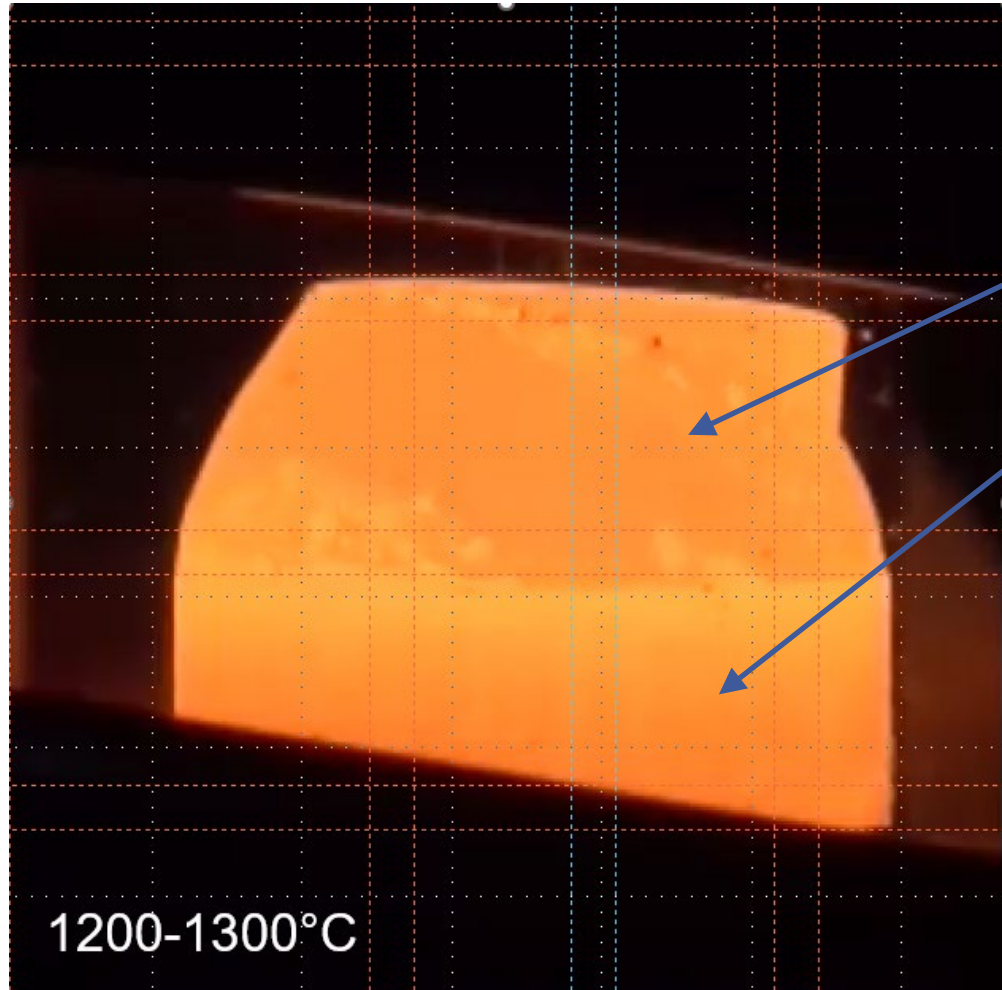
Complete  
liquefaction of  
stainless steel



1/3 of SS liquefied



# Eutectic interaction of stainless steel with $B_4C$ (kinetics)



Rapid and complete melting of SS at 1250°C starting at  $B_4C$ /SS interface

# Degradation of boron carbide control rods (pellet size)



1000 °C



1200 °C



1300 °C



1400 °C



1500 °C



1600 °C

- Apparently intact samples up to 1400 °C, but...

$T \leq 1200 \text{ °C}$ :

- Intact specimen with  $B_4C/SS/Zry-4$

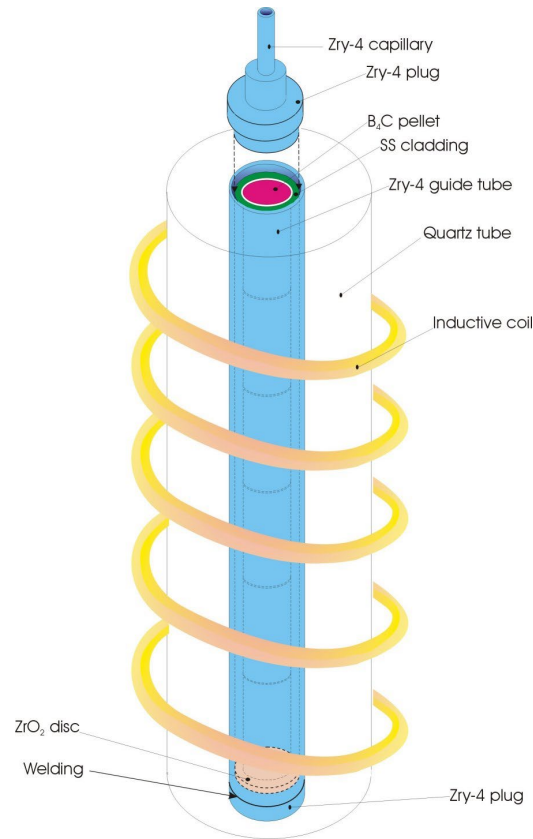
$T \leq 1400 \text{ °C}$ :

- Intact specimen due to “crucible effect” (melt kept by the external  $ZrO_2$  scale)

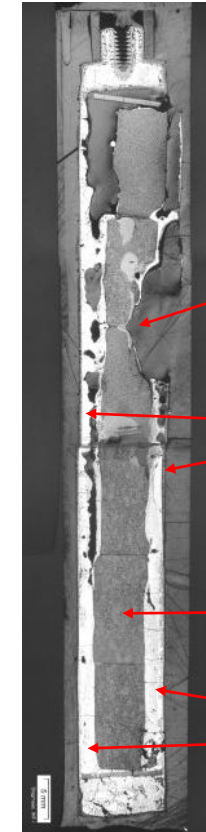
$T \geq 1500 \text{ °C}$ :

- Failure of the oxide shell and rapid oxidation of absorber melt and  $B_4C$  pellet

# Degradation of B<sub>4</sub>C control rods (single rod)



Inductive heating of the specimen in the QUENCH rig



Local oxidation of B<sub>4</sub>C

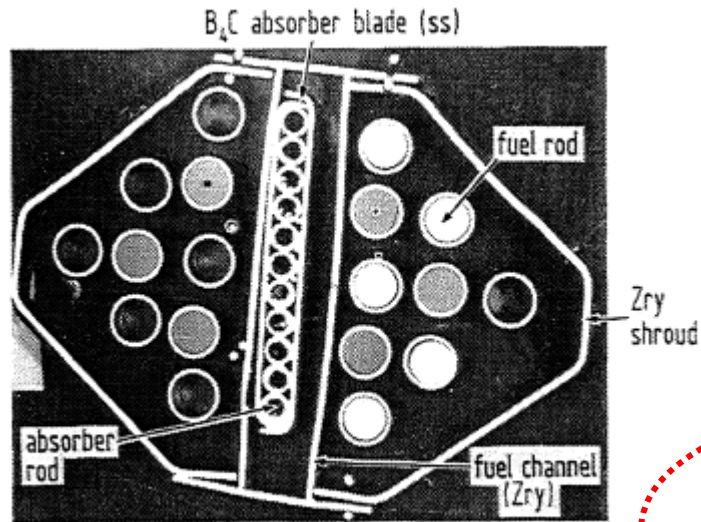
ZrO<sub>2</sub> scale enclosing the absorber melt

Partly dissolved B<sub>4</sub>C pellet

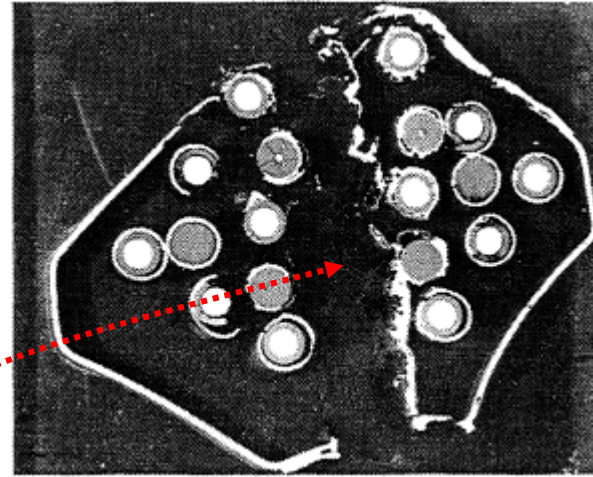
Relocated absorber melt

Post-test appearance and axial cross-section of a specimen after 30 min isothermal test at 1470 °C

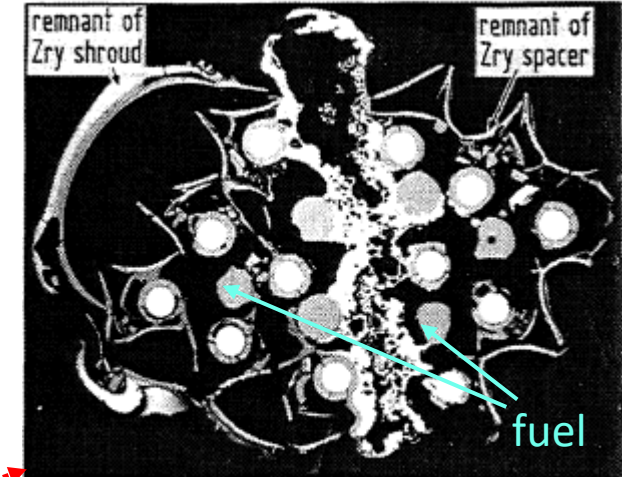
# Degradation of B<sub>4</sub>C control blade (BWR bundle test CORA-16)



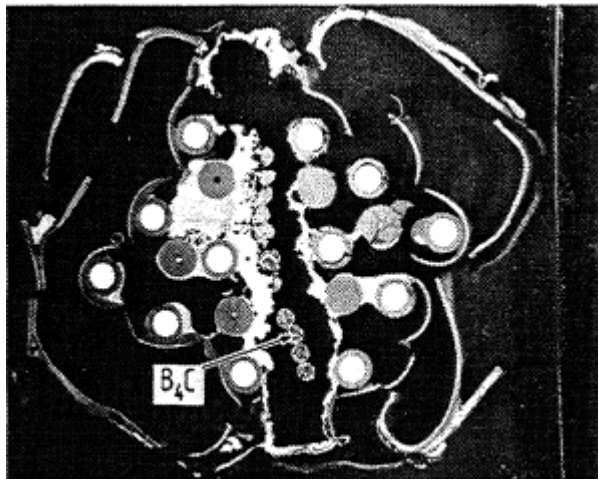
16-08 (1145mm), bottom view



16-07 (963mm), top view

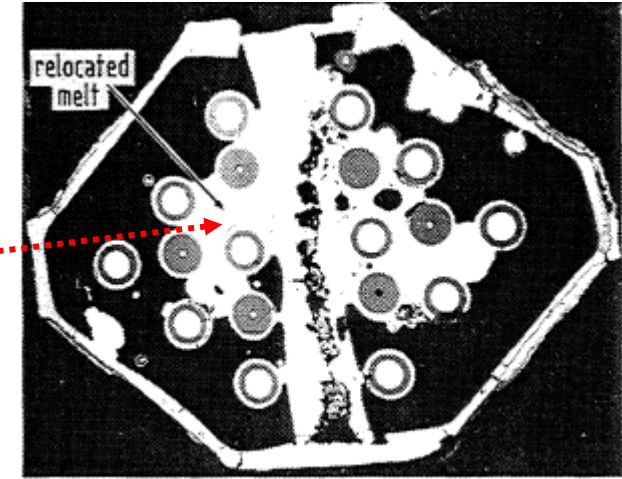


16-09 (525mm), top view  
center grid spacer elevation



16-03 (310mm), top view

- Complete loss of absorber blade
- Dissolution of cladding and fuel
- Massive melt relocation (SS, Zry, UO<sub>2</sub>)

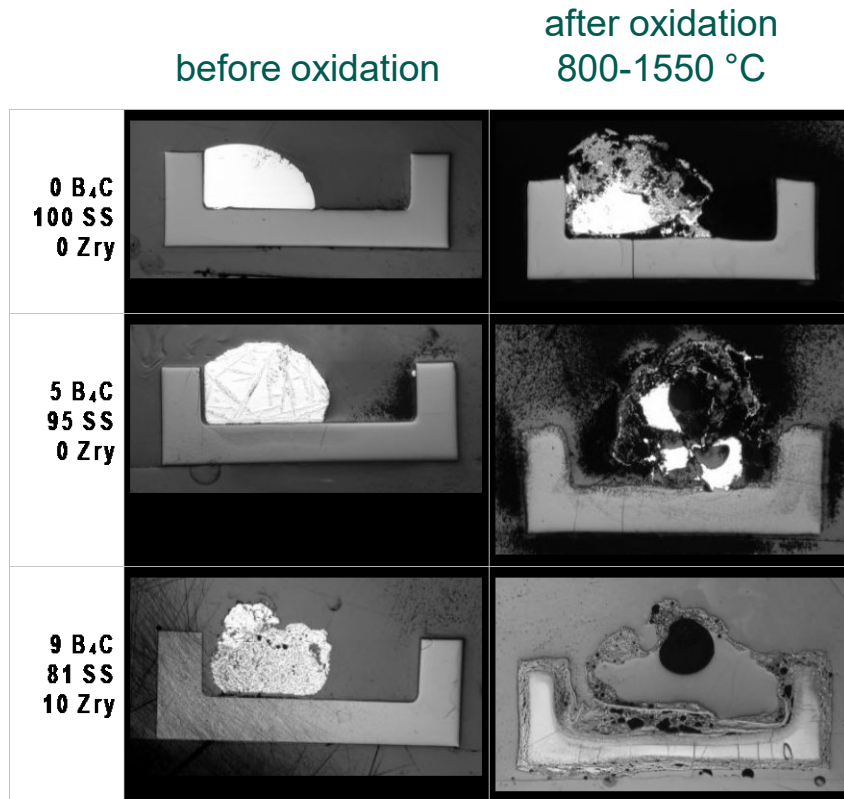


16-01 (110mm), top view

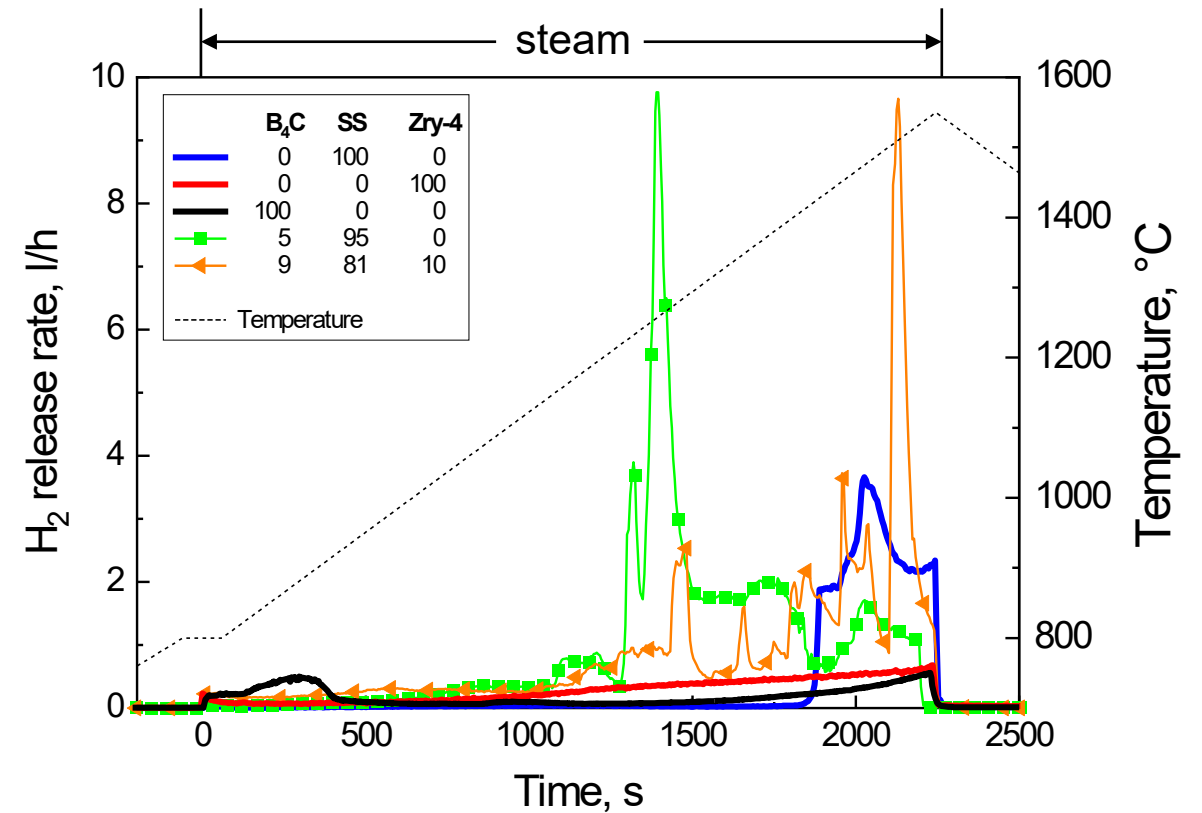
21/01/20



# Oxidation of eutectic melts



Strong interaction of oxidized melt with ZrO<sub>2</sub> crucible



High oxidation rates beyond melting temperature

# Summary of B<sub>4</sub>C effects in severe accidents

- Low-temperature eutectic melts form at temperatures several hundred Kelvin below the melting temperatures of the materials involved
- These chemically aggressive melts may attack surrounding core structures including fuel, thus influencing corium behavior and the FP source term
- Oxidation of B<sub>4</sub>C and B<sub>4</sub>C-containing melts results in the release of large amounts of hydrogen and heat
- Further reaction products (CO, CO<sub>2</sub>, boric acids) have to be taken into account for accident analyses as well
- No methane (relevant for FP chemistry) is produced during high-temperature oxidation of B<sub>4</sub>C

# Takeaways

- ❑ Not everything is as it seems at first glance
- ❑ Experiments must be designed to be as prototypical as possible
- ❑ Equilibrium thermodynamics (also locally!) and kinetics must be considered
- ❑ The key to the success of the QUENCH program lies in the interlocking of large-scale bundle experiments, separate-effects tests, modelling, and code validation and application

# Acknowledgement

- Helmholtz Association for funding program NUSAFE at KIT
- Program NUSAFE and IAM institute's management for broad support of our activities
- Funding and supporting organizations as German ministries, EURATOM program, OECD-NEA, etc.
- And last but not least the QUENCH team





**Juri Stuckert**

KIT

## **The importance of the temperature gradient for the processes occurring during high-temperature oxidation of the cladding, its mechanical deformation and oxidation of the melt**

Unlike isothermal conditions in some single effect tests, prototypical reactor conditions and the bundle tests simulating them always exhibit both axial and radial temperature gradients. Such gradients are crucial for a number of effects observed in accident conditions at high temperatures. This presentation describes three such effects: (1) Redistribution of oxygen in cladding under steam starvation conditions; (2) Growth of ceramic precipitates in a metal melt during its oxidation; (3) Dependence of cladding deformation on radial temperature gradient.

In the first case, the heat flow from the pellet to the outer surface of the cladding creates a temperature gradient across the outer cladding oxide layer. In areas of steam starvation, this leads to the formation of metal precipitates in the oxide layer already at temperature (at  $T \geq 1200$  °C), and not only during the cooling stage.

The second case involves the release of molten cladding metal (through the degrading oxide cladding layer) into the interrod space and its oxidation in the steam. Due to the pronounced exothermic oxidation reaction, the temperature at the surface of the resulting molten pool is higher than in its bulk. This drives the formation of ceramic precipitates within the melt already at temperature, leading to its complete transition to the ceramic phase.

The third case concerns the formation of asymmetric cladding ballooning during a design basis accident. Fuel pellets can maintain their geometric shape up to burnups of 30 MWd/kgU, and a gap remains between the pellet and the cladding. Several pellets are displaced from their axisymmetrical arrangement and touch the cladding at a specific point, forming a hot spot there. As a result, the cladding begins to plastically deform at  $T > 600$  °C, primarily near this hot spot. As a result, the circumferential strain of the cladding can remain below 40%, significantly lower than in single rod tests with direct current heating of the cladding.

# The importance of the temperature gradient for the processes occurring during high-temperature oxidation of the cladding, its mechanical deformation and oxidation of the melt

J. Stuckert

Institute for Applied Materials; Program NUSAFE

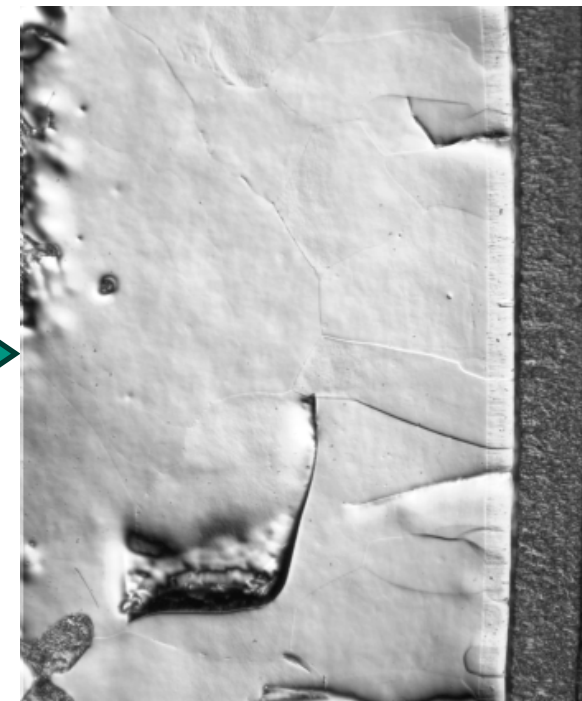
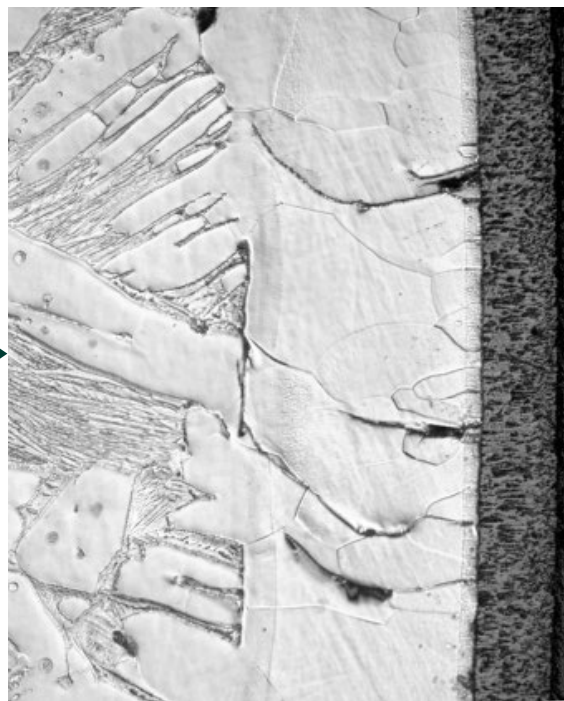


## Outline

- (1) Redistribution of oxygen in cladding under steam starvation conditions.**
- (2) Growth of ceramic precipitates in a metal melt during its oxidation.**
- (3) Dependence of cladding deformation on radial temperature gradient.**



# Evolution of outer oxide layer annealed in Ar at $T \approx 1150 \text{ }^\circ\text{C}$ without radial temperature gradient: gradual diffusion of oxygen into the metal layers with decrease of $\text{ZrO}_2$ and increase of $\alpha\text{-Zr(O)}$



**prior  $\beta\text{-Zr}$   $\alpha\text{-Zr(O)}$   $\text{ZrO}_2$**   
 after oxidation in steam:  
 $\text{ZrO}_2$  73  $\mu\text{m}$ ,  $\alpha\text{-Zr(O)}$  83  $\mu\text{m}$ ,  
 $\beta\text{-Zr}$  residual

**$\alpha\text{-Zr(O)}$   $\text{ZrO}_2$**   
 after annealing in Ar during 900 s:  
 $\text{ZrO}_2$  52  $\mu\text{m}$ ,  $\alpha\text{-Zr(O)}$  165  $\mu\text{m}$ ,  
 $\beta\text{-Zr}$  residual

**$\alpha\text{-Zr(O)}$   $\text{ZrO}_2$**   
 after annealing in Ar during 1800 s:  
 $\text{ZrO}_2$  43  $\mu\text{m}$ ,  $\alpha\text{-Zr(O)}$  329  $\mu\text{m}$ ,  
 $\beta\text{-Zr}$  residual

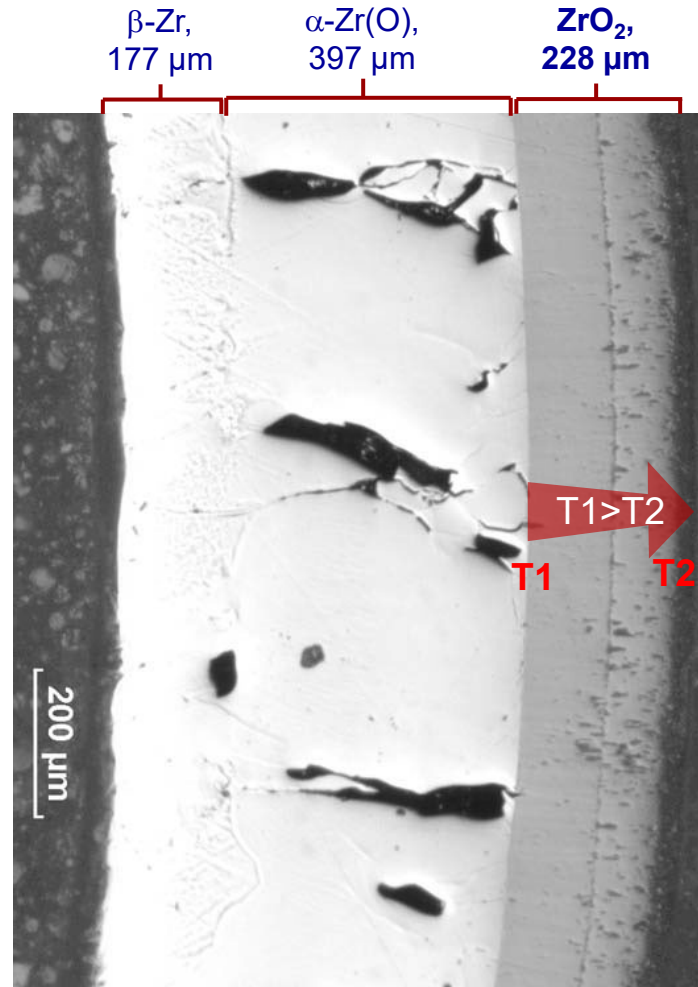
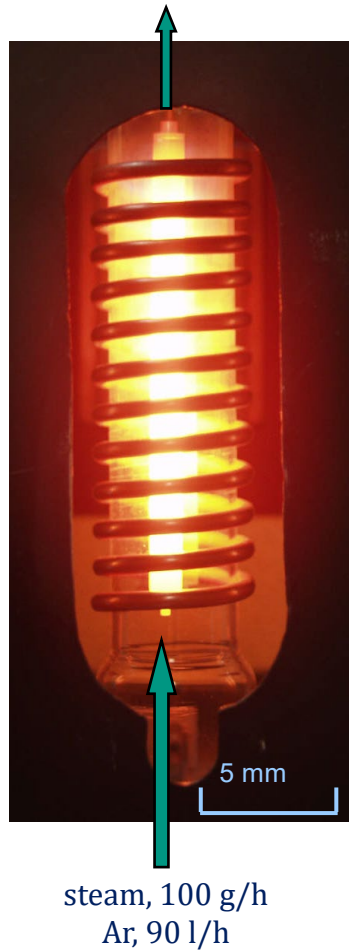
J. Stuckert et al.,  
 Kinetics of dissolution of oxide layer on cladding  
 surface under oxygen starvation conditions  
 at temperatures between  $900^\circ\text{C}$  and  $1200^\circ\text{C}$ ,  
 QUENCH-Workshop 20 (2014),  
<https://www.doi.org/10.13140/RG.2.2.25819.05925>

$$\text{decrease of } \text{ZrO}_2: \Delta d_{\text{ox}} / t^{1/2} = 287 \cdot \exp(-8473/T) = 287 \cdot \exp(-70326/RT),$$

$$\text{increase of } \alpha\text{-Zr(O)}: \Delta d_{\alpha} / t^{1/2} = 5 \cdot 10^6 \cdot \exp(-19679/T) = 5 \cdot 10^6 \cdot \exp(-163611/RT),$$

$$\text{with } R = 8.314 \text{ J/(mol}\cdot\text{K)}$$

# Radial temperature gradient across the cladding oxide layer in single rod and bundle tests ( $T > 1100^\circ\text{C}$ ) with flowing steam



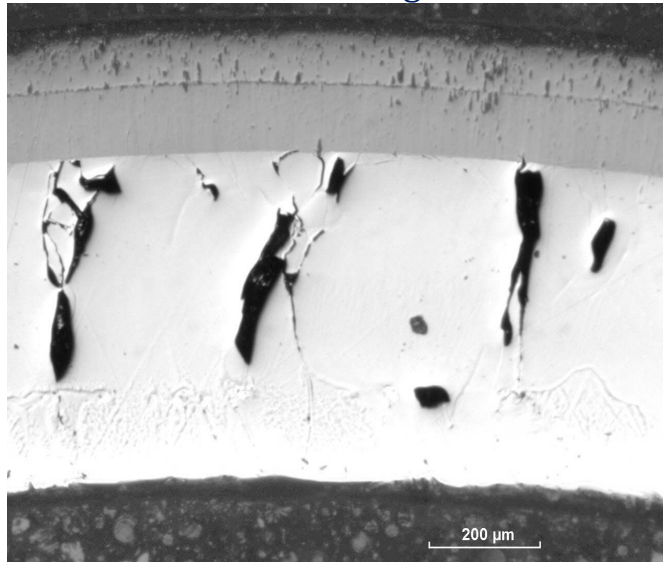
$$|\nabla T| \approx -0.2 \text{ K}/\mu\text{m}$$



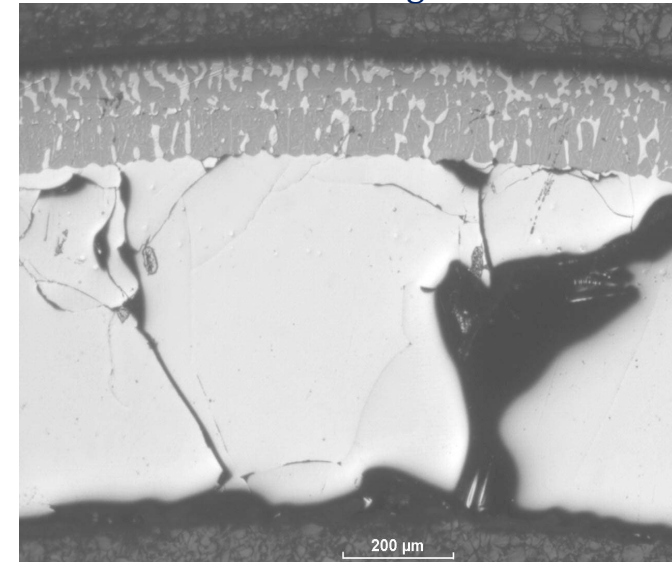
QUENCH-07 bundle:  
thick oxide layers  
after oxidation in steam

# Evolution of outer oxide layer annealed in Ar at $T \approx 1430 \text{ }^\circ\text{C}$ during 1 h with radial temperature gradient: gradual diffusion of oxygen into the metal layers

reference sample after oxidation in steam during 750 s



test sample after following annealing in Ar during 3 h



duplex layer  
 $\text{ZrO}_2$ ,  
228  $\mu\text{m}$

$\alpha$ -Zr(O),  
397  $\mu\text{m}$

$\beta$ -Zr,  
177  $\mu\text{m}$

$\text{ZrO}_2$ ,  
186  $\mu\text{m}$

$\alpha$ -Zr(O),  
646  $\mu\text{m}$

J. Stuckert and M. Veshchunov,  
Behaviour of Oxide Layer of Zirconium-Based  
Fuel Rod Cladding under Steam Starvation  
Conditions,  
FZKA-7373 (2008),  
<https://www.doi.org/10.5445/IR/270071587>

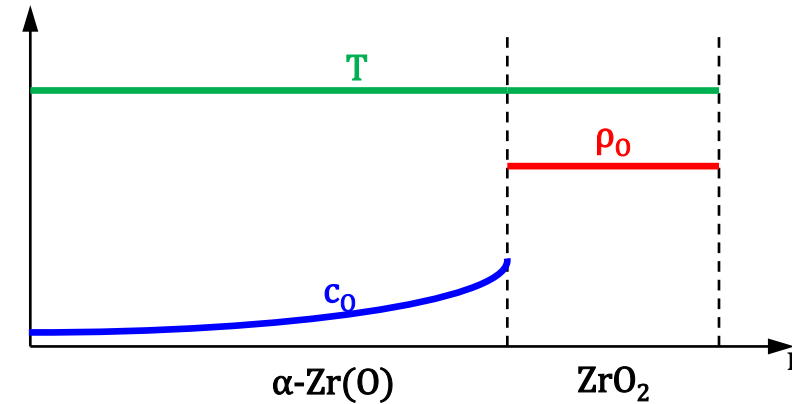
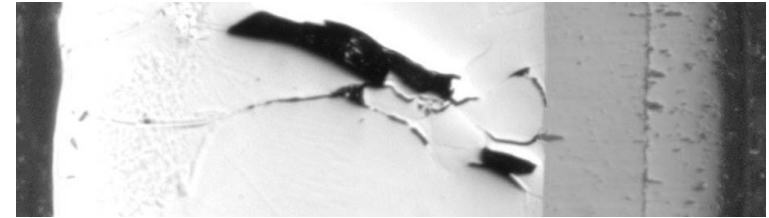
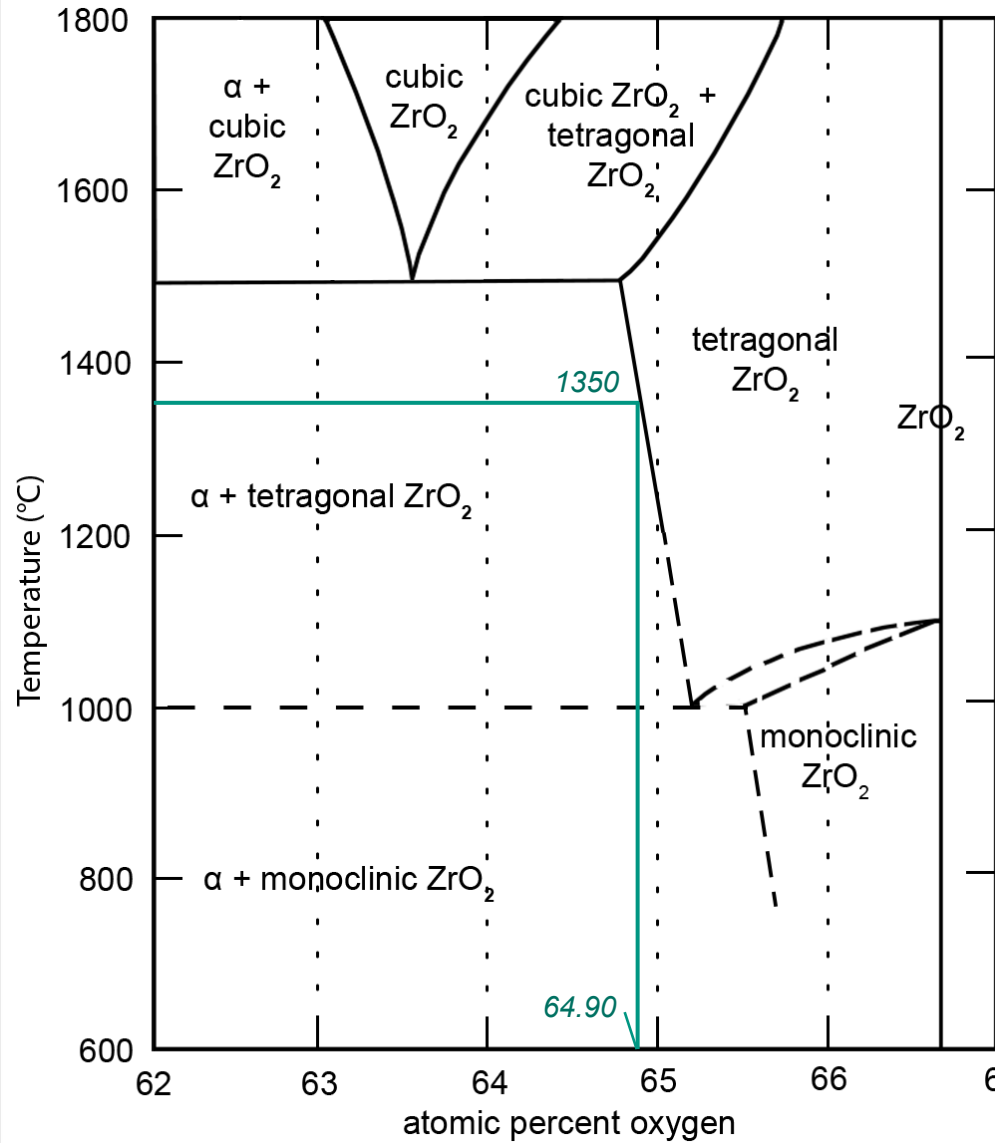
moderate decrease of the  $\text{ZrO}_2$  layer thickness;

disappearance of  $\beta$ -Zr layer;

formation of  $\alpha$ -Zr(O) precipitates inside  $\text{ZrO}_2$  at temperature  
*/it is not the eutectoid phase, which can be formed due to decomposition of the sub-stoichiometric  $\text{ZrO}_{2-x}$  during the cooldown/;*

relative large area of precipitates: 24%

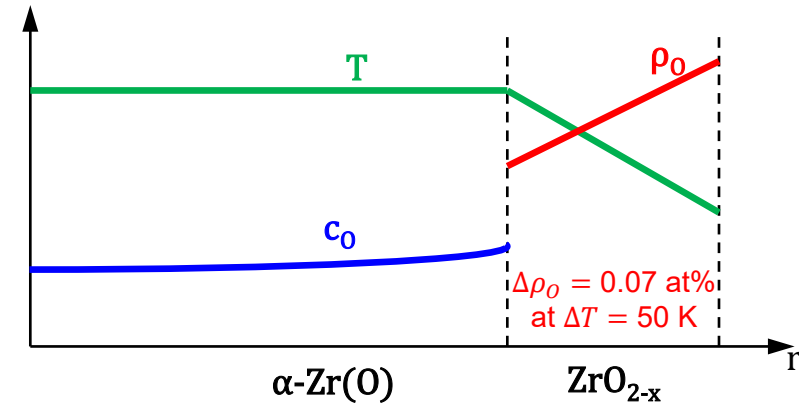
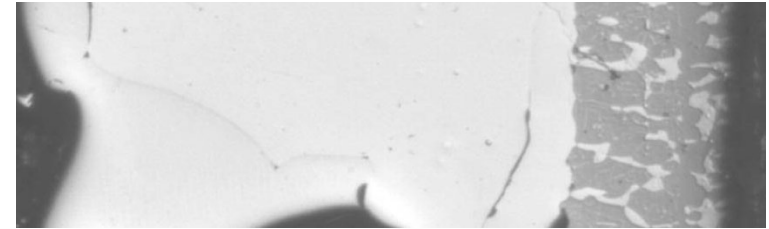
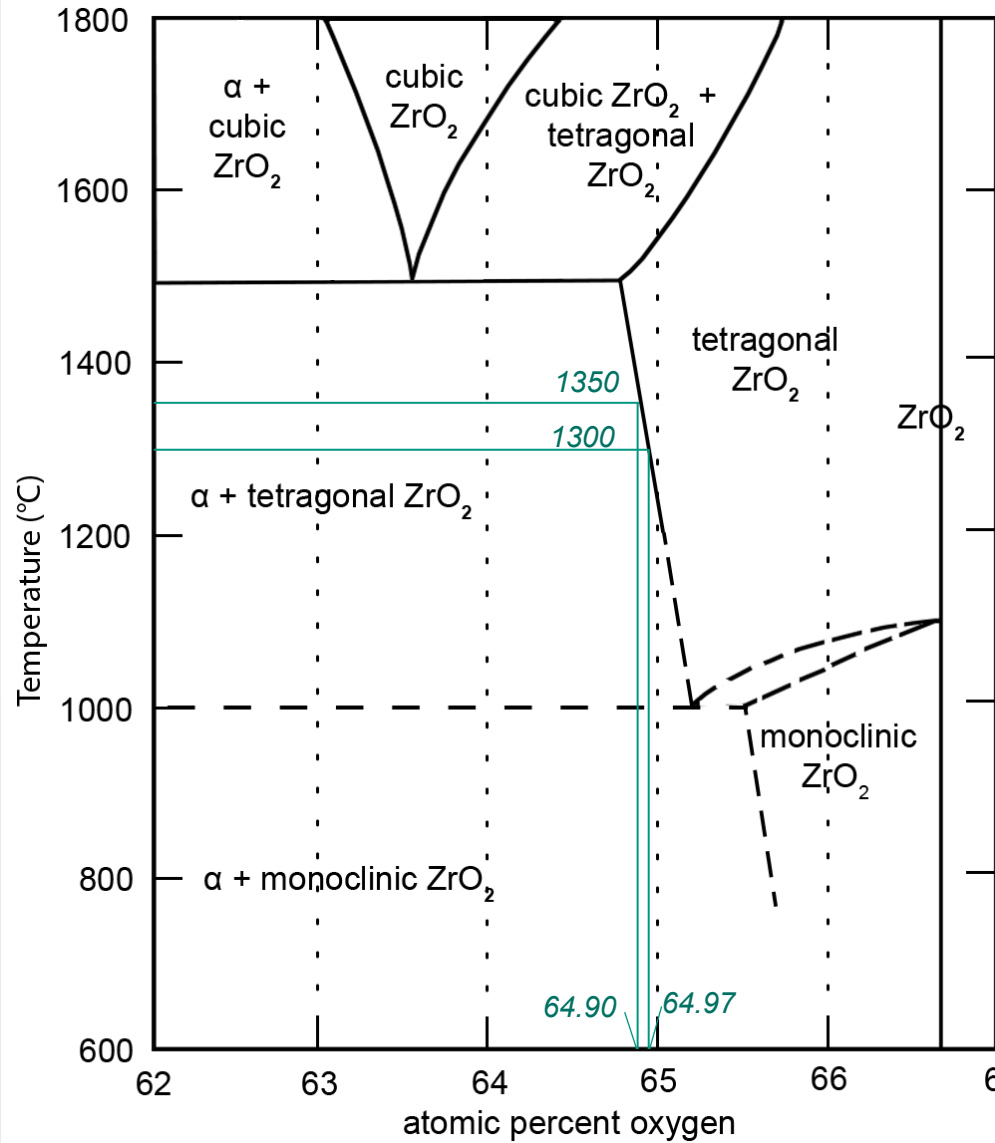
# A probable explanation for the observed phenomenon is the peculiarity of the phase diagram at the sub-stoichiometric boundary of tetragonal $ZrO_2$



Isothermal conditions

part of Zr-O phase diagram acc. to [Domagala and McPherson](#), [Ruh and Garrett](#)

# A probable explanation for the observed phenomenon is the peculiarity of the phase diagram at the sub-stoichiometric boundary of tetragonal $ZrO_2$



Temperature gradient

Gradient of oxygen concentration

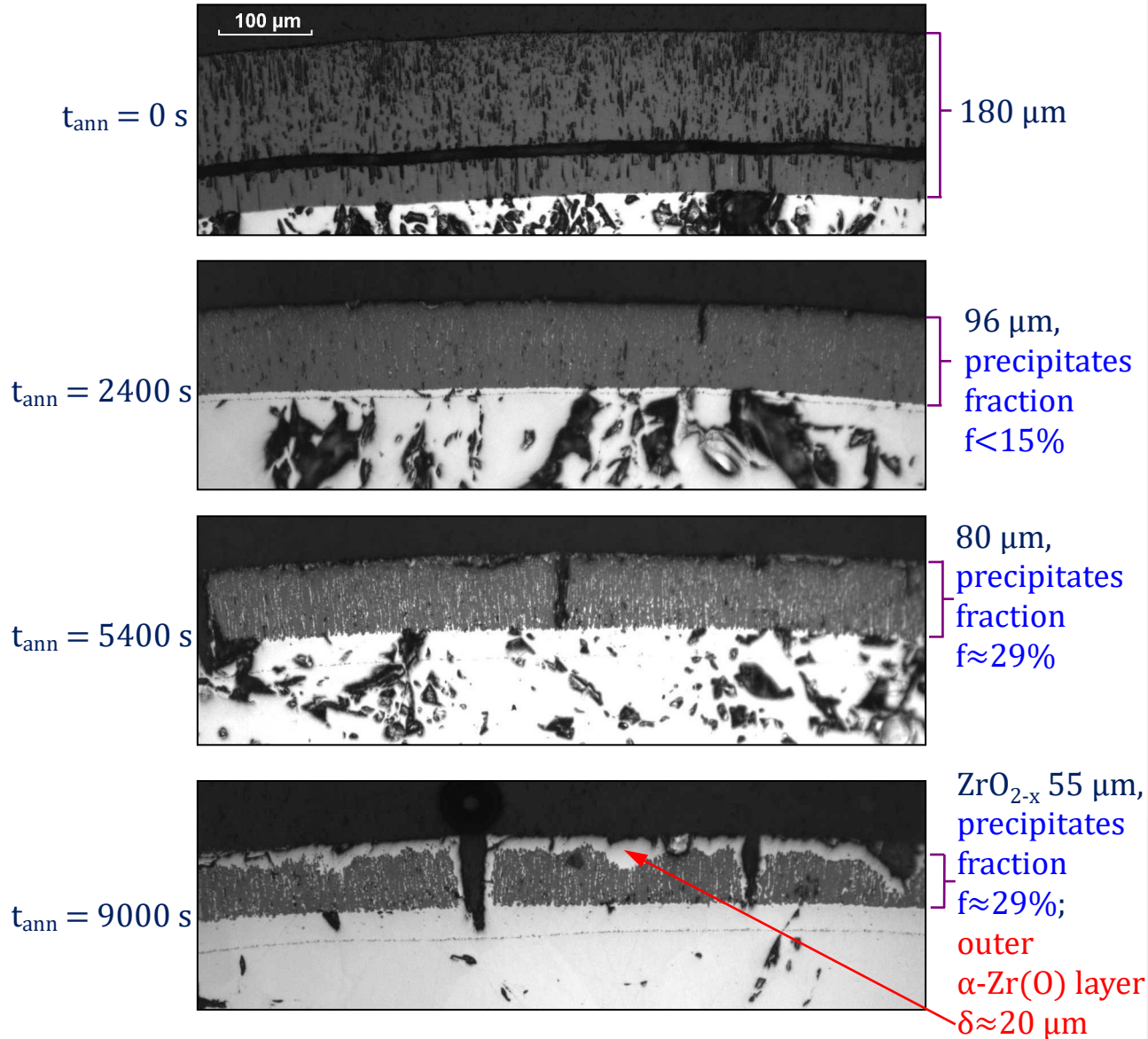
Diffusion of oxygen across the oxide

part of Zr-O phase diagram acc. to [Domagala and McPherson](#), [Ruh and Garrett](#)

# Experiments at 1300 °C: formation of the outer $\alpha$ -Zr(O) layer after formation of $\alpha$ -Zr(O) precipitates

change of oxide layer after 720 s oxidation during annealing:

- monotonous decrease of the layer thickness
- formation of bulk  $\alpha$ -Zr(O) precipitates
- formation of  $\alpha$ -Zr(O) layer on outer surface of oxide



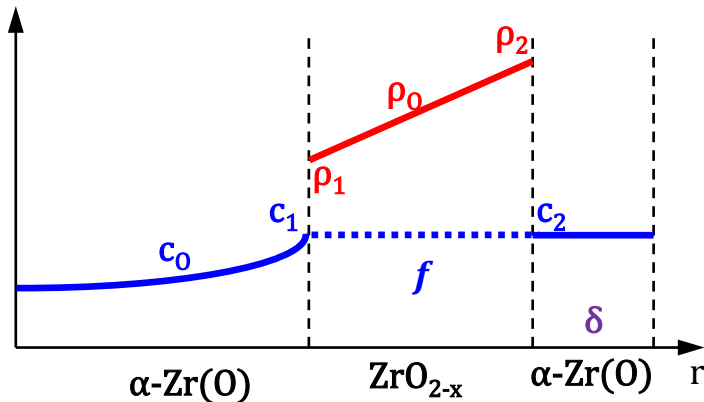
According to the Veshchunov's approach:

*fraction of  $\alpha$ -Zr(O) precipitates in  $ZrO_2$ :*

$$f \approx \frac{D_0^{ox}}{L_{final}} \cdot \frac{\Delta\rho_o(t)}{L(t)} \cdot \frac{\rho_{Zr}}{c_{Zr}\rho_2 - c_2\rho_{Zr}} \cdot t$$

*thickness of outer  $\alpha$ -Zr(O) layer formed after cessation of  $f$  increase (due to relaxation of compressive stresses):*

$$\delta_\alpha^{out} \approx D_0^{ox} \cdot \frac{\Delta\rho_o(t)}{L(t)} \cdot \frac{\rho_{Zr}}{c_{Zr}\rho_2 - c_2\rho_{Zr}} \cdot t$$



Oxygen concentration profiles in layers of the oxidized cladding after equilibration of  $ZrO_{2-x}$  phase under a temperature gradient

where  $\rho_{Zr}=35, c_{Zr} = 70, \rho_2=65, c_2=30$ ;

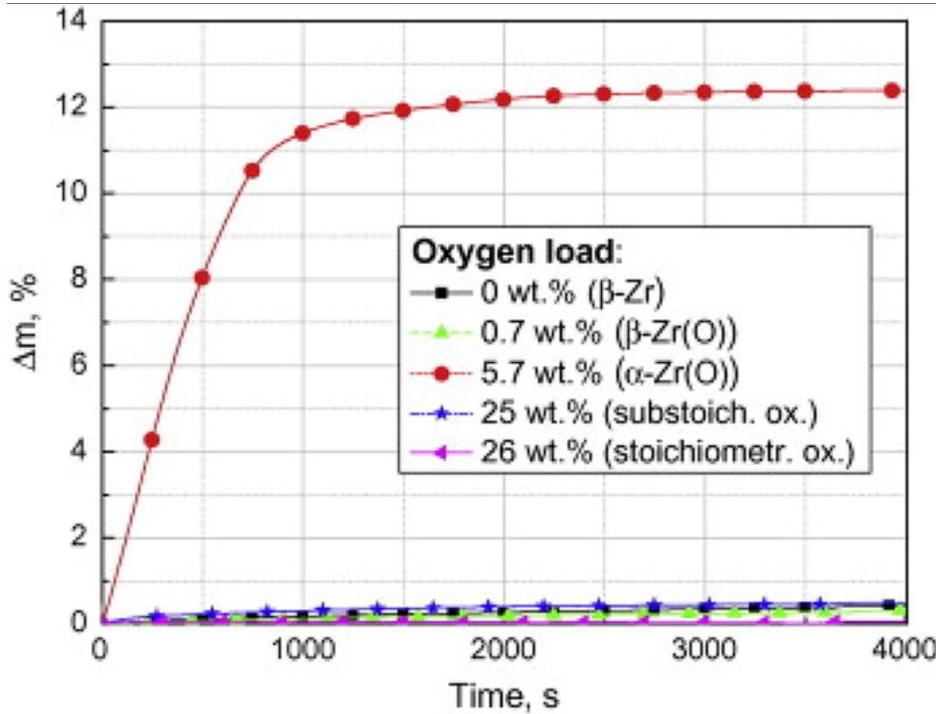
for tetr.  $ZrO_2$ :  $D_0^{ox}[\frac{cm^2}{s}] = 8.67 \cdot \exp(-\frac{20380}{T})$ ,

$D_0^{ox} = 2.05 \cdot 10^3 \mu m^2/s$  @ 1300 °C;

$$\frac{\Delta\rho_o(t)}{L(t)} = const = \frac{0.07}{250} = 2.8 \cdot 10^{-3} \frac{\%}{\mu m} \quad (\text{due to } |\nabla T| \approx 0.2 \frac{K}{\mu m})$$

- The corresponding calculations give values of  $f=31\%$  (after  $t=5400$  s, i.e.  $L_{final}=80 \mu m$ ) and  $\delta=21 \mu m$  (after following  $t=3600$  s), which agrees with the experiment performed at  $T_{pct}=1300$  °C (previous slide)

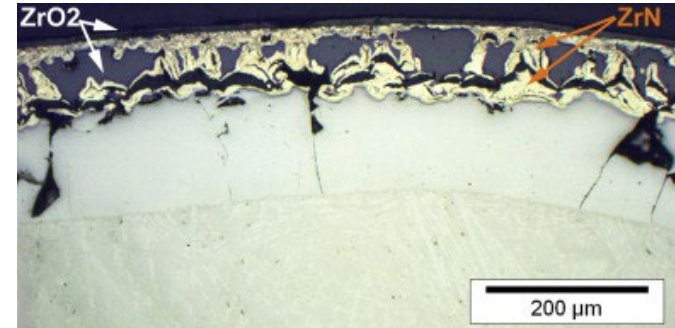
# Influence on air ingress after steam starvation



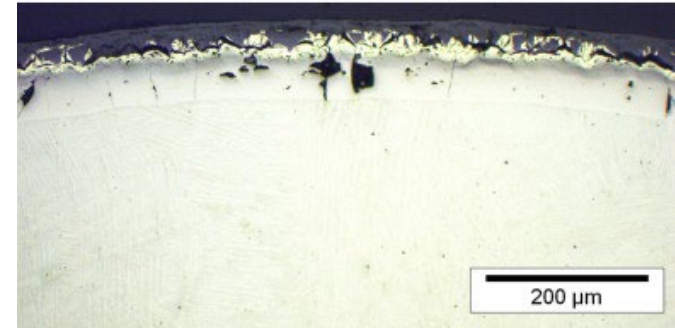
N<sub>2</sub> interaction only with α-Zr(O)

Martin Steinbrück,  
High-temperature reaction of oxygen-stabilized  
α-Zr(O) with nitrogen, JNM 447 (2014), 46-55,  
<https://doi.org/10.1016/j.jnucmat.2013.12.024>

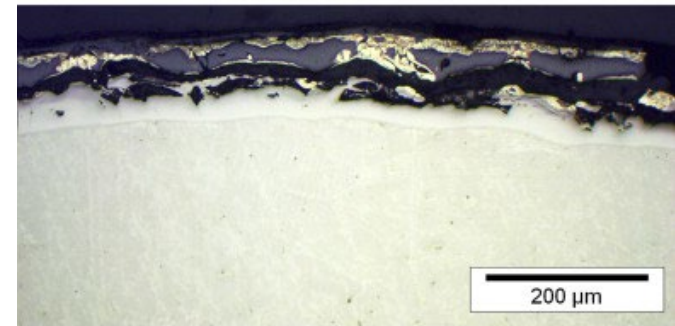
J. Stuckert, M. Steinbrück,  
Experimental results of the QUENCH-16 bundle  
test on air ingress, PNE 71 (2014), 134-141,  
<https://doi.org/10.1016/j.pnucene.2013.12.001>



elevation: 850 mm



elevation: 550 mm



elevation: 350 mm

N<sub>2</sub> interaction with α-Zr(O) formed during the  
steam starvation stage of the QUENCH-16 test



# Sequence of phenomena in the $\text{ZrO}_2$ layer due to oxygen diffusion into the inner metallic layers during steam starvation

➤ For  $T \gtrsim 1400 \text{ }^\circ\text{C}$

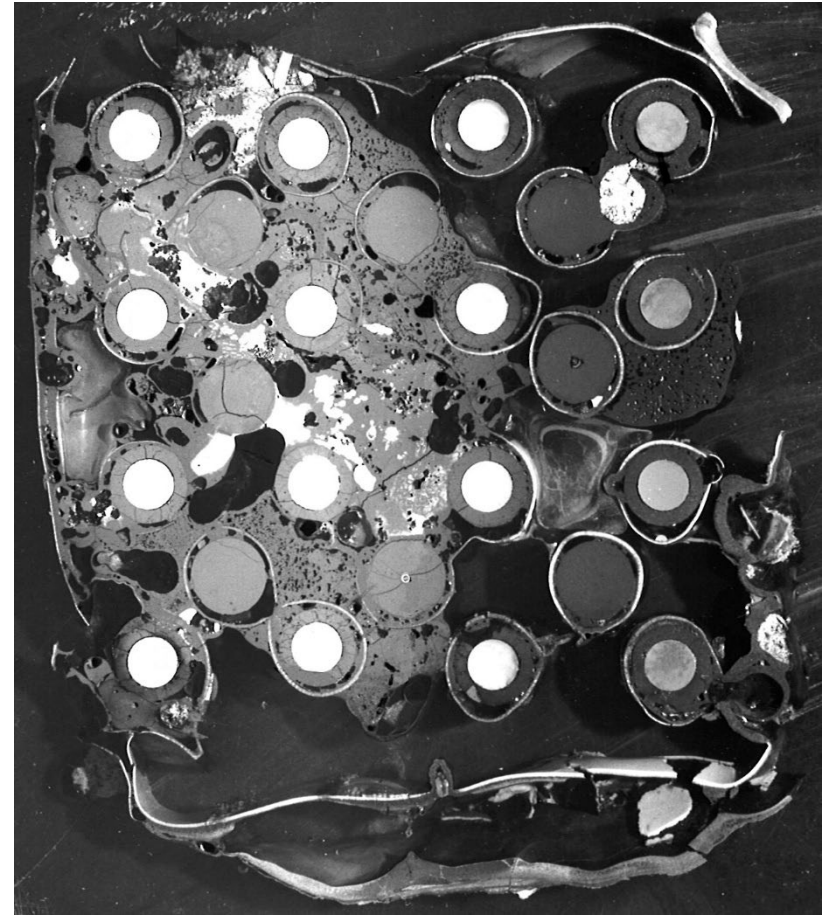
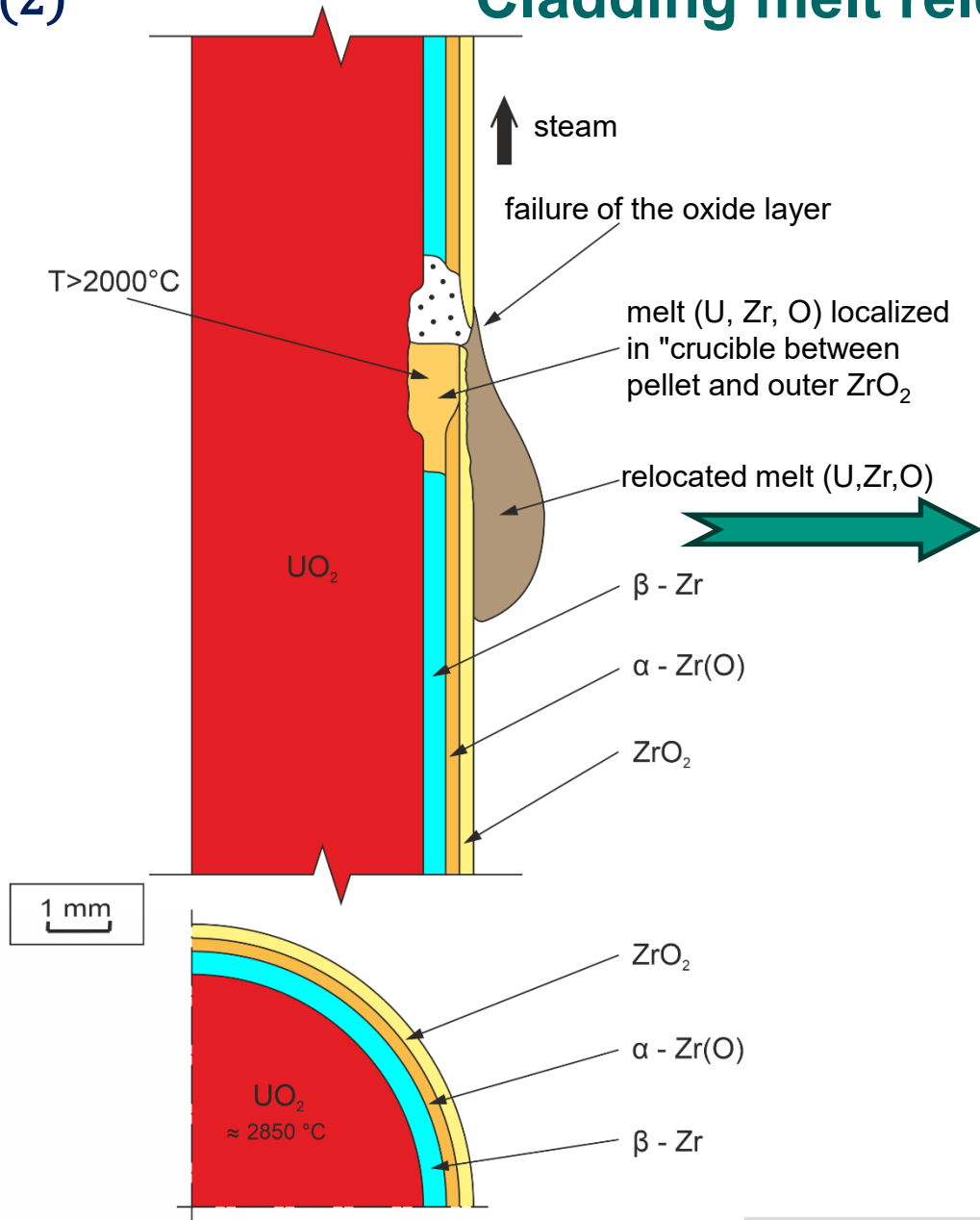
- Equilibration of  $\text{ZrO}_{2-x}$  phase (transition from stoichiometric  $\text{ZrO}_2$  to substoichiometric  $\text{ZrO}_{2-x}$ ).
- Movement of the boundary between  $\text{ZrO}_{2-x}$  and  $\alpha\text{-Zr(O)}$  layers, growth of  $\alpha\text{-Zr(O)}$  precipitates inside the  $\text{ZrO}_{2-x}$  layer until the internal  $\alpha\text{-Zr(O)}$  layer is saturated with oxygen.

➤ For  $T \lesssim 1400 \text{ }^\circ\text{C}$

- Equilibration of  $\text{ZrO}_{2-x}$  phase.
- Thickness decrease of the  $\text{ZrO}_{2-x}$  layer, growth of  $\alpha\text{-Zr(O)}$  precipitates inside the  $\text{ZrO}_{2-x}$  layer.
- Cessation of  $\alpha\text{-Zr(O)}$  precipitates growth due to relaxation of compressive stresses inside the oxide layer.
- Growth of the outer  $\alpha\text{-Zr(O)}$  layer until the internal  $\alpha\text{-Zr(O)}$  layer is saturated with oxygen.

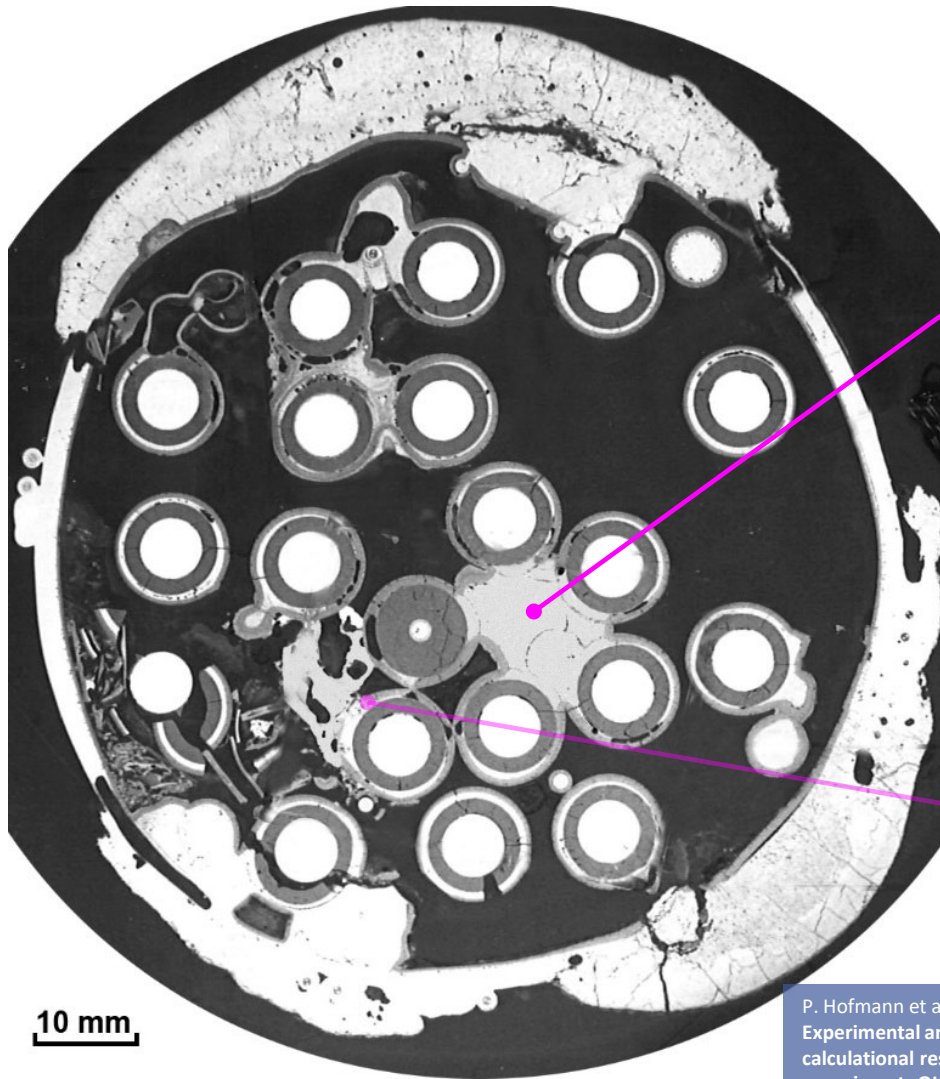
(2)

# Cladding melt release and relocation



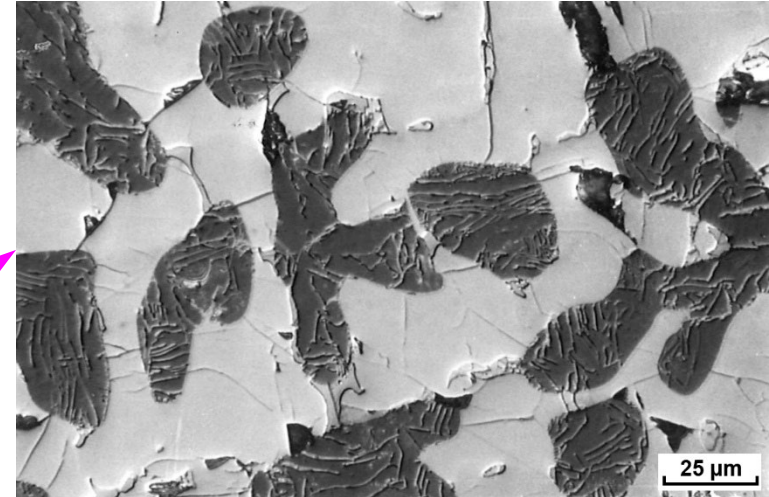
**partial blockage of the CORA-05 bundle at the bundle elevation 408 mm with the melt relocated from upper elevations**

# Structure of frozen melt in molten pools and inside pellet/cladding gap in the QUENCH-02 bundle



QUENCH-02 bundle, elevation 850 mm

P. Hofmann et al.,  
Experimental and  
calculational results of the  
experiments QUENCH-02  
and QUENCH-03, FZKA-  
6295 (2000)



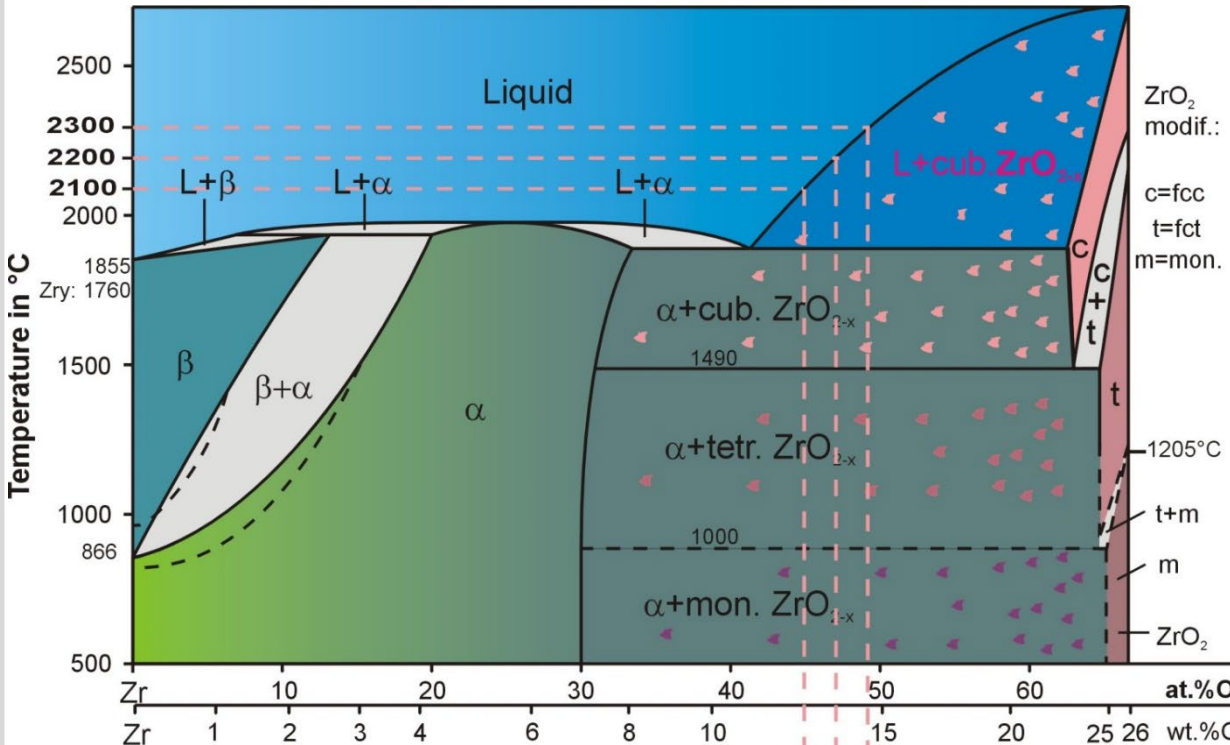
ceramic precipitates in molten pool:  
43% area acc. to image analysis



ceramic precipitates in the cladding-pellet gap:  
35% area acc. to image analysis

# Determination of oxygen content in oxidized Zr melt

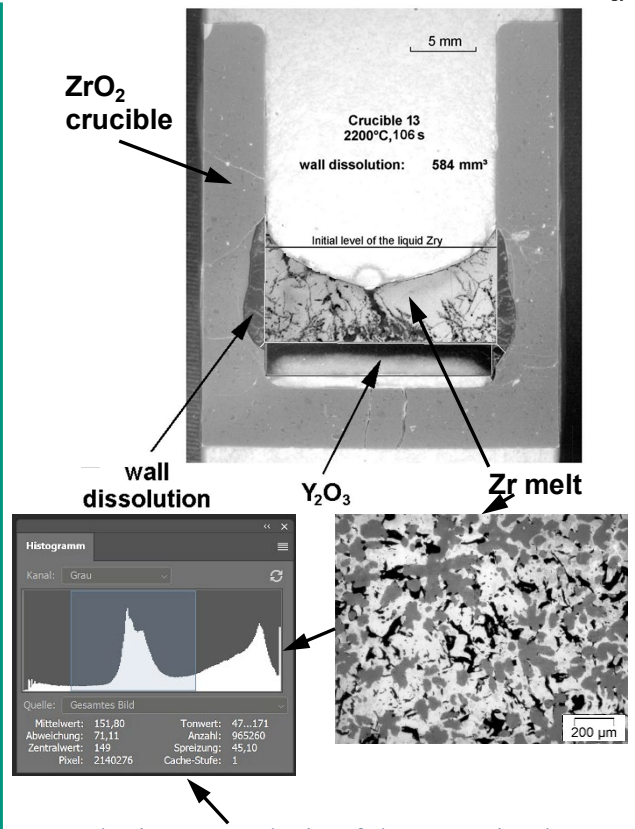
## Simplified equilibrium Zr-O phase diagram



**Solubility of oxygen in Zr liquid at 2100, 2200, 2300 °C:**

45.3	47	49.5	at.% O
12.7	13.5	14.7	wt.% O

P. Hofmann, J. Stuckert, A. Miassoedov, M. Veshchunov, A. Berdyshev, A. Boldyrev, ZrO<sub>2</sub> dissolution by molten zircaloy and cladding oxide shell failure. New experimental results and modelling, FZKA-6383 (1999), <https://doi.org/10.5445/IR/270046616>

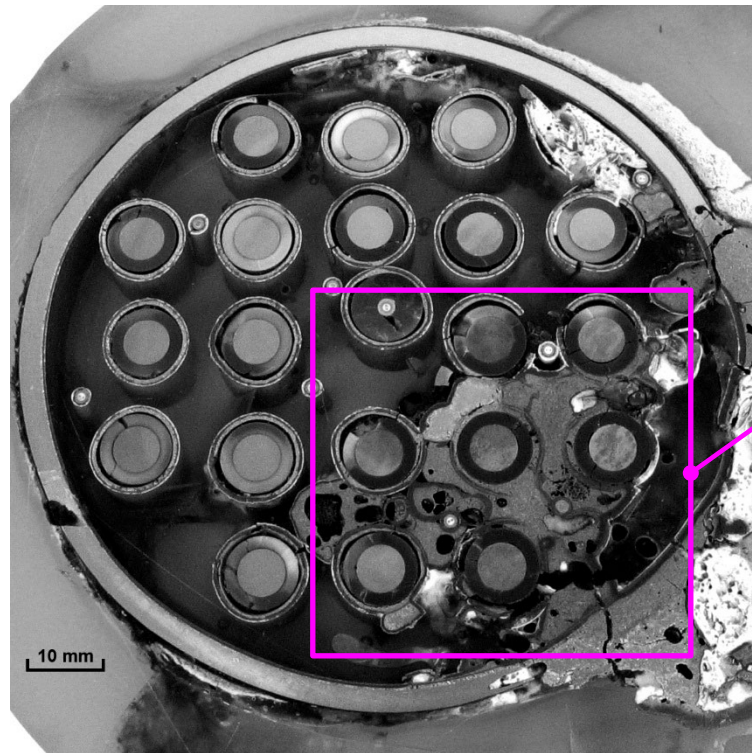


From the image analysis of the ceramic phase content in crucible tests with known relationship between dissolved ZrO<sub>2</sub> and the resulting amount of ceramic precipitated in the solidified melt, the following formula was derived:

$$O = 0.186 \cdot (A + 34)$$

where O is in weight %, A – in area %.

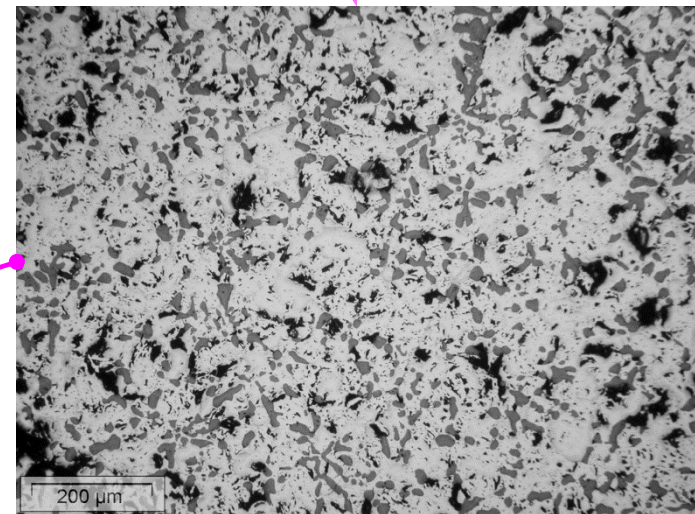
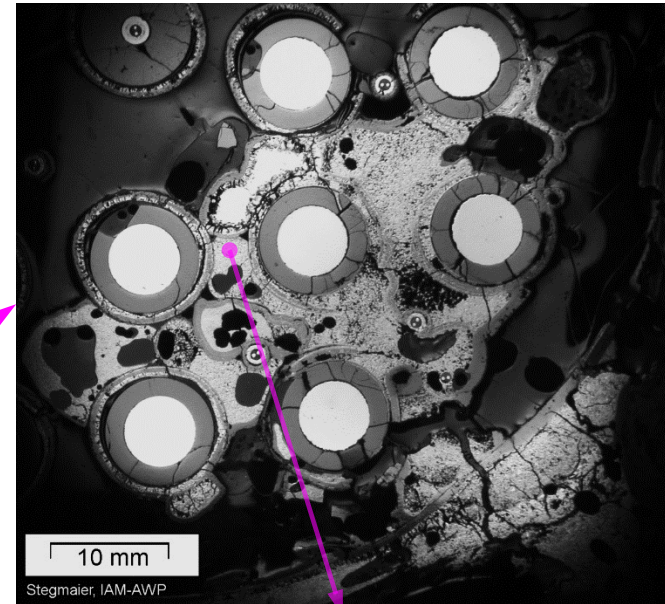
# Structure of frozen melt formed as molten pool in the QUENCH-16 bundle



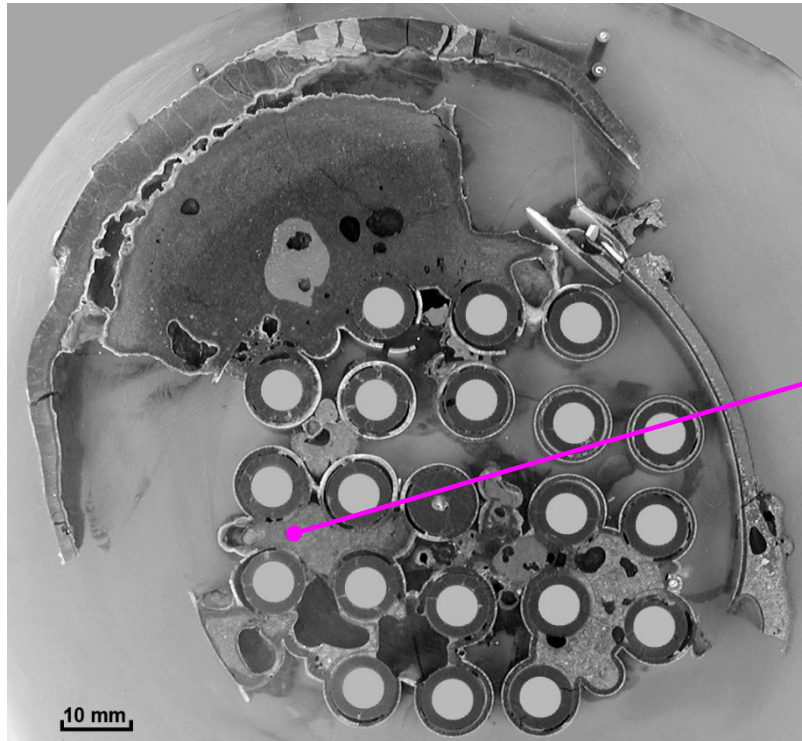
QUENCH-16, elevation 450 mm

J. Stuckert, M. Steinbrück,  
Experimental results of the QUENCH-16  
bundle test on air ingress, PNE 71 (2014),  
134-141

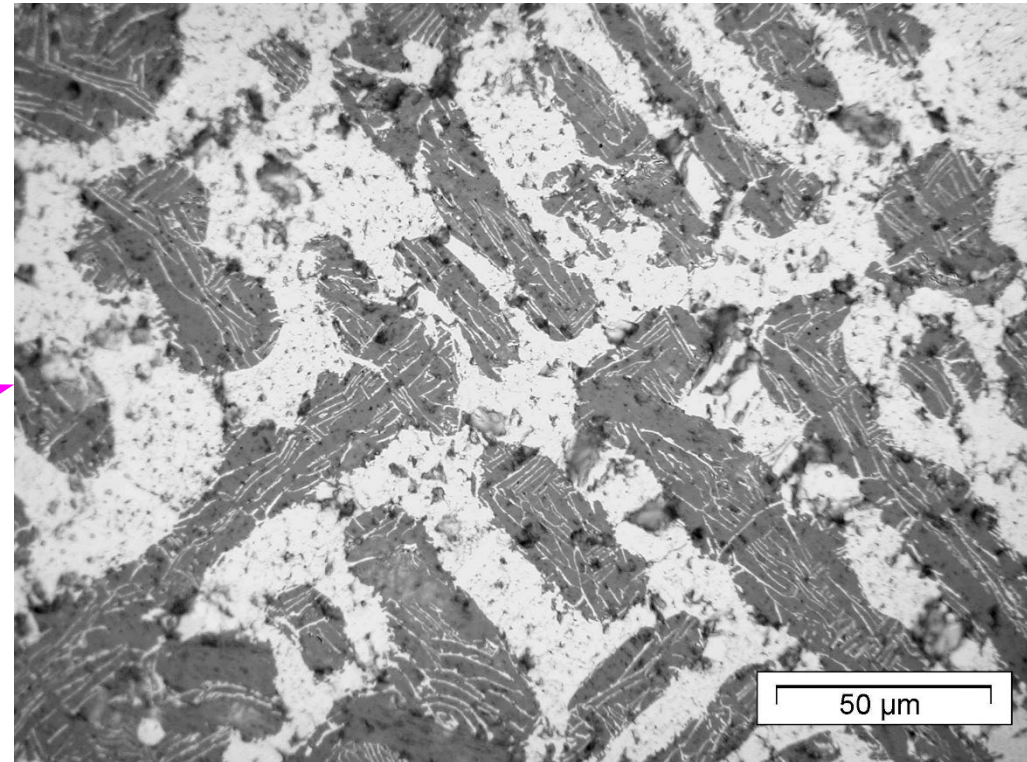
area of ceramic precipitates 23%  $\Rightarrow$  10.6 wt% of O,  
this is below the solubility limit (12.7 wt% at 2100 °C)



# Structure of frozen melt formed as molten pool in the QUENCH-11 bundle



QUENCH-11 bundle test, elevation 850 mm

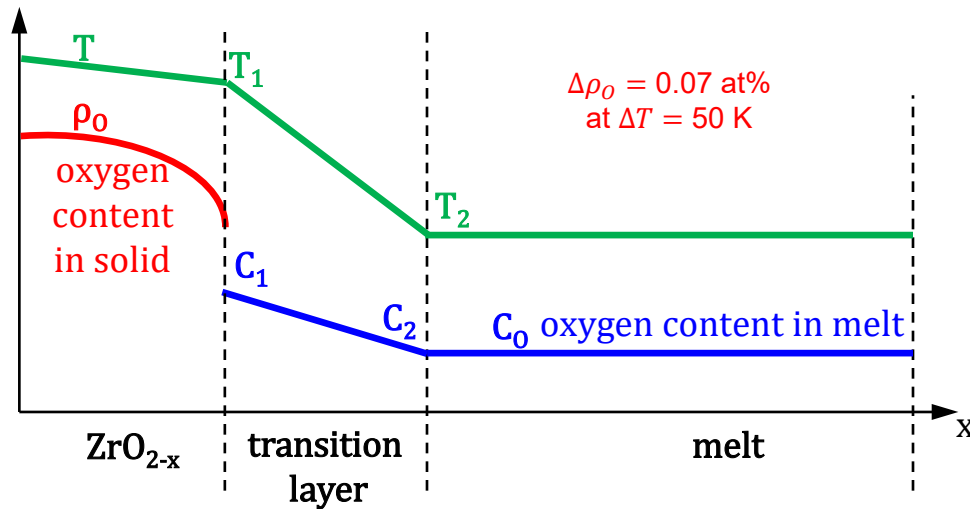
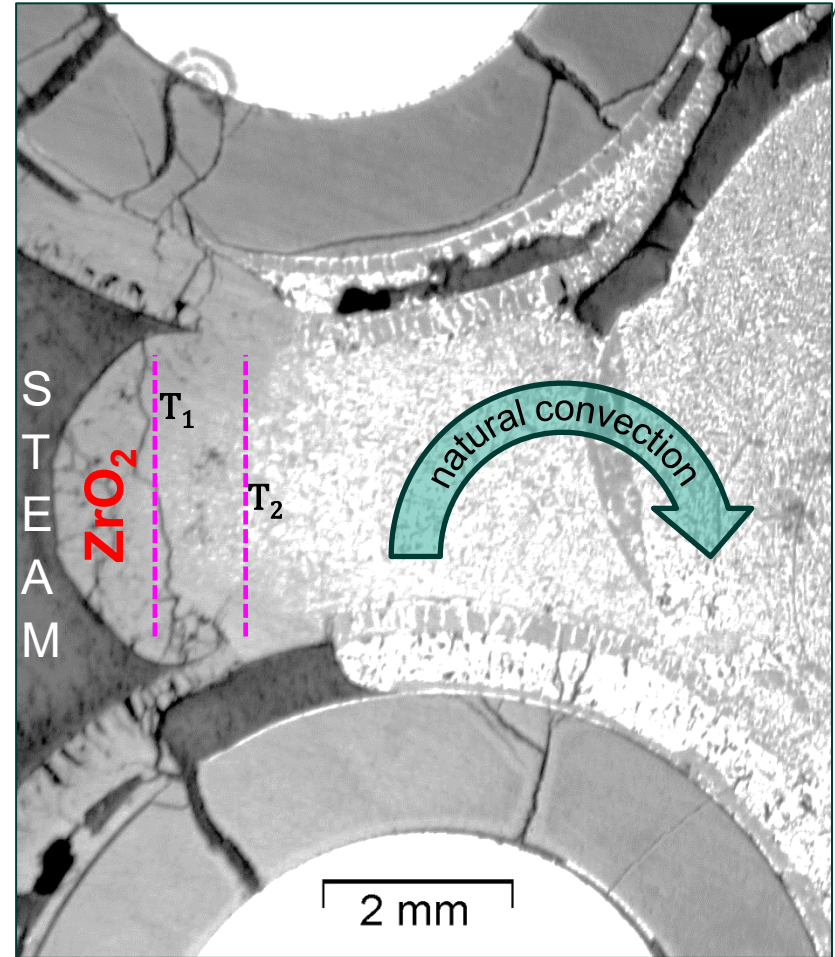
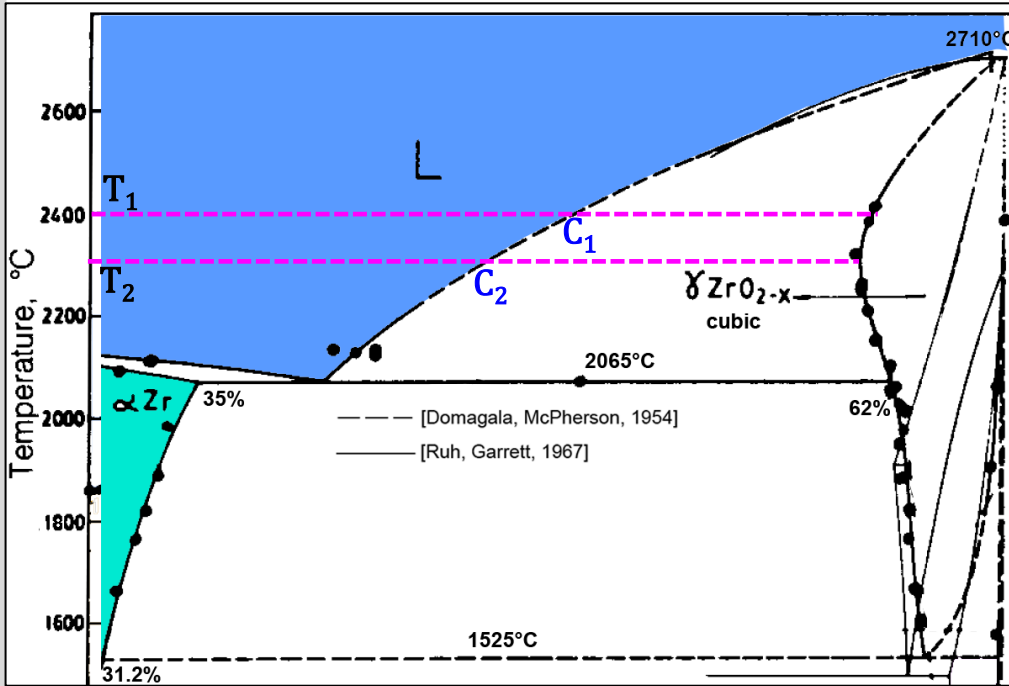


area of ceramic precipitates 56%  $\Rightarrow$  16.7 wt% of O,

this is **above** the oxygen solubility limit

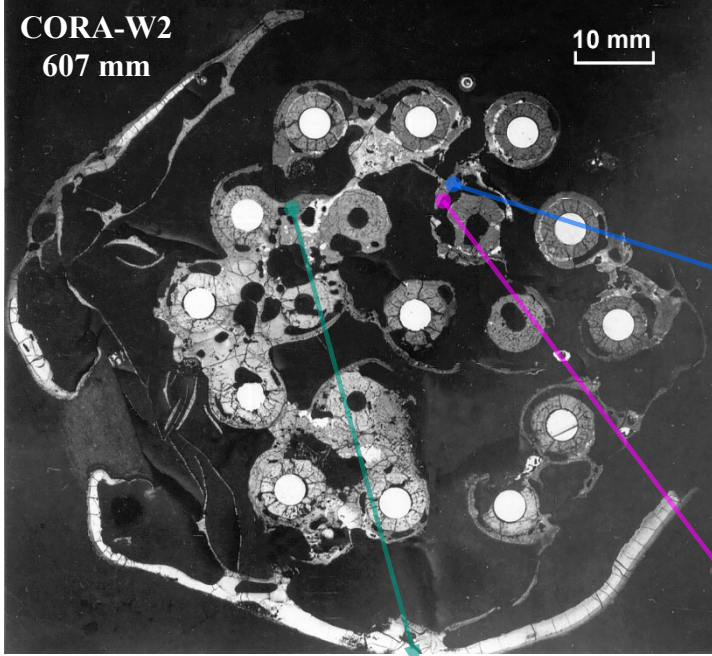
(14.7 wt% at 2100 °C)

# Oxygen diffusion to the saturated melt due to T gradient

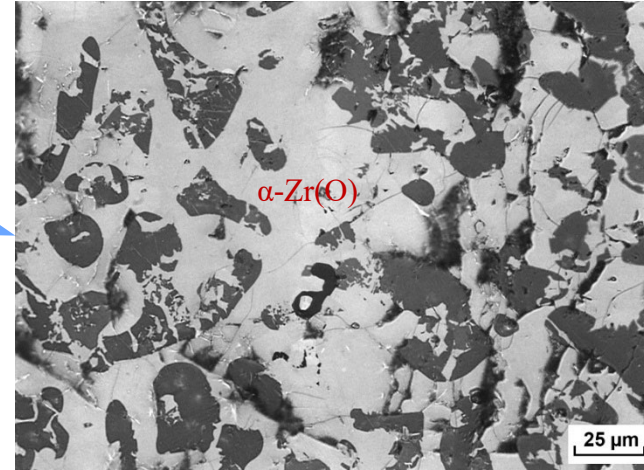


**$T_1 > T_2$  due to exothermic reaction of steam with molten Zr**

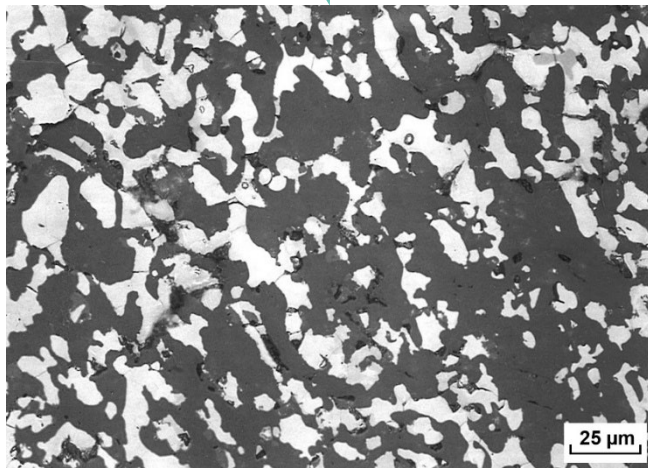
M. Veshchunov, J. Stuckert, A. Berdyshev, Modelling of Zr-O and U-Zr-O melts oxidation and new crucible tests, FZKA-6792 (2002), <https://doi.org/10.5445/IR/270046616>



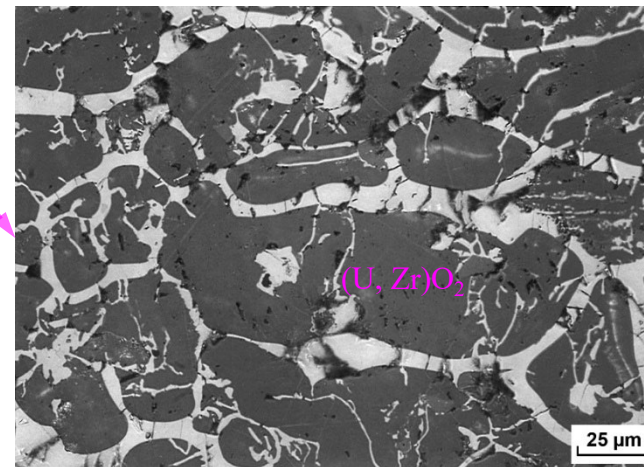
## Structure of frozen melt formed in the CORA-W2 bundle at temperature and during cooldown



ceramic precipitates 34% → melt saturated with oxygen



ceramic precipitates 56% → oversaturated melt

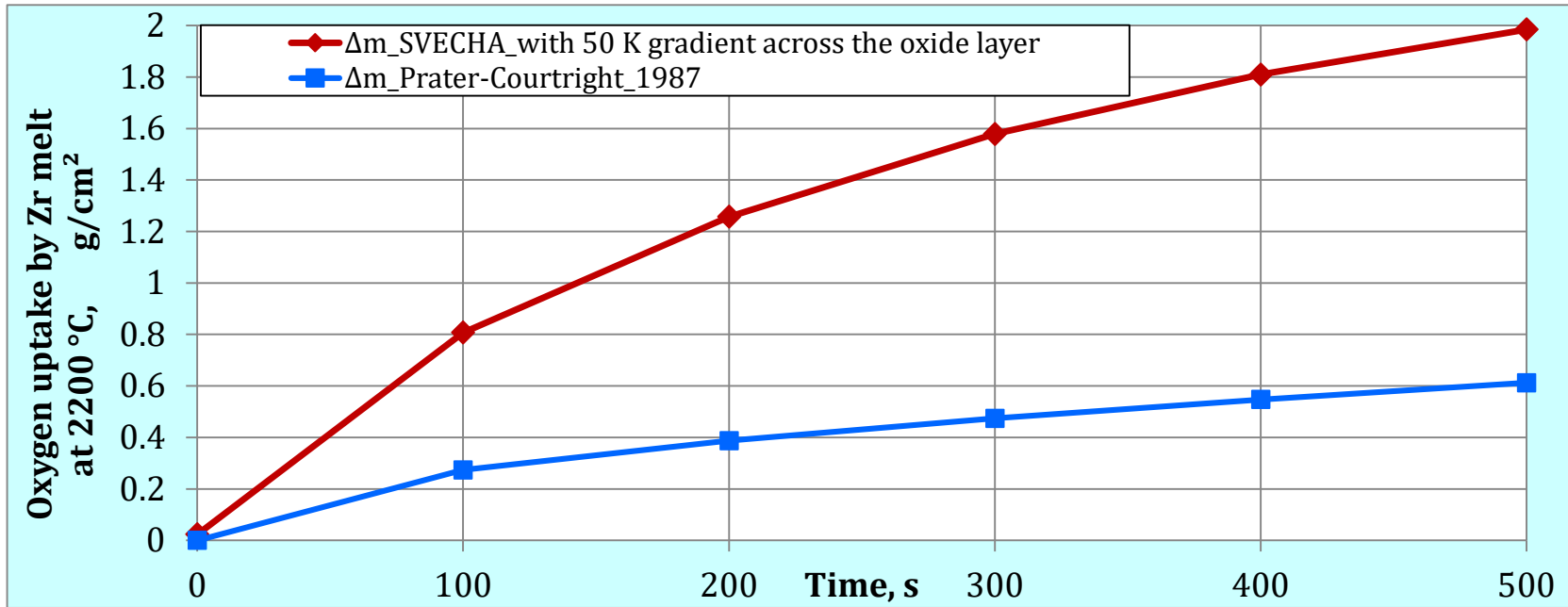


ceramic precipitates 68% → oversaturated melt

*According to the EDX analysis of the oxidized melt, the zirconium content in it (in at%) is 4-8 times higher than the uranium (which entered the melt due to the dissolution of the pellets). Therefore, the presence of zirconium is the determining factor.*



# Oxygen uptake by molten pools at 2200 °C: comparison of two models (SVECHA mechanistical model vs. engineering approach)



t, s	mass gain by ZrO <sub>2</sub> layer $\Delta m_{R-T}$ , g/cm <sup>2</sup>	mass gain by ZrO <sub>2</sub> precipitates in melt $m_f$ , g/cm <sup>2</sup>	total mass gain $\Delta m_{\text{SVECHA}}$ , g/cm <sup>2</sup>	Prater-Courtright mass gain $\Delta m_{\text{PC}}$ , g/cm <sup>2</sup>	$\Delta m_{\text{SVECHA}}/\Delta m_{\text{PC}}$
0	0.023	0	<b>0.023</b>	0	
100	0.057	0.751	<b>0.807</b>	0.274	3.0
200	0.088	1.169	<b>1.257</b>	0.387	3.2
300	0.120	1.458	<b>1.578</b>	0.474	3.3
400	0.153	1.657	<b>1.809</b>	0.547	3.3
500	0.182	1.803	<b>1.984</b>	0.612	3.2

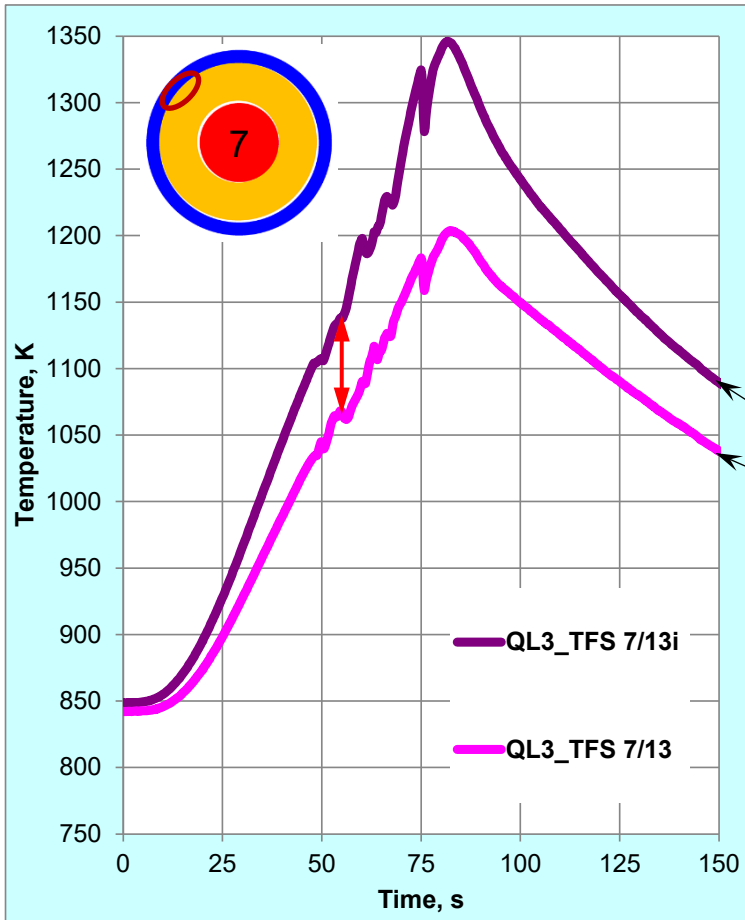
➤ **accelerated melt oxidation due to formation of ceramic precipitates: factor 3 in comparison to the Prater-Courtright**

➤ **suggested kinetics:  $K_{\text{mod}} = 5.74 \cdot \exp(-85900/RT)$ , g/cm<sup>2</sup>/s<sup>0.5</sup> (instead  $K_{\text{PC}} = 5.74 \cdot \exp(-109911/RT)$ , g/cm<sup>2</sup>/s<sup>0.5</sup>)**

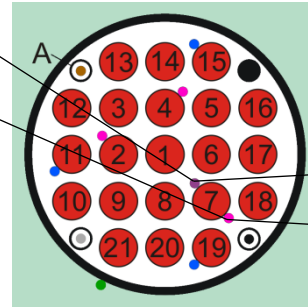
## Phenomena occurring in an oxidizing melt

- The analysis of the viscous melt behavior in bundles and the image analysis of the frozen melt show the formation of ceramic precipitates in the melt even in the molten state (not only during the cooldown).
- The driving mechanism for the formation of melt oversaturated with oxygen and precipitation of ceramic phase is the temperature gradient at the oxide-melt interface of the molten pool.
- According to the Zr-O phase diagram, this ensures a decreasing oxygen concentration in the transition layer and therefore diffusion of oxygen from the oxide to the saturated melt, which is then mixed as a result of natural convection.
- A numerical calculation carried out for the case with an operating temperature of 2200 °C and a temperature gradient at the melt boundary of 50 K showed that the oxidation process occurs parabolically and three times faster than predicted by the Prater-Courtright oxidation correlation used usually in computer codes at  $T \geq 1800$  °C.

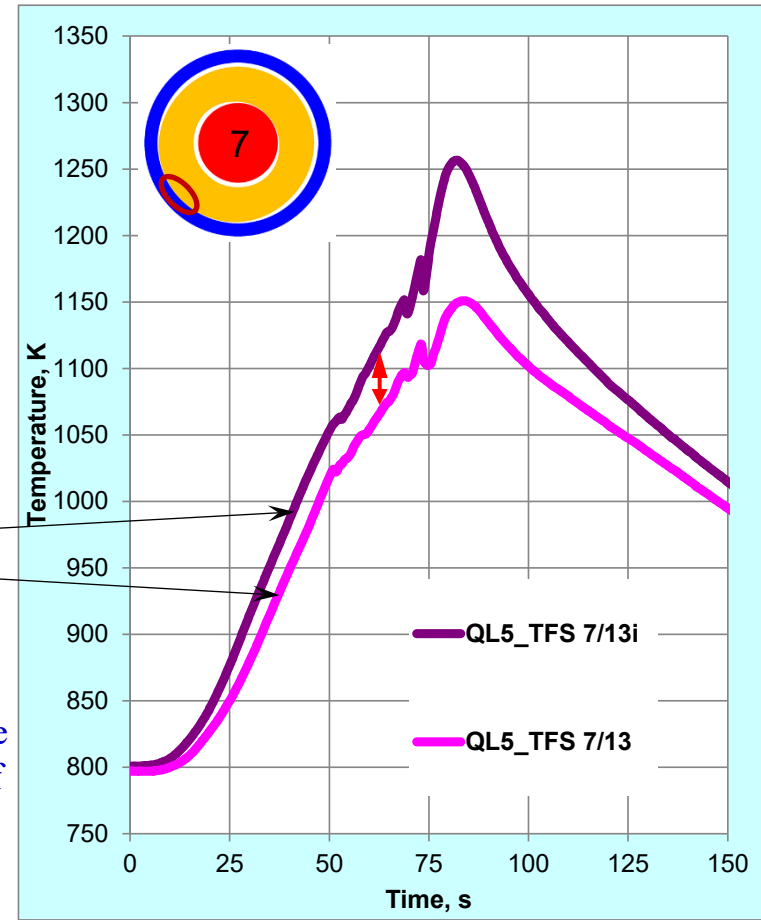
# Dependence of the circumferential temperature difference on the position of **contact** between the pellet and the cladding



**QL-3 bundle:**  
large circumferential difference  $\Delta T=70$  K



positions of two diametrically opposite TCs on the surface of the rod 7



**QL-5 bundle:**  
moderate circumferential gradient  $\Delta T=50$  K

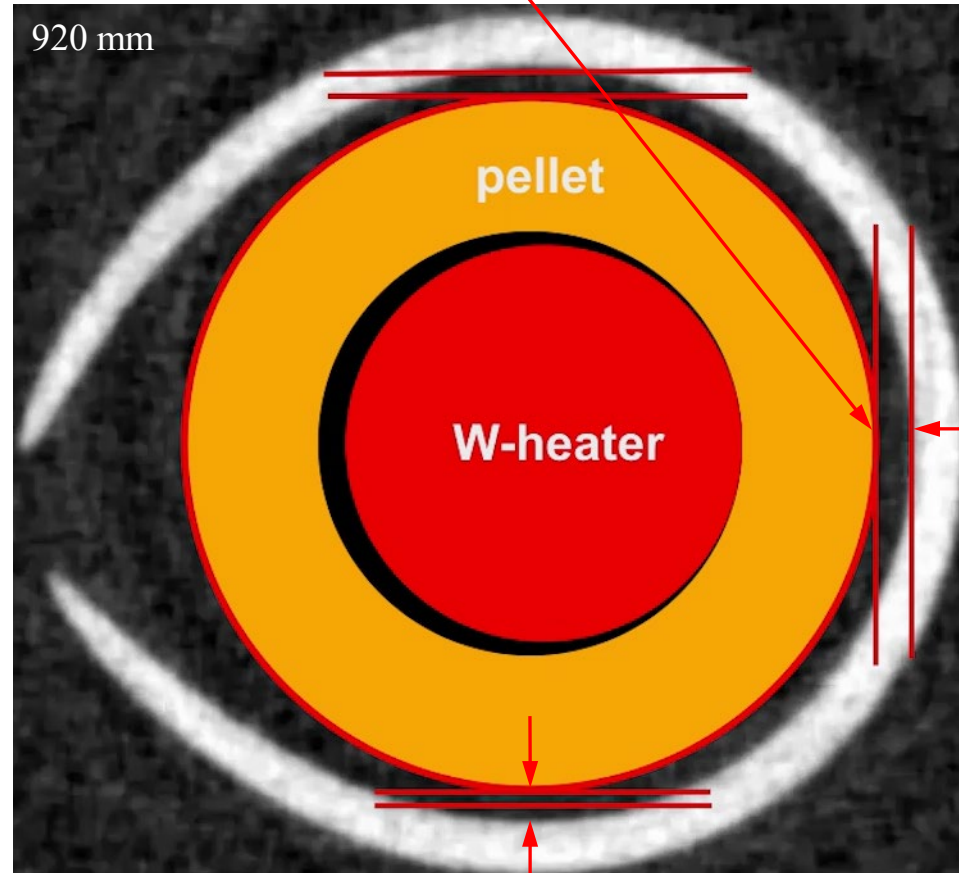
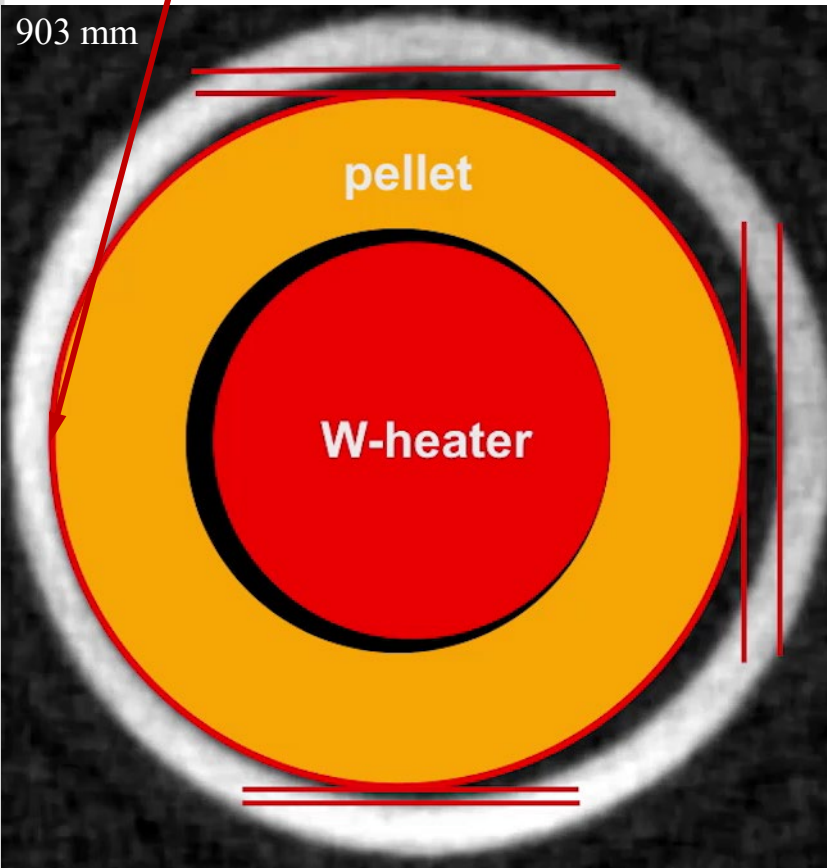
# Not symmetrical cladding ballooning due to point contact between pellet and cladding (QL4 bundle, rod 1, tomography of rod between 903 and 920 mm)

*optical view of clad inner surface below the burst opening at 920 mm*



**hot spot: pellet-cladding contact**

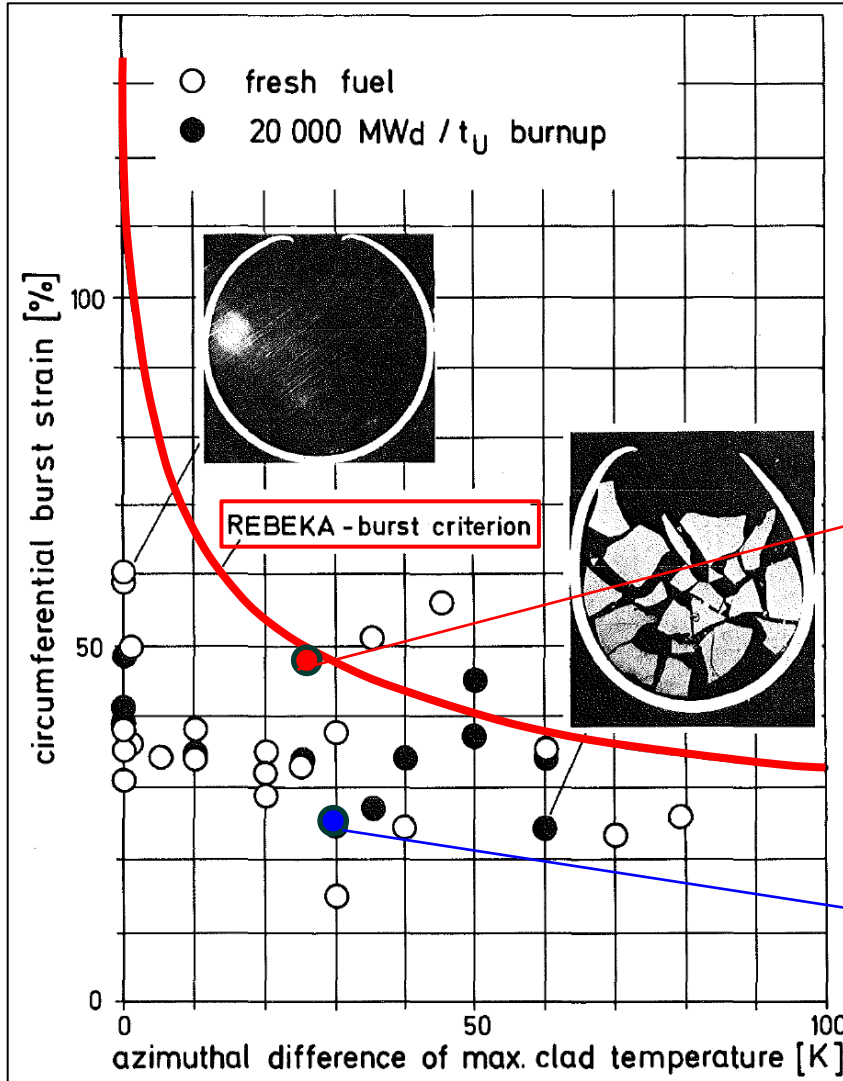
*the gap is present until burnouts of 30 MWd/kgU*  
**max gap 150  $\mu$ m**  
**not changed during ballooning**



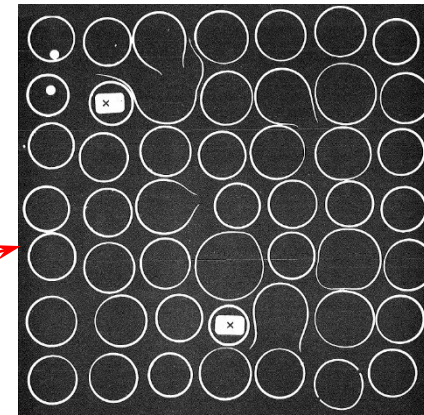
Link to movie: <http://www.doi.org/10.5445/IR/1000189456>

**gap increased during ballooning**

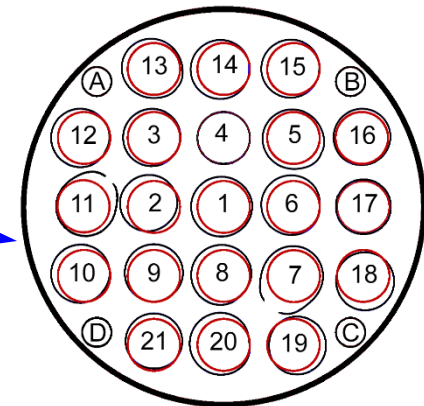
# REBEKA burst criterion (burst strain vs. circumferential $\Delta T$ ) and FR2 in-pile test data



The circumferential burst strains of cladding tubes are kept relatively small due to *temperature differences* on the cladding circumference and the anisotropic strain behavior of Zr alloys.



REBEKA-5 bundle at 2000 mm with maximum bundle blockage of 52%: maximum clad strain 49%



*original clad*  
*ballooned clad*

QUENCH-LOCA-4 bundle at 924 mm with maximum bundle blockage of 19%: maximum clad strain 23%

comparison of FR2 data with REBEKA burst criterium

## Cladding deformation under circumferential temperature gradient

- Up to burnups of 30 MWd/kgU, fuel pellets can only have point contact with the cladding (and not along their entire perimeter), which leads to a hot spot in this place.
- The cladding begins to unsymmetrical stretch in directions perpendicular to the tangent line of contact between the pellet and the cladding, and then ruptures near the contact point with additional outward deformation of the burst opening edges.
- The circumferential strains of the claddings are generally no more than 40%, which leads to maximum blockades of the bundle cross-section of about 60%, which in turn ensures full coolability of the bundle during reflood.

## Acknowledgment

The author would like to thank the entire QUENCH team for their intensive work during the test preparations and post-test investigations.

*Thank you for your attention*

<https://www.iam.kit.edu/awp/english/163.php>

<http://quench.forschung.kit.edu/>



**Mirco Große**

KIT

## **Neutron Imaging Investigations of Hydrogen in Cladding Tube Materials**

The paper gives an overview about 20 years of neutron imaging investigations by the QUENCH team of KIT. After an introduction into neutron radiography and tomography, examples of the results concerning:

- The hydrogen uptake during oxidation of cladding materials by steam, particularly the effect of breakaway on the hydrogen concentration.
- The hydrogen diffusion at temperatures between 900 and 1300°C.
- The hydrogen distribution around a crack tip at 350°C.
- The effect of the total gas flow rate on the oxidation of Zircaloy-4 in steam-nitrogen mixtures.
- The hydrogen enrichments in cladding tubes after LOCA simulation tests.
- The effect of elastic strain on the hydrogen distribution in pure zirconium.

were given. Hydrogen concentrations were determined quantitatively. Results of in-situ investigations are shown as movies in the paper.

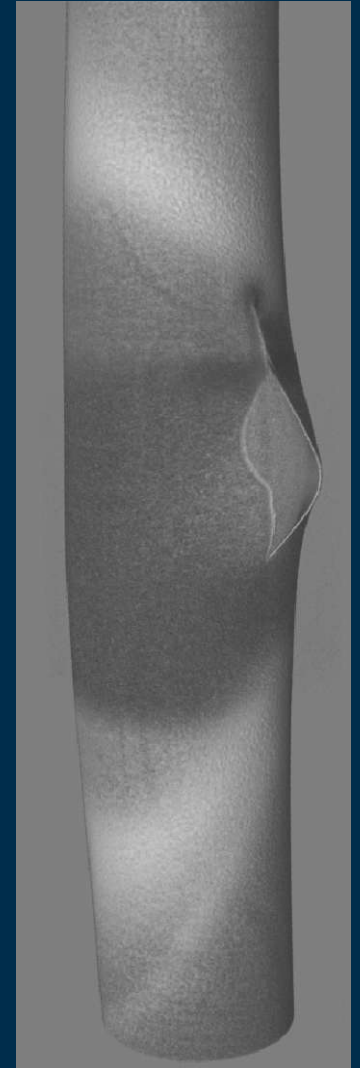
The examples demonstrate the power of neutron imaging not only to investigate the behaviour and distribution of hydrogen in zirconium, but also to obtain new insights into the kinetic of processes occurring in cladding tubes under operational accidental conditions.



# Neutron Imaging Investigations of Hydrogen in Cladding Tube Materials

Mirco Grosse, et al.,

30. Intern. QUENCH Workshop,  
KIT Campus North, 2025/12/16



# Basis Neutron Imaging

X-ray radiography



1895/12/22

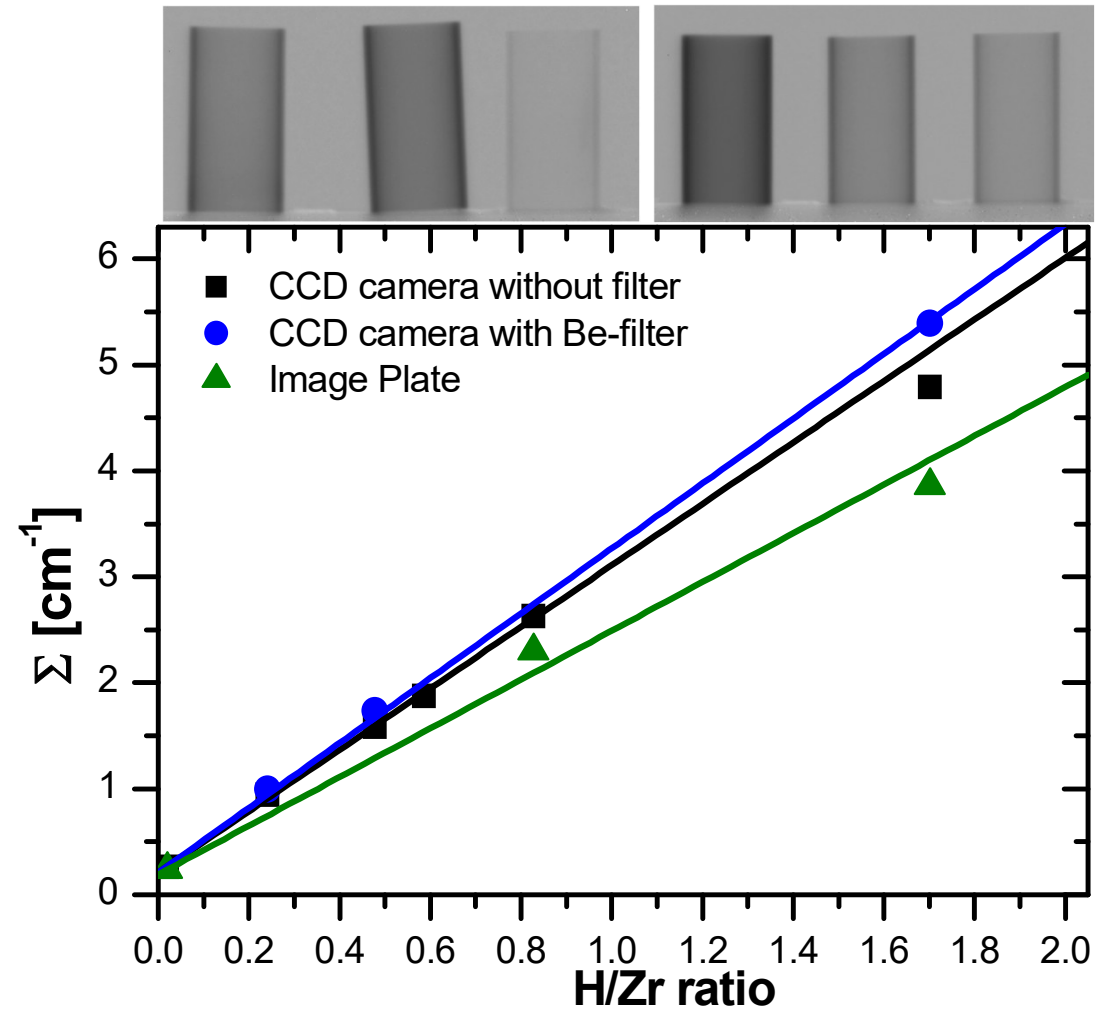
neutron radiography



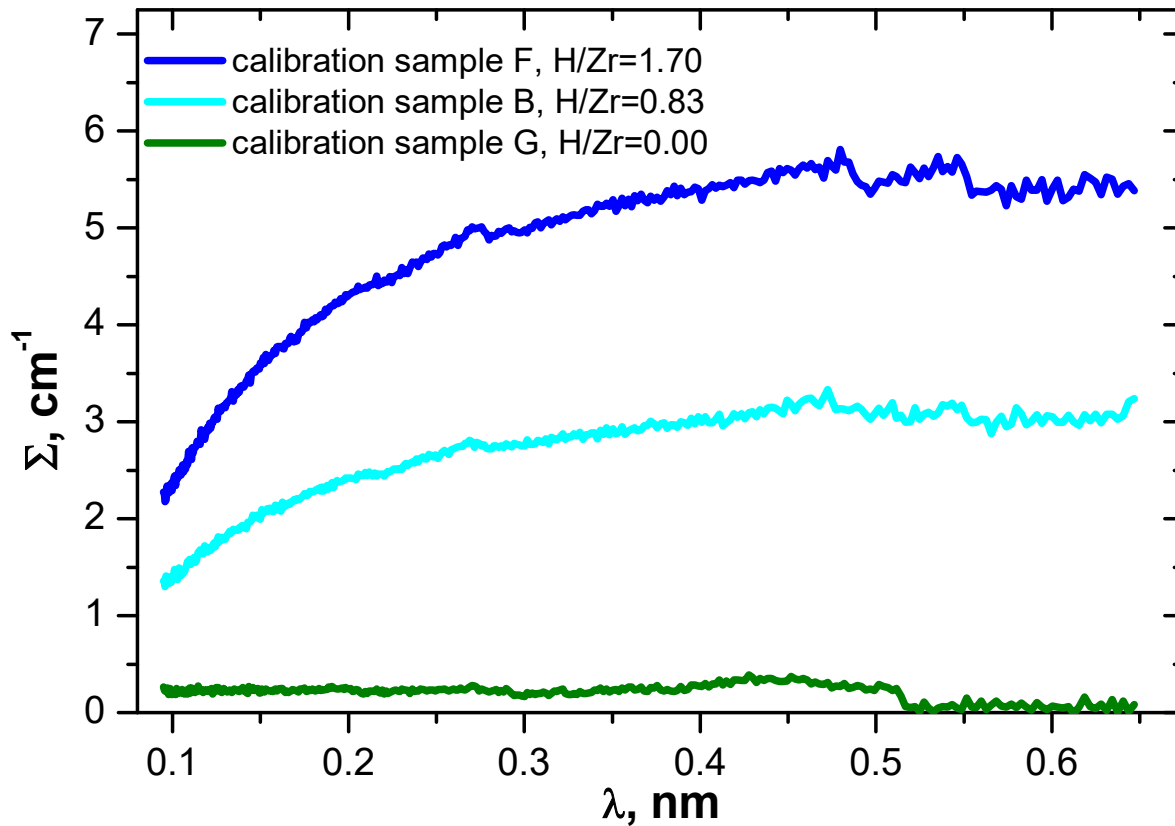
GKSS Geesthacht 1991

# Basis Neutron Imaging

$$\begin{aligned} \Sigma_{total} &= \frac{-\ln\left(\frac{I - I_B}{I_0 - I_B}\right)}{s} \\ &= \sum_i N_i \sigma_i \\ &= \underbrace{N_{Zr} \sigma_{Zr} + \dots}_{\Sigma_{Zry}} + N_H \sigma_H + N_O \sigma_O \end{aligned}$$



# Basis Neutron Imaging



Generally:

$$\sigma_{total} \sim \lambda^4$$

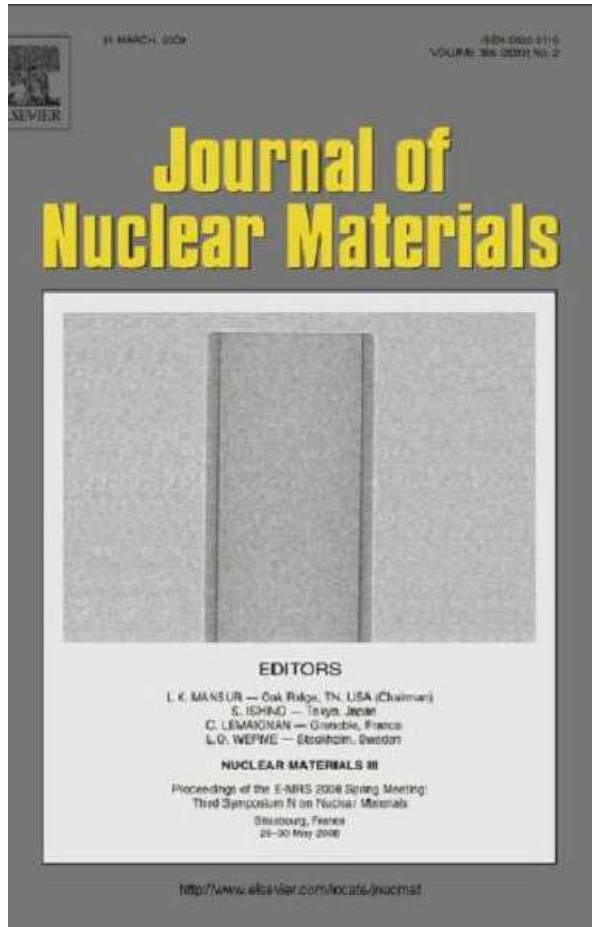
$$\sigma_{total} = \sigma_{ab.} + \sigma_{coh.sc.} + \sigma_{inc.sc.}$$



$$\sin(\theta) = \frac{\lambda}{2d}$$

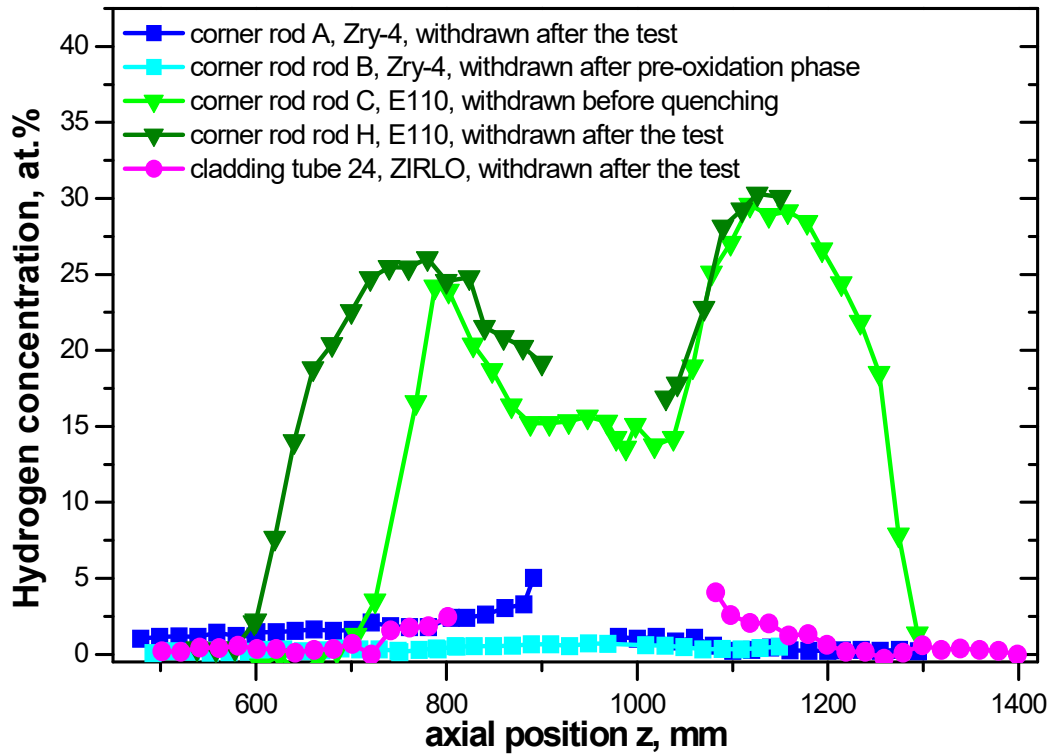
Neutron energy/wavelength  
dependence of total neutron cross  
section

# Hydrogen uptake during oxidation by steam

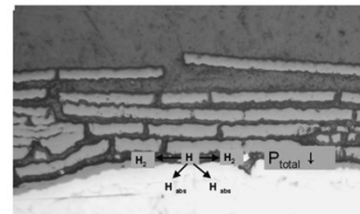


- Various ex-situ investigations of the hydrogen uptake during the oxidation in steam
- The zirconium community was sceptical about this method and our results
- Discussions about the possibility to apply this method to investigate DHC with the colleagues from PSI at the ASTM Symposia in Chengdu 2010
- Since this time groups from France, Switzerland, Czech Republic, Hungary, USA, Canada, China, South Africa, Australia and Argentina has applied neutron imaging methods to investigate hydrogen in Zirconium

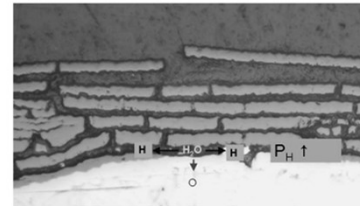
# Hydrogen uptake during oxidation by steam



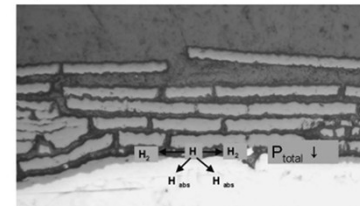
Neutron radiography investigations of the hydrogen uptake of cladding tubes tested in the QUENCH-ACM sub-programme



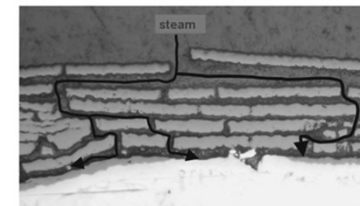
a)



b)



c)



d)

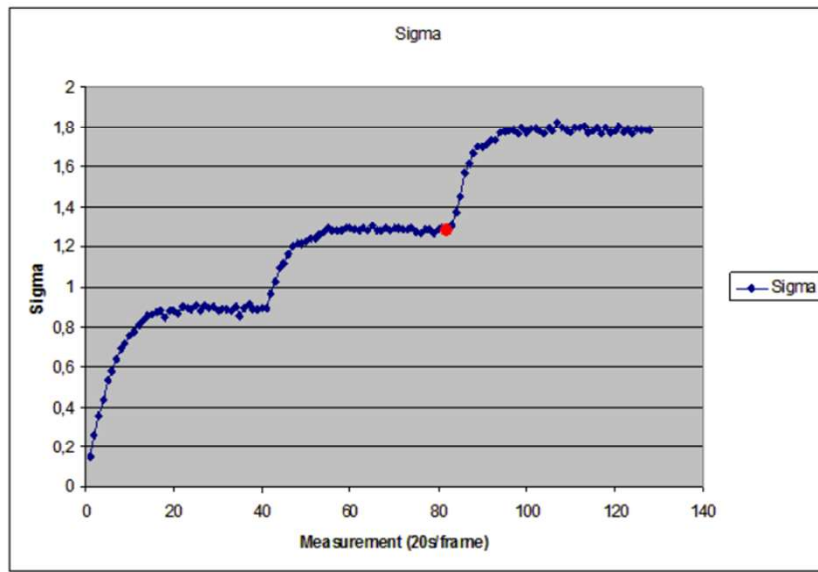
Hydrogen pump effect occurring at breakaway oxides

# Calibration at high temperatures

Sieverts' law:

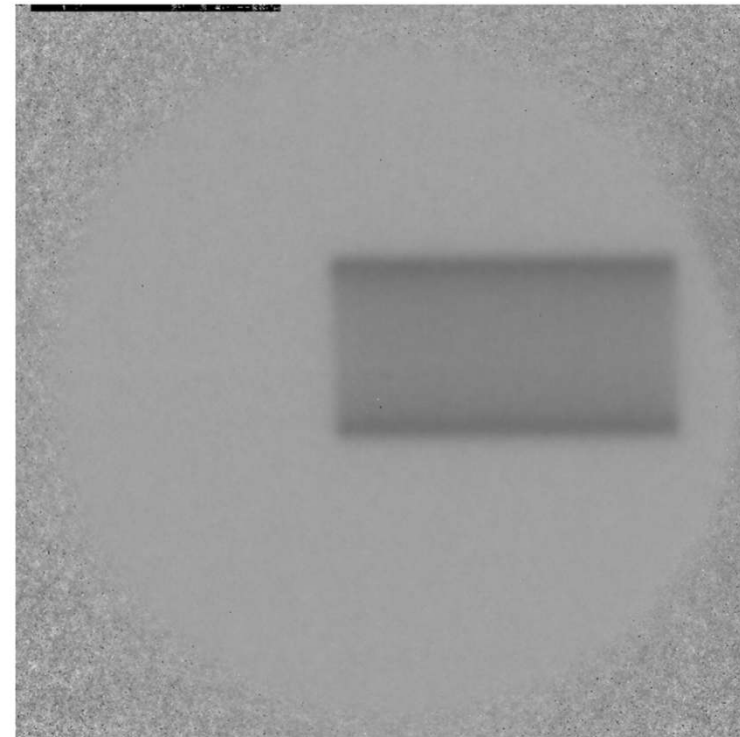
$$C_H^{(m)} = K_S \cdot \sqrt{p_{H_2}}$$

$$K_S = \exp\left(\frac{\Delta_S S}{R} - \frac{\Delta_S H}{R \cdot T}\right)$$

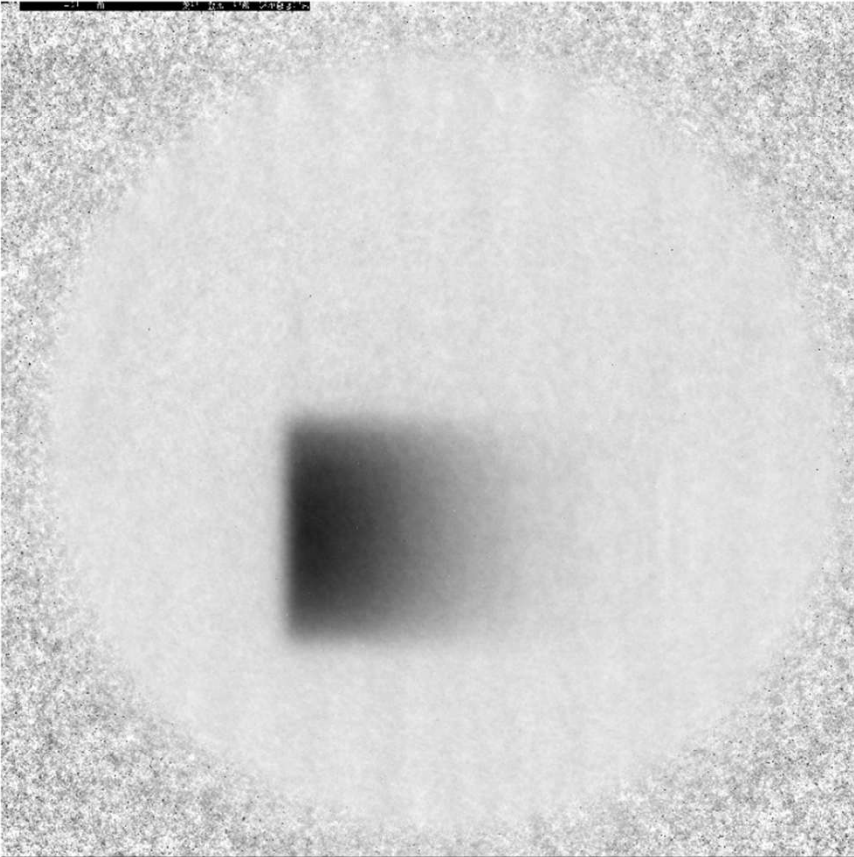


2 l/h    4 l/h    8 l/h H<sub>2</sub>, 50 l/h Ar

1000°C



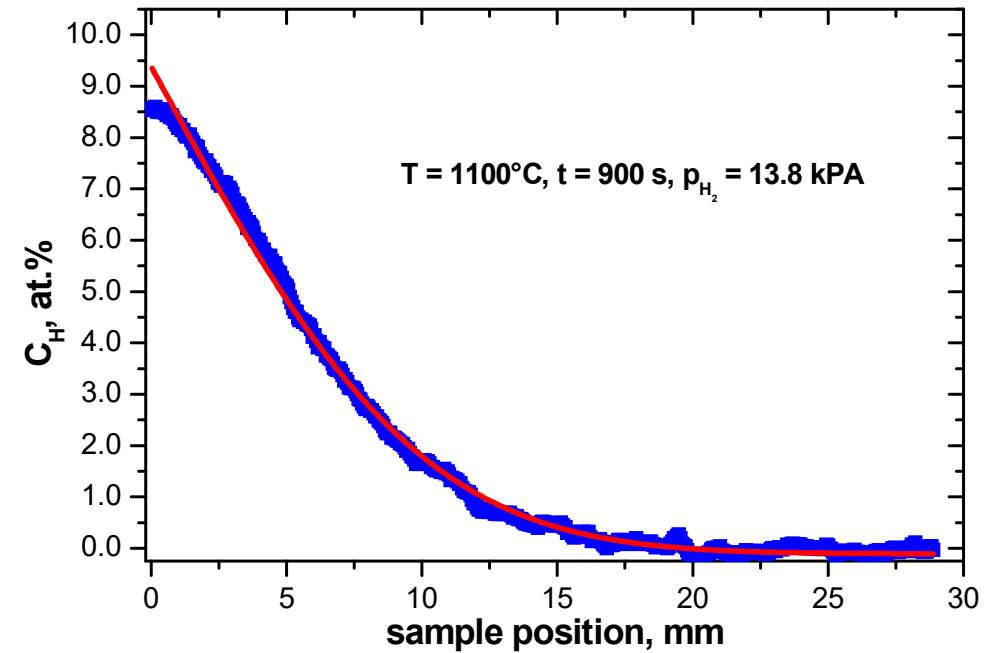
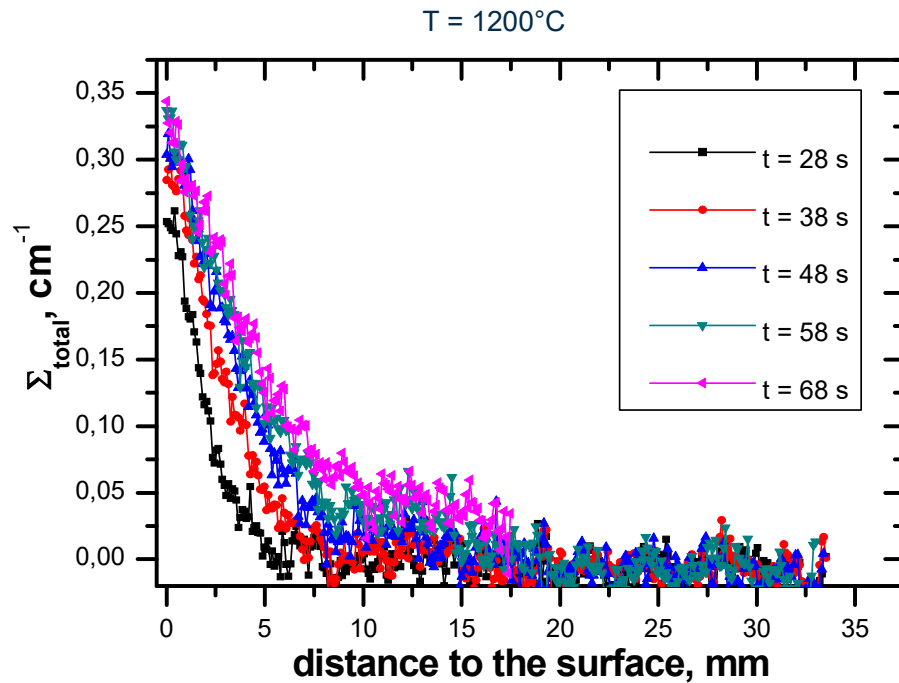
# Hydrogen diffusion at high temperatures



- Sample: solid cylinder pre-oxidized in Ar/O<sub>2</sub>, at one base plane the oxide layer was removed by grinding and polishing allowing hydrogen uptake through this face
- In-situ annealing's in Ar/H<sub>2</sub> atmosphere at 900, 1000, 1100, 1200 and 1300°C
- Frame repetition time was 10 s.

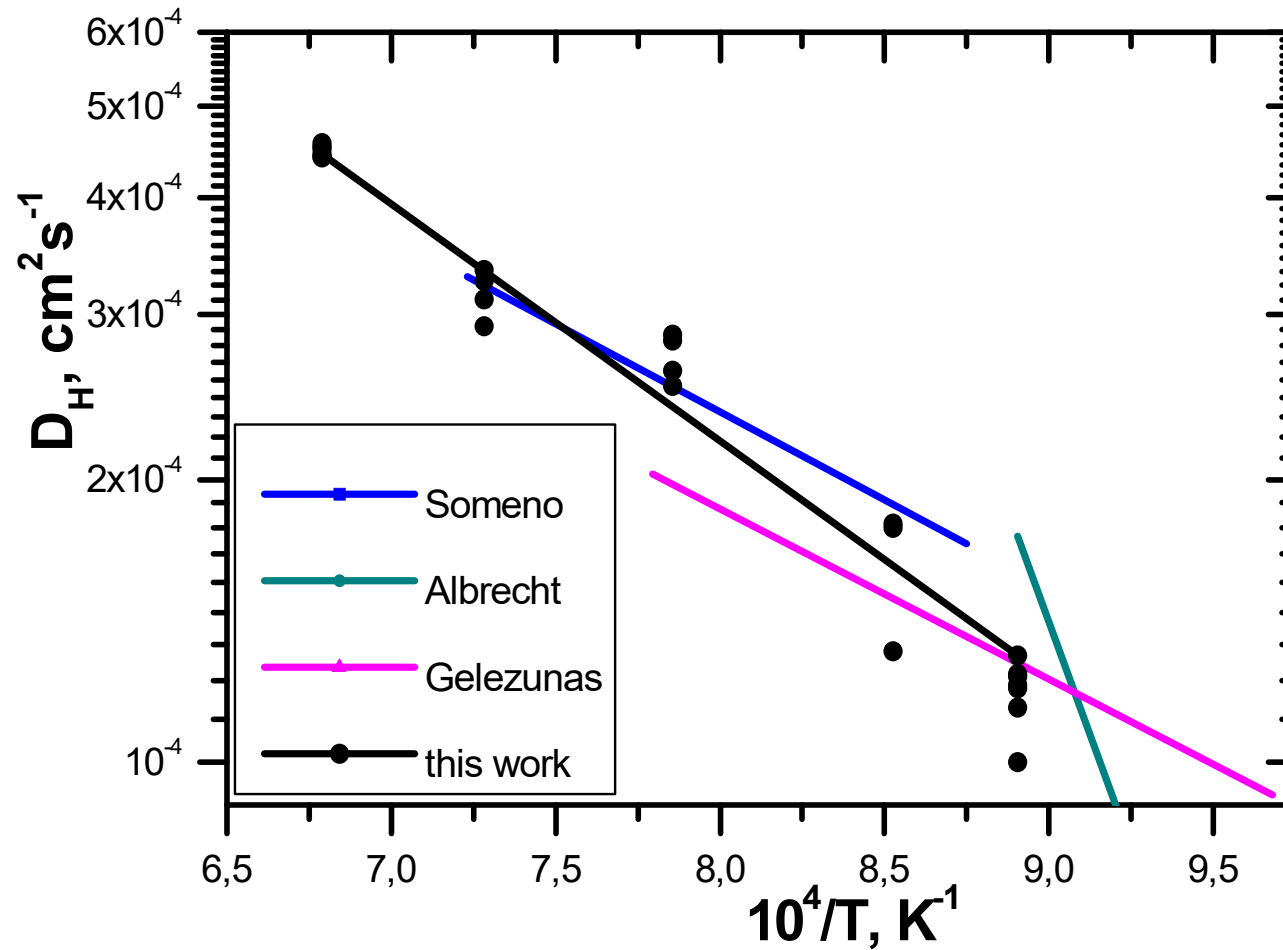


# Hydrogen diffusion at high temperatures

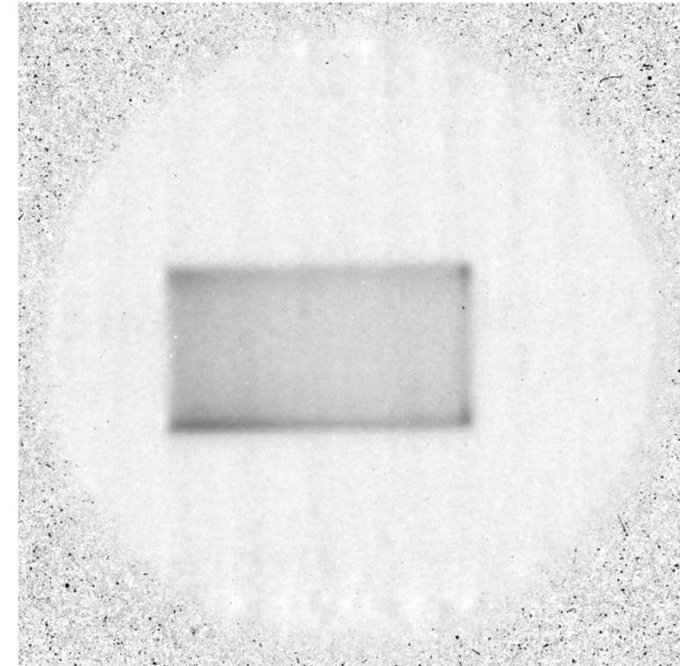
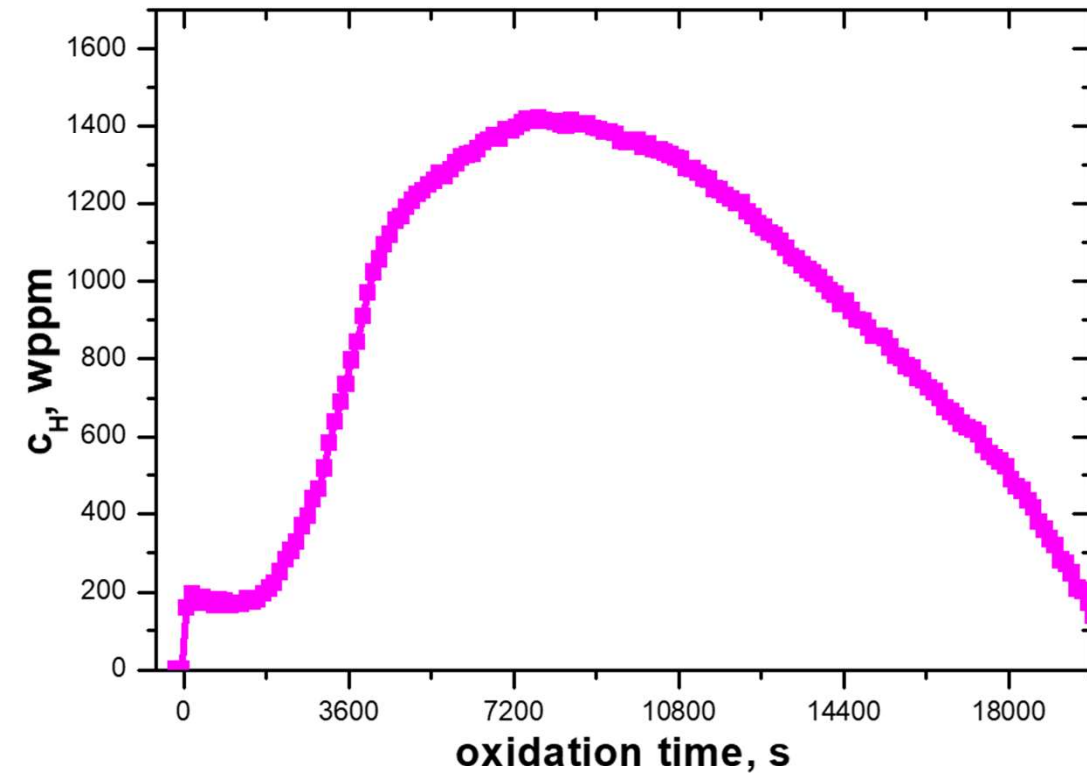


Axial distributions of the total macroscopic neutron cross section and of the hydrogen concentration

# Hydrogen diffusion at high temperatures

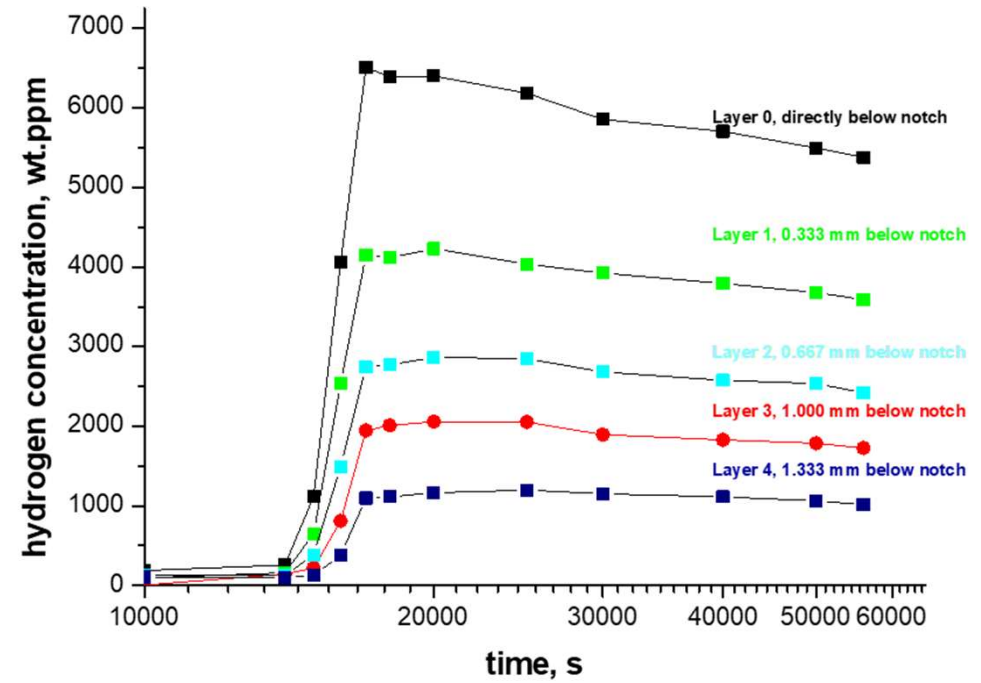
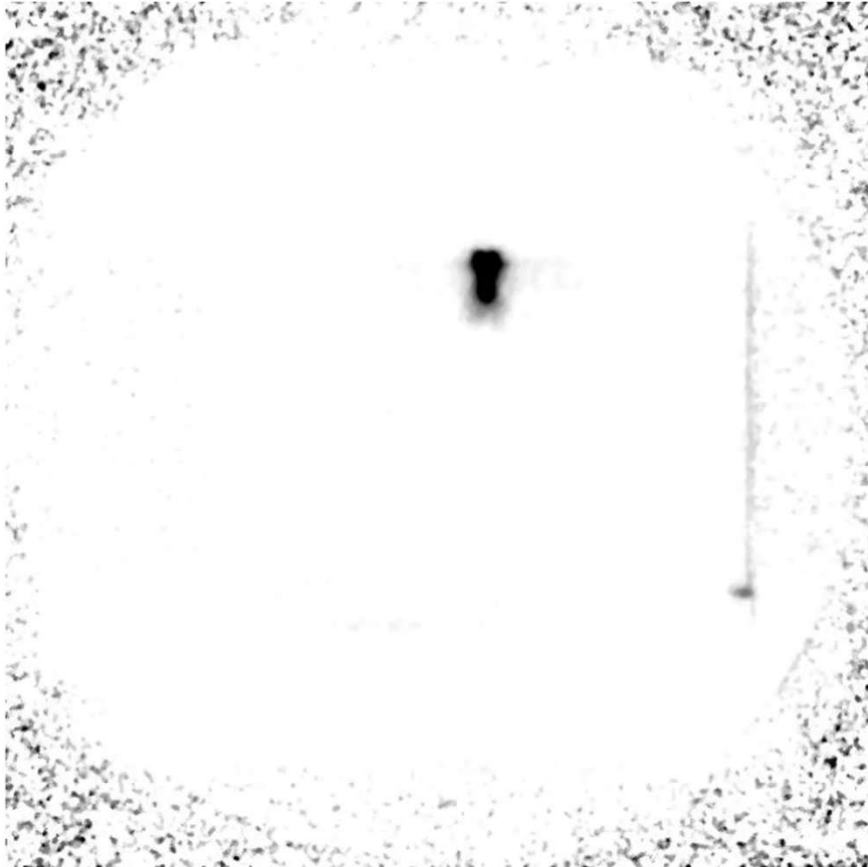


# Hydrogen uptake during oxidation by steam



Breakaway oxidation at 1000°C

# Hydrogen in zirconium

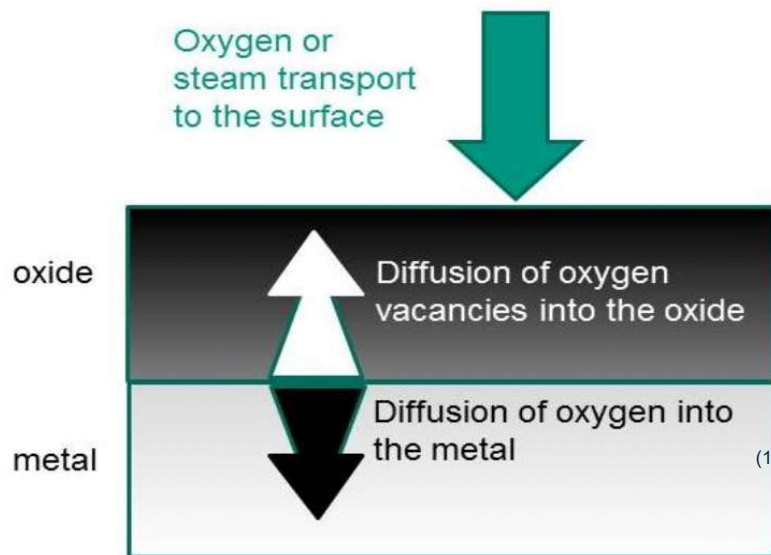


Attempts to investigate DHC by means of in-situ neutron radiography investigations

# Effects of nitrogen

## Flow rate model

[M. Grosse et al. ICAPP 2016]



- Basic reaction with steam if an oxide layer is already formed



- $\dot{n}_{\text{V}_\text{o}^{2+}} = \dot{n}_{\text{oxygen,react}} = \frac{K_{n_{\text{ox}}}}{2\sqrt{t}}$  for saturation

- In the case of steam + oxygen starvation

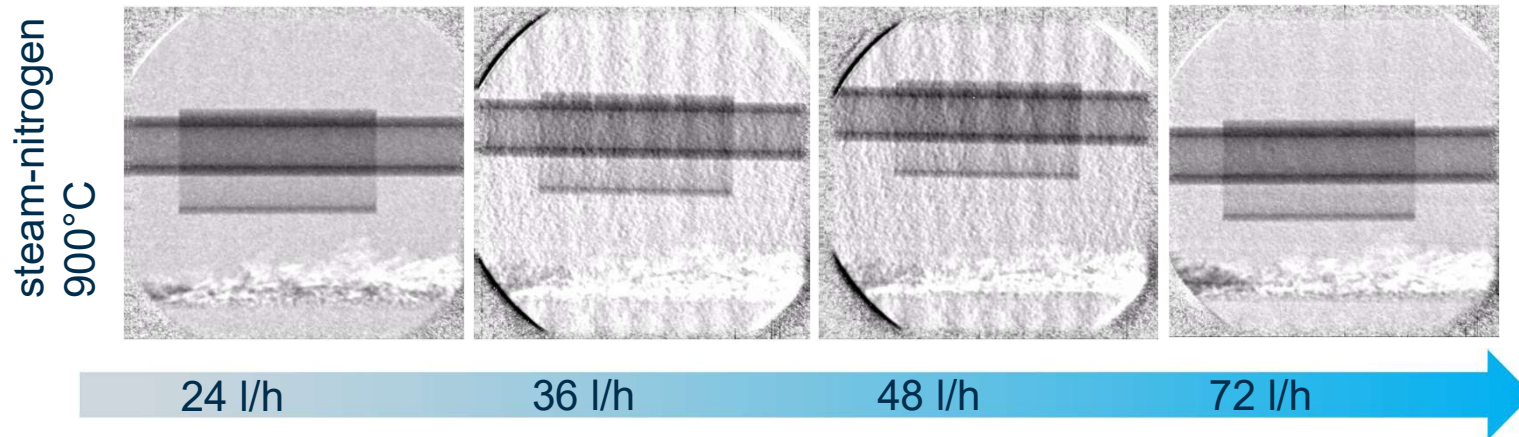
$$\rightarrow \frac{K_{n_{\text{ox}}}}{2\sqrt{t}} - \frac{\dot{n}_{\text{O}_2}}{2} - \dot{n}_{\text{H}_2\text{O}} = \frac{\dot{n}_{\text{N}_2}}{4}$$

- If  $c_{\text{N}} > c_{\text{N,critical}}$  -> ZrN precipitation and formation of cracks

- $\dot{x}_{\text{res}} = IF_{\text{cracks}} * \dot{x}_{\text{linear}} + (1 - IF_{\text{cracks}}) * \dot{x}_{\text{parabolic}}$

- cracks results in higher reaction rate

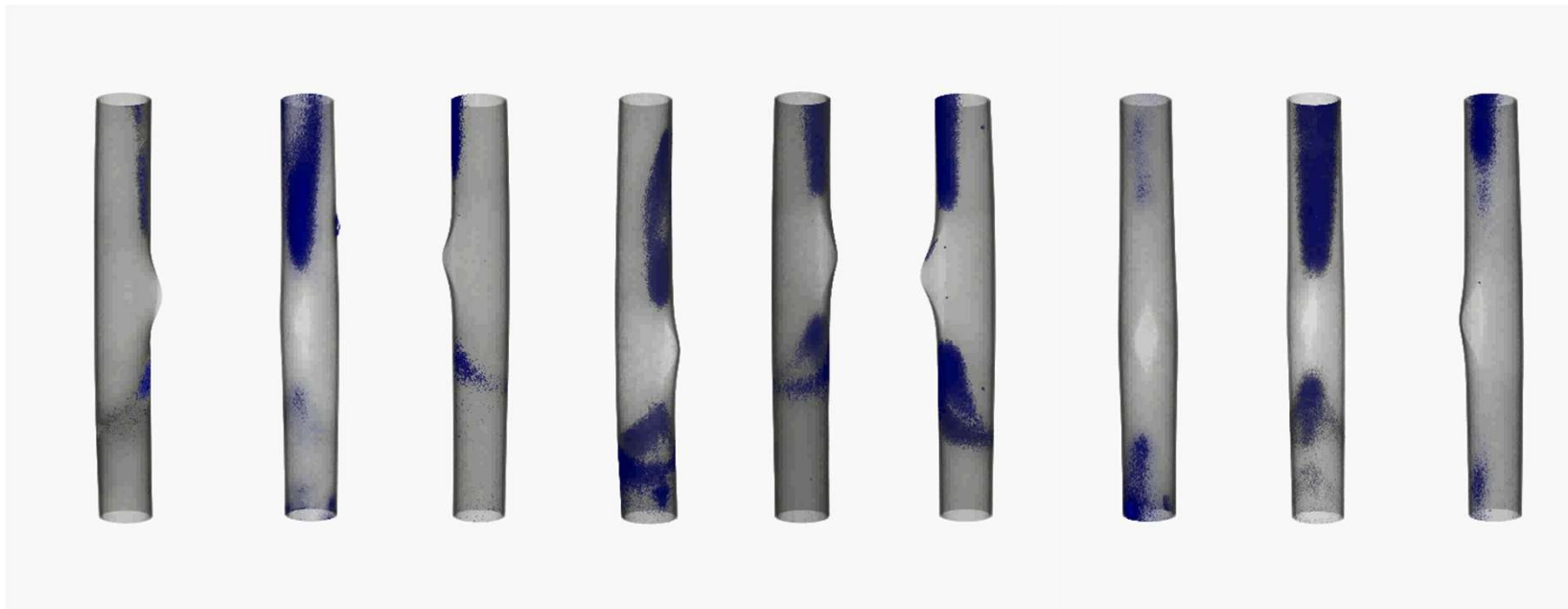
# Effects of nitrogen



Effect of the total gas flow rate on the reaction of Zry-4 in steam nitrogen atmosphere

# Post-test examinations of claddings from our LOCA tests

inner rods



01

02

03

04

05

06

07

08

09

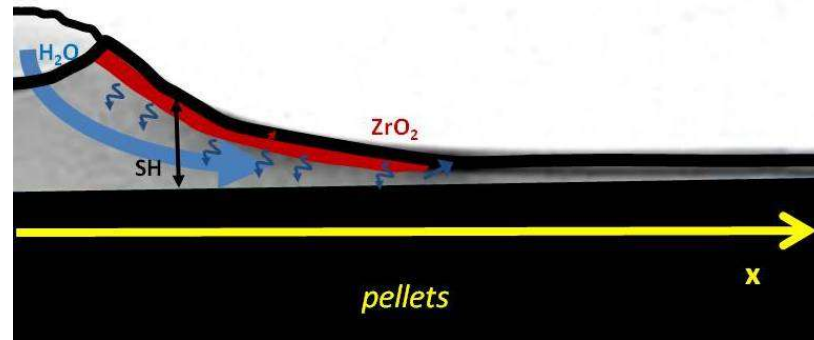
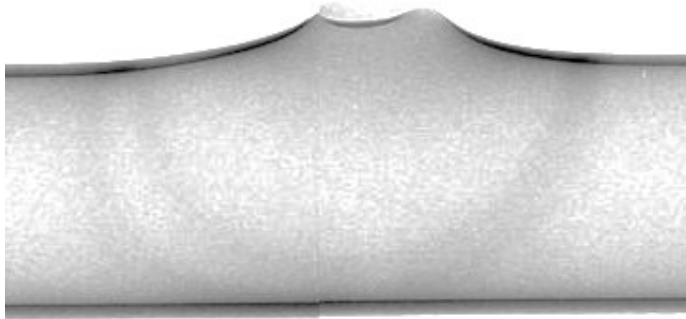
Samples from the inner part of the QUENCH-LOCA-3 test

# Post-test examinations of claddings from our LOCA tests

- Band shaped hydrogen enrichments are formed around the burst opening non-perpendicular to the tube axis.
- Enrichments occur where the inner oxide layer ends.
- Compared to the determinations before by hot extraction, the hydrogen enrichments are lateral smaller but with higher hydrogen concentrations
- Hydrogen enrichments occur at temperatures above 1000°C (tetragonal ZrO<sub>2</sub>)



# Modeling of the hydrogen distribution



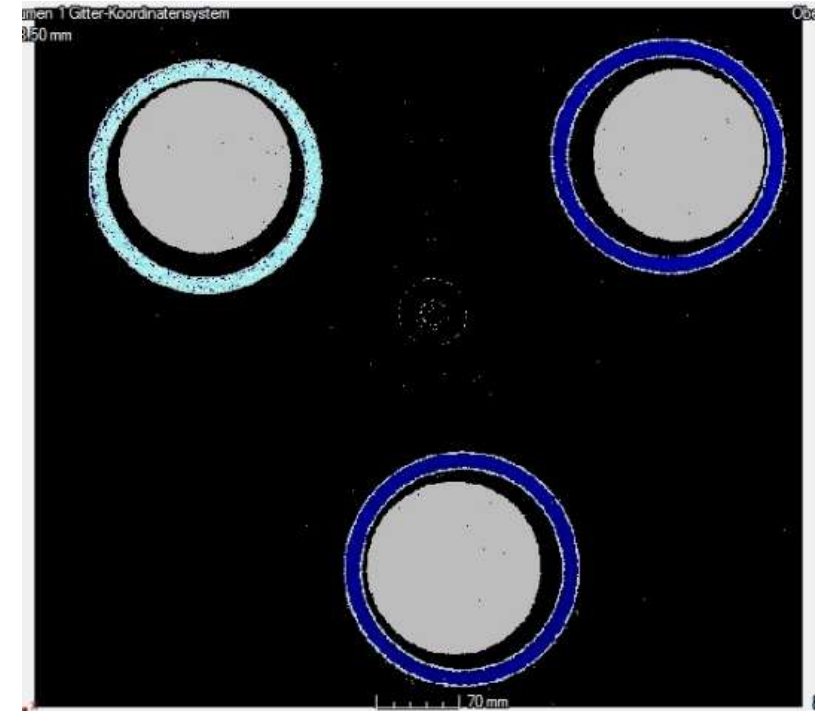
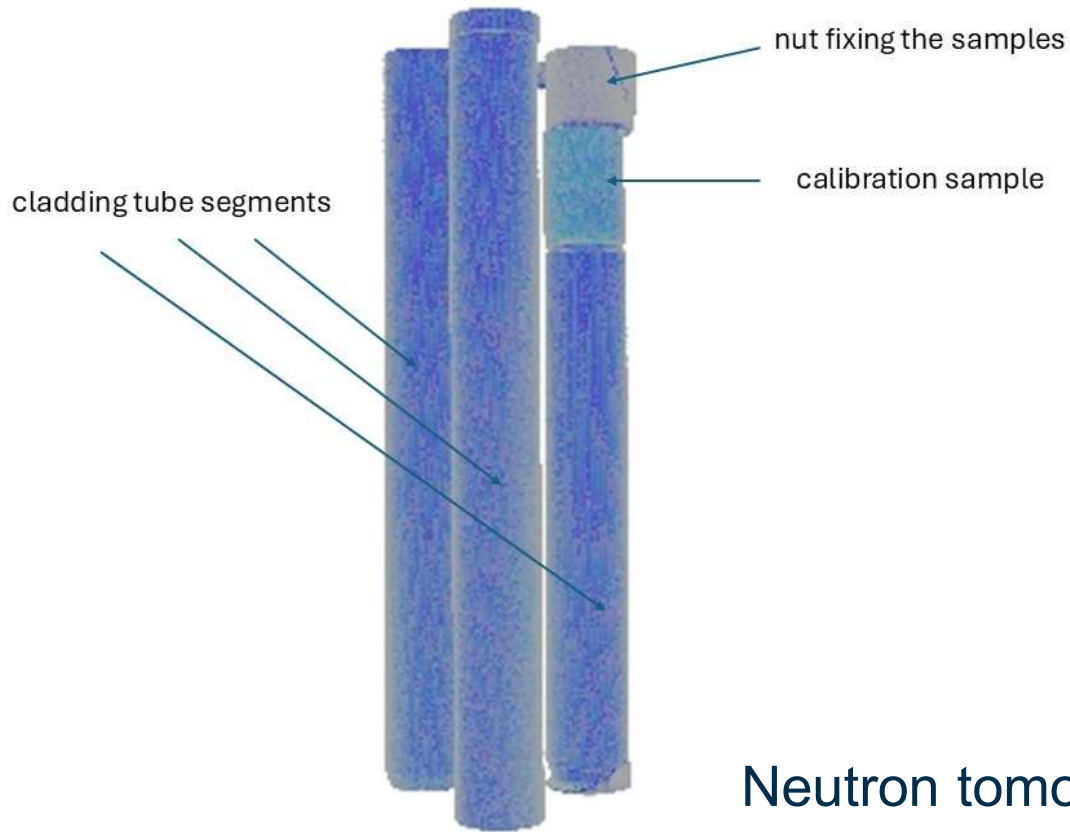
$$dc_{H_2=O}(x) = \text{Max} \left( \begin{array}{c} \left( D \frac{\delta^2 c_{H_2O}}{\delta x^2} - \frac{K_{ox}}{2\sqrt{t}} \right) dt \\ 0 \end{array} \right) \quad \text{Steam transport and consumption in the gap}$$

$$dc_{H_2}(x) = \left( \frac{K_{ox}}{2\sqrt{t}} + D \frac{\delta^2 c_{H_2}(x)}{\delta x^2} \right) dt \quad \text{Free hydrogen production and transport}$$

$$c_H^m(x, r=0) = \frac{K_S \sqrt{p_{total}} * c_{H_2}(x)}{\quad} \quad \text{Hydrogen uptake (amount of hydrogen in the gap has to be taken into account)}$$

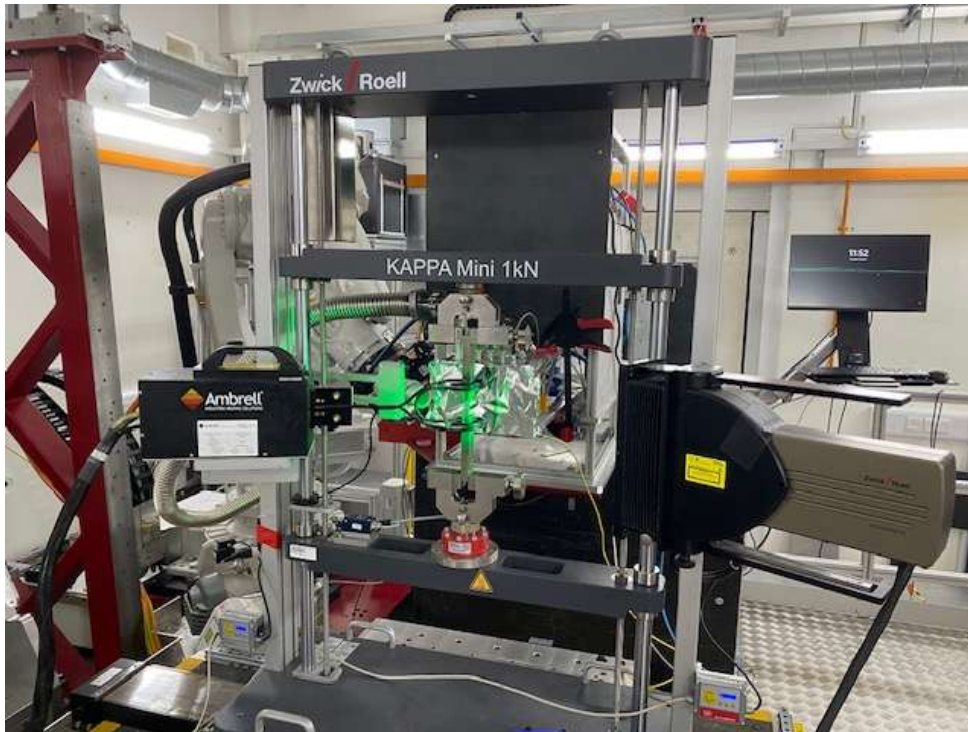
$$dc_H^m(x, r) = D \frac{\delta^2 c_H^m(x, r)}{\delta x^2} \quad \text{Hydrogen diffusion in the tube wall}$$

# Actual applications



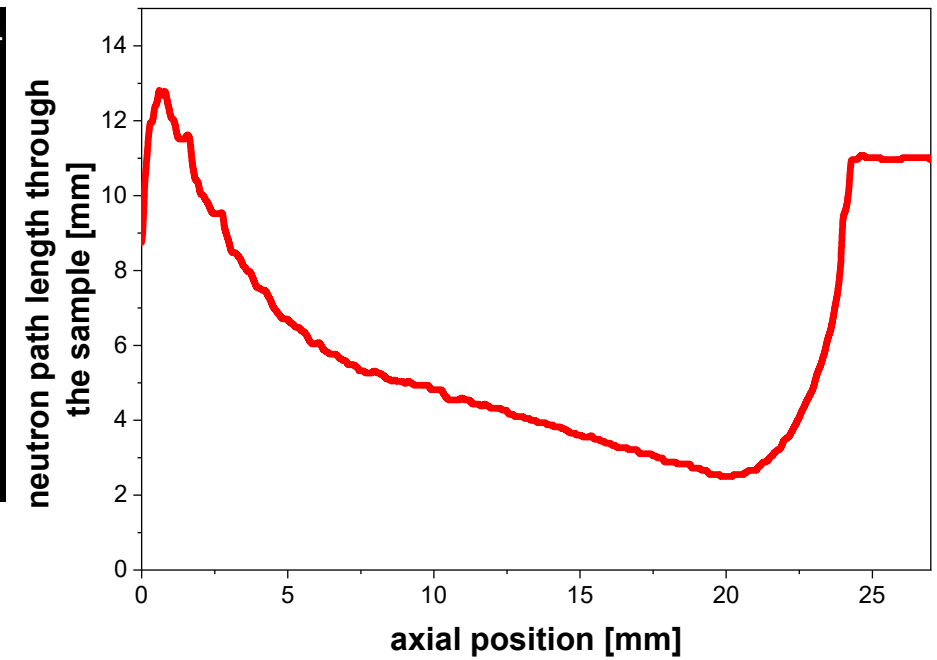
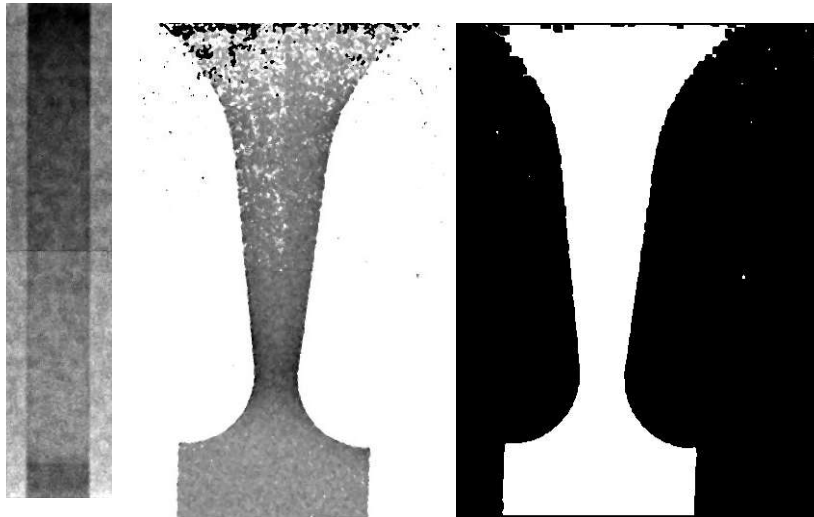
Neutron tomography measurements at SPIZWURZ samples at PorTO (ILL, France, September 2025)

# Actual applications



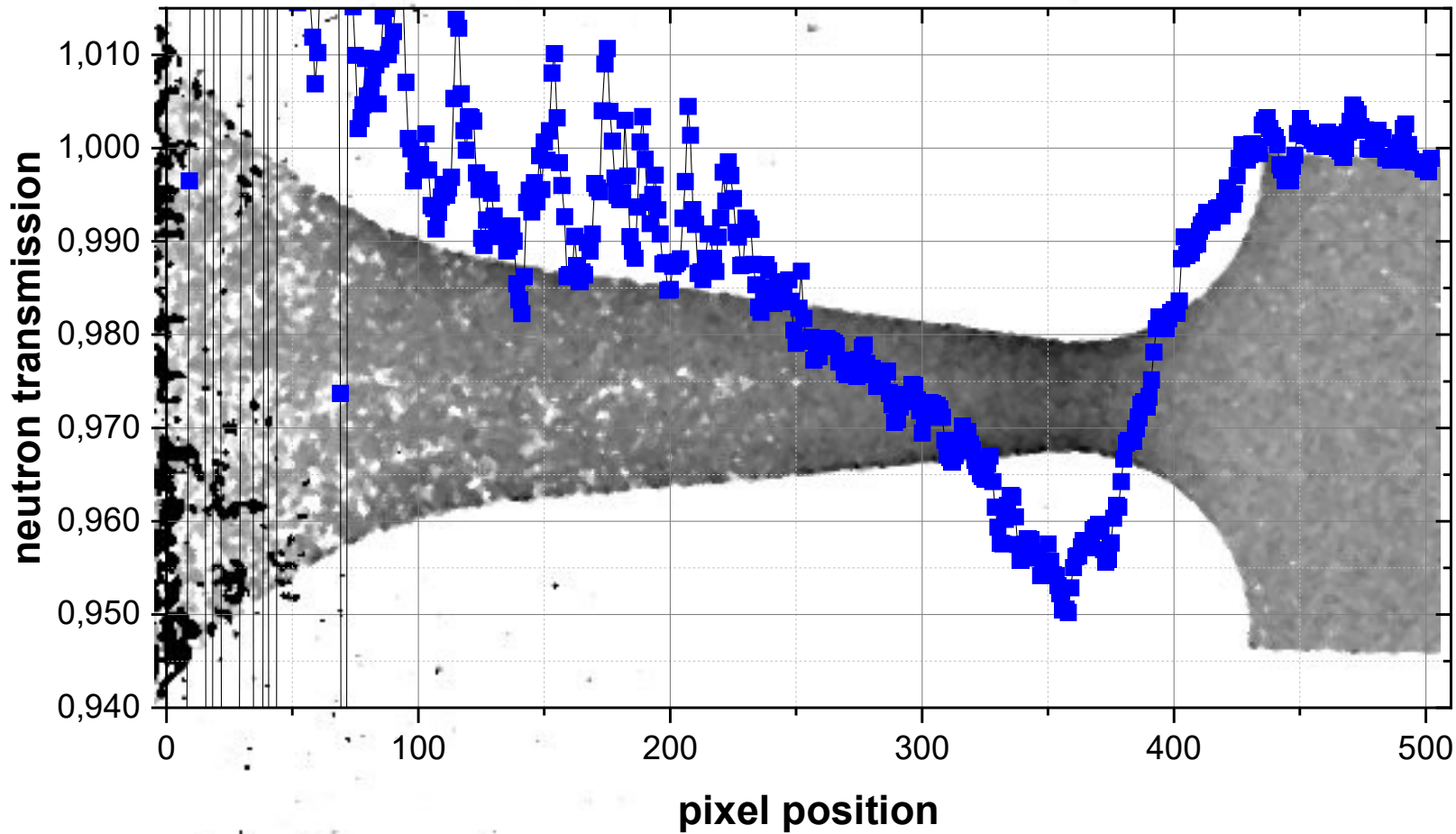
In-situ radiography measurements at the IMAT facility (ISIS, RAL, Harwell, UK, October 2025) with our INCHAMEL tensile machine

# Actual applications



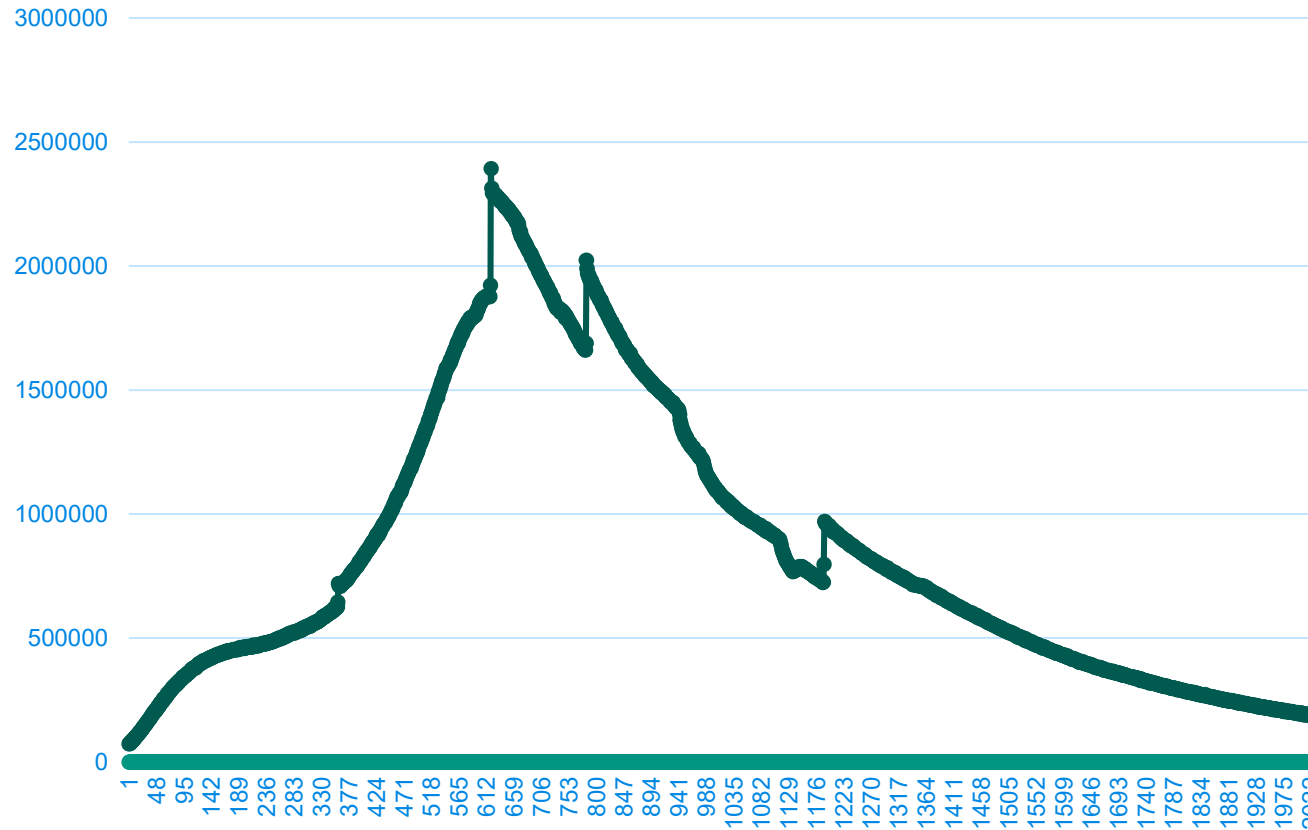
Tensile samples with stress/strain gradient

# Actual applications



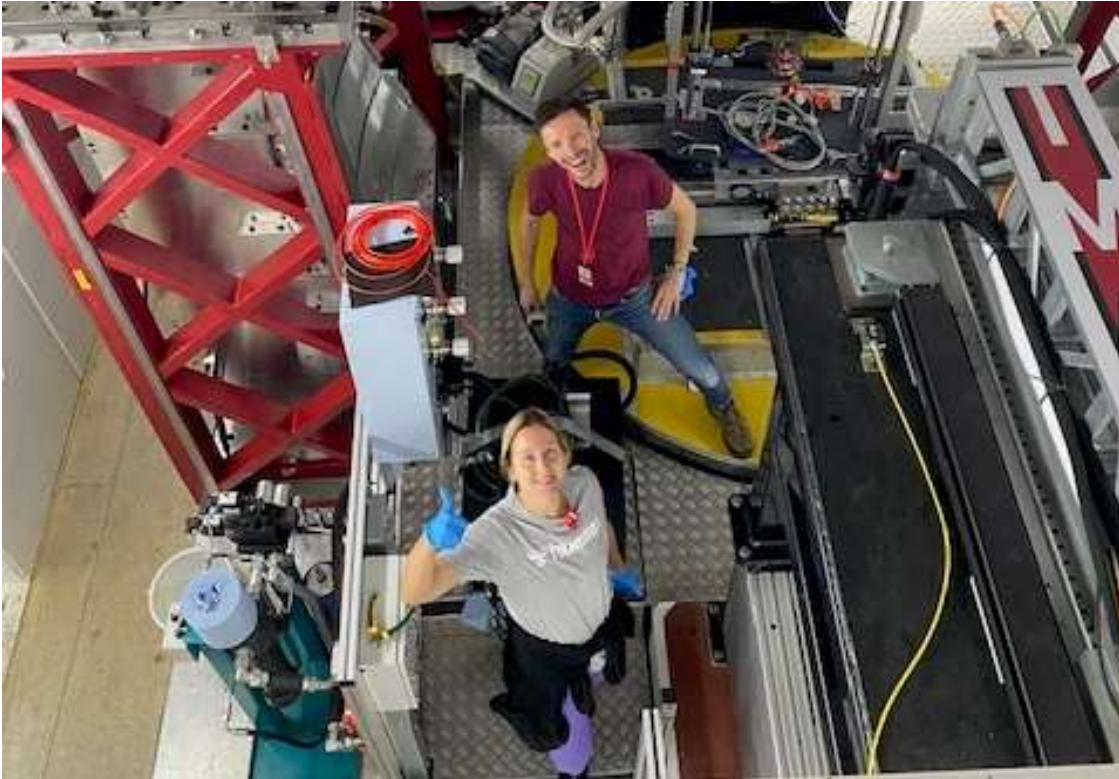
Distribution of the neutron transmission of the sample

# Actual applications



Bragg edges measured at the sample allowing to measure the strain, the temperature distribution and may be give hints on the hydrogen in solution

## Actual applications



We are happy about this results even the experimental setup has to be improved.

# People involved

- **Colleagues from KIT**
  - Sarah Weick
  - Conrado Roessger
  - Martin Steinbrueck
  - Ulrike Stegmaier
  - Chongchong Tang
  - Diana Bachurina
- **Placement or internchip students**
  - Marius van den Berg
  - Leaticia Ott
  - Camille Goulet
  - Enzo Muttini
  - Samuel Pulvermacher
  - Stefan Prestel

## Neutron Imaging Facilities

- ConRad @ HMI
  - Nikolai Kartschilov
- ANTARES @ TUM
  - Burkhard Schillinger, Michael Schulz
- ICON, NEUTRA and BOA @ PSI
  - Anders Kaetner, Pawel Trtik, David Mannes, Jan Hovid
- ENGINE-X and IMAT @ RAL
  - Javier Santisteban
  - Winfried Kockelmann, Sylvia Britto
- PorTo and NEXT @ ILL
  - Alessandro Tengattini, Anna Fredrigo,
  - Bratislav Lukic, Lukas Helfen

## Cooperations

- CNEA (Argentina)
  - Javier Santisteban
  - Pablo Vizcaino, Adrian Gomez, Sergio Soria, ...
- NECSA (South Africa)
  - Robert Nshirimana
- ASNR (France)
  - Martial Kpemou
  - Severine Guilbert
- CEA (France)
  - Frederic Ott
- PSI (Switzerland)
  - Johannes Bertsch, Stefan Valence, Weija Gong, Aaron Coldeweih, Okan Yetik, Liliana Duarte



# Acknowledgements

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**Thank you for your attention**



**Thorsten Hollands**

GRS

## **From QUENCH-01 to QUENCH-ATF-2: Three Decades of AC<sup>2</sup>/ATHLET-CD Validation using QUENCH Experiments**

For the development of software tools applied in the field of nuclear safety requirements and procedures are defined for quality assurance purposes. For example, the IAEA published a general document concerning requirements, that need to be fulfilled during code development, including verification and validation (IAEA SAFETY STANDARDS SERIES No. SSG-2). In general development, verification and validation should be separated, while the validation process should cover a phenomena orientated validation matrix, SET), and integral tests.

The QUENCH test matrix shows that several topics are covered in the history of the test series to investigate the material behaviour of fuel rod simulators during flooding of superheated cores. First, classical PWR tests were performed, followed by three tests focusing on B<sub>4</sub>C oxidation. Additionally, the scope was on the investigation of different cladding materials like E110, Zirlo™ or M5°. Furthermore, three air-ingress tests were conducted as well as one debris test. Beside one BWR test ATF claddings become focus of the latest test campaign. Starting with one test using FeCrAl cladding two tests were already performed and one severe accident experiment is pending on Cr-coated claddings in the frame of the OECD/NSC QUENCH-ATF project. Finally, LOCA tests were carried out using different claddings for scenarios up to extended DBA. Several tests were used as benchmarks or even one ISP.

Based on the performed test matrix at KIT a validation matrix was derived for AC<sup>2</sup>/ATHLET-CD which covers most of the conducted experiments leading to several simulations using different code versions from the very beginning of the QUENCH programme and code development up to latest developments – e. g. for Cr-coated claddings – by GRS as well as national partners like RUB and KIT since the late 1990s.

Current simulations using the last code version (ATHLET-CD 3.5) compared to one released in 2012 (ATHLET-CD 2.2C) show that for QUENCH-06 (ISP-45) with nearly no severe core damage the code version does not differ which approves an already good model basis at that time. For experiments with stronger core degradation like QUENCH-03 and -11 the current code version predicts e. g. less hydrogen compared to the older test. This might look strange, because newer code version should be better. And exactly this is the case, because an error during oxidation was fixed, but leads to less hydrogen. These results show that a permanent code validation on as much as possible experiments dealing with a wide range of phenomena and validity ranges of properties is necessary to ensure a good code performance.

# From QUENCH-01 to QUENCH-ATF-2: Three Decades of AC<sup>2</sup>/ATHLET-CD Validation using QUENCH Experiments

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Thorsten Hollands

30th International QUENCH Workshop

Karlsruhe Institute of Technology, Campus North

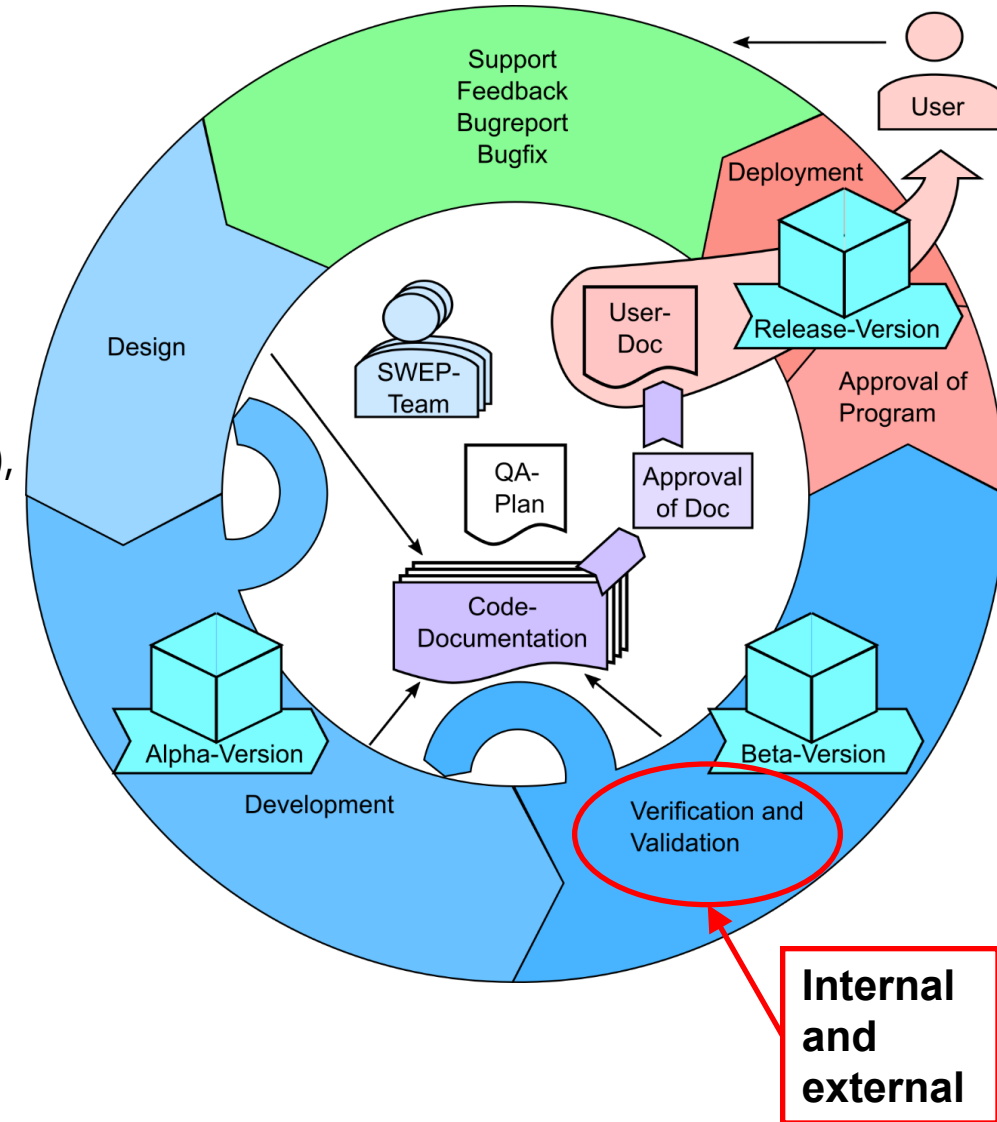
16-18 December 2025

# Outline

- Impact of QUENCH Experiments for ISP, Benchmarks and Code Validation
  - Validation of Computer Codes
  - QUENCH Matrix and Application
- Progress of AC<sup>2</sup>/ATHLET-CD Validation
  - Test Matrix
  - QUENCH-03
  - QUENCH-06
  - QUENCH-11
- Conclusions and Outlook

# General Guidelines for Computer Codes (IAEA SSG-2)

- QM Guidelines for computer programs.
- Separation of **Development and Verification vs. Validation**.
  - **Verification:** check, whether models are implemented correctly,
  - **Validation:** check, whether physical phenomena are described by the appropriate models (in terms of correctness),
    - Phenomena orientated validation matrix,
    - Single effect tests (SET): selected effects, clearly defined initial and boundary conditions, high instrumentation density and quality,
    - Integral tests: interaction of different effects, normally scaled test facilities, common special instrumentation.



# Validation of Computer Codes - Requirements for Code Validation

- IAEA SAFETY STANDARDS SERIES No. SSG-2
- OECD/CSNI In-Vessel Core Degradation Code Validation Matrix (NEA/CSNI/R(2000)21)
  - **Category 1** experiments are amongst the best qualified for code validation in their field. ISPs normally fall into this category. Data are well documented and boundary conditions are well defined (these conditions may be relaxed if there are specific unique features). Category 1 tests are strongly recommended for the validation of system codes (depending on their specific objectives)
  - **Category 2** experiments are well qualified for code validation, and could be used to increase the degree of confidence in a code's suitability for a given application. The experiment may not be unique, but valuable in the sense of parameter range.
  - **Category 3** and **4** were not considered due to the database and quality of the evaluated experiments.
  - **Cross References Matrices** were generated to evaluate the investigated experiments

# QUENCH Matrix and Application (I)

Experiment	Topic	Used for
QUENCH-01	partial fragmentation of pre-oxidized cladding	Validation
QUENCH-02	no additional pre-oxidation; quenching from high temperatures	Validation
QUENCH-03	delayed flooding; 240 s after temperature escalation has started	Validation
QUENCH-04	cool-down behavior of slightly pre-oxidized cladding by injected cold steam	Validation
QUENCH-05	cool-down behavior of pre-oxidized cladding by injected cold steam	Validation
QUENCH-06	prediction of H <sub>2</sub> source term by different code systems	<b>ISP-45</b>
QUENCH-07	impact of B4C absorber rod failure on H <sub>2</sub> , CO, CO <sub>2</sub> and CH <sub>4</sub> generation	Validation
QUENCH-08	Reference test to QU-07 without absorber rod	Validation
QUENCH-09	impact of B4C absorber rod failure on H <sub>2</sub> , CO, CO <sub>2</sub> and CH <sub>4</sub> generation in steam-starved conditions	Validation
QUENCH-10	air ingress during spent fuel storage container accident	<b>SARNET Benchmark</b>

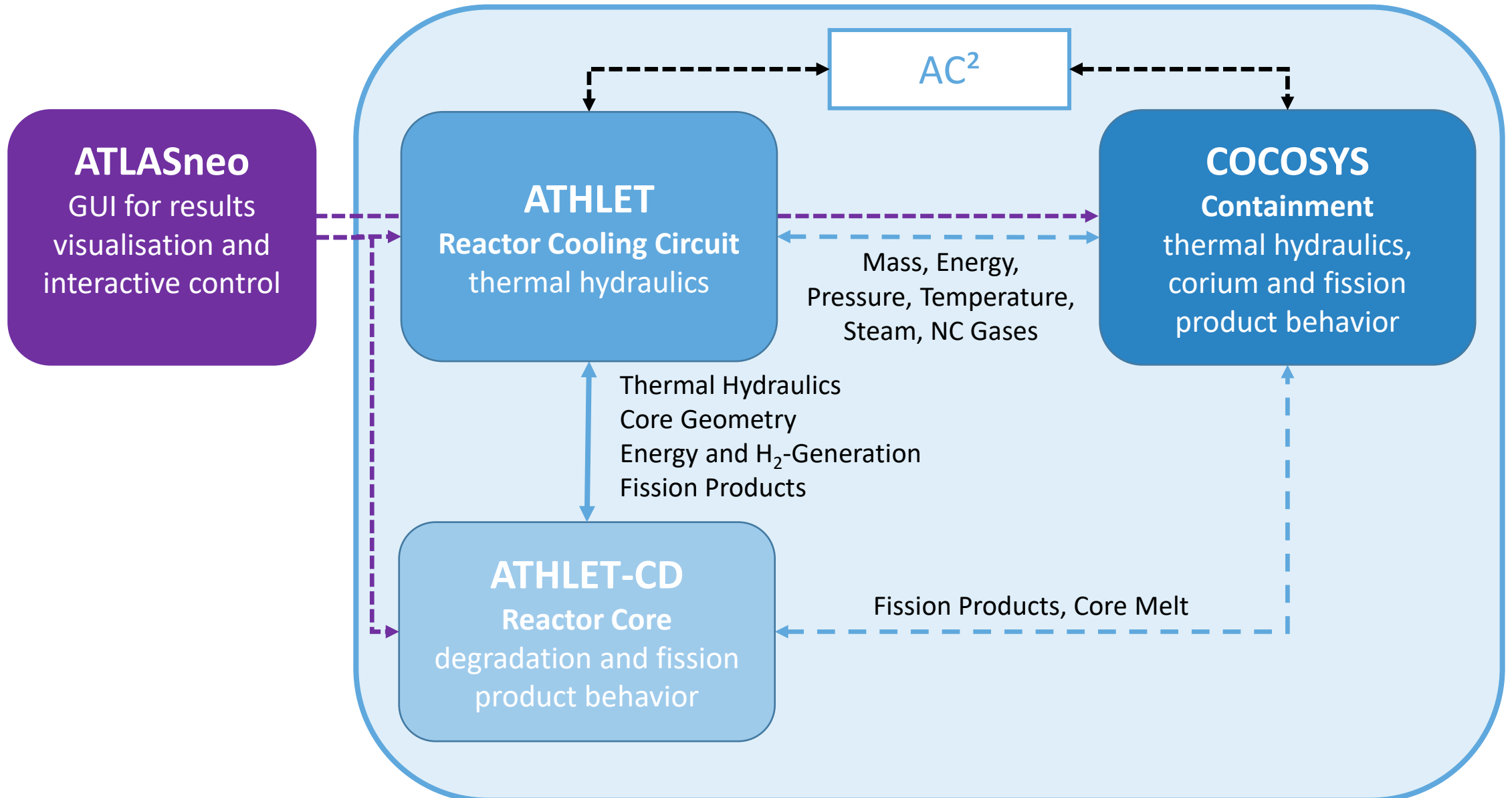
## QUENCH Matrix and Application (II)

Experiment	Topic	Used for
QUENCH-11	boil-off test with subsequent flooding	<b>SARNET Benchmark</b>
QUENCH-12	physico-chemical behavior of VVER type cladding (Zr1%Nb) during flooding	Validation
QUENCH-13	AgInCd absorber rod, aerosol	Validation
QUENCH-14	ACM series, M5 <sup>®</sup> cladding	Validation
QUENCH-15	ACM series, ZIRLO <sup>™</sup> cladding	Validation
QUENCH-16	air ingress	<b>SARNET Benchmark</b>
QUENCH-17	debris formation and coolability	Validation
QUENCH-18	air ingress, AgInCd absorber rods	<b>NUGENIA QUESA Benchmark</b>
QUENCH-19	ATF, FeCrAl cladding	<b>IAEA Benchmark</b>
QUENCH-20	BWR configuration	Validation

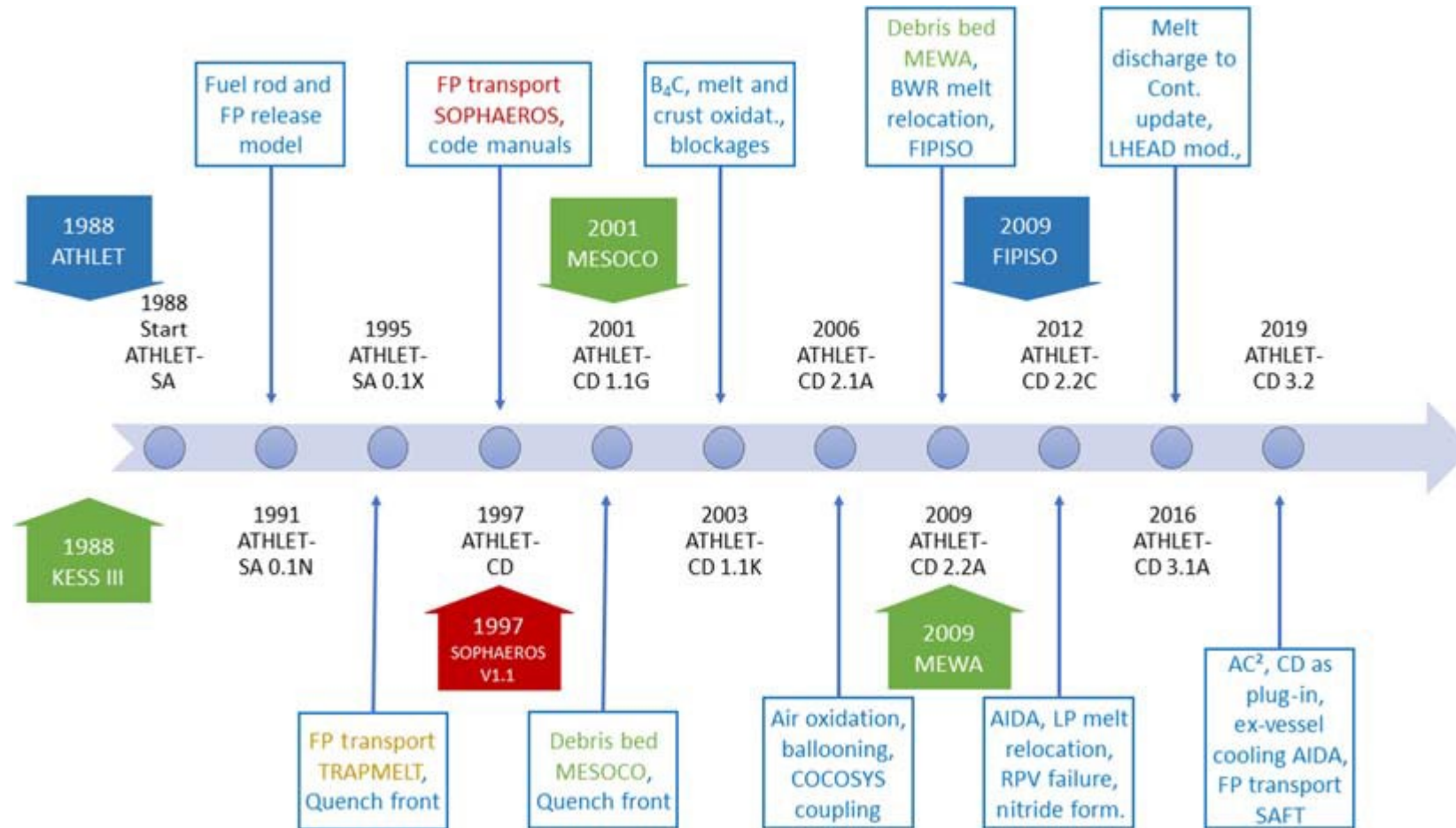


# QUENCH Matrix and Application – Special Test Series

Experiment	Topic	Used for
QUENCH-L0	LOCA bundle commissioning test with Zircaloy-4 claddings	Validation
QUENCH-L1	LOCA bundle reference test with Zircaloy-4 claddings	<b>IAEA FUMAC Benchmark</b>
QUENCH-L2	LOCA bundle test QUENCH-L2 with M5 <sup>®</sup> claddings	Validation
QUENCH-L3	LOCA bundle test with optimised ZIRLO <sup>™</sup> cladding	Validation
QUENCH-L3HT	Extended LOCA bundle test with optimised ZIRLO <sup>™</sup> cladding	Validation
QUENCH-L4	LOCA bundle test with pre-hydrogenated M5 <sup>®</sup> claddings	Validation
QUENCH-L5	LOCA bundle test with pre-hydrogenated optimised ZIRLO <sup>™</sup> claddings	Validation
QUENCH-ATF-1	Cr-coated, Extended DBA	<b>OECD QUENCH-ATF Benchmark</b>
QUENCH-ATF-2	Cr-coated, QUENCH-15 like scenario	<b>OECD QUENCH-ATF Benchmark</b>
QUENCH-ATF-3	Cr-coated, boil-off scenario with subsequent flooding	



# History of AC<sup>2</sup>/ATHLET-CD



# AC<sup>2</sup>/ATHLET-CD – QUENCH Validation Matrix (I)

Experiment	Calculations done by	Code Version	First Documented
QUENCH-01	GRS	1.2G	2001
QUENCH-03	RUB	1.1F, 1.2C	2001
QUENCH-04	RUB	3.1A	2002
QUENCH-05	RUB	1.1G	2002
QUENCH-06	GRS, RUB	1.1H, 3.2, 3.3	2002
QUENCH-07	GRS, RUB	1.1J, 2.0, 3.2	2006
QUENCH-08	GRS, RUB	1.1L, 2.1	2006
QUENCH-09	GRS	1.1K	2006
QUENCH-10	GRS	2.0B, 3.2	2006

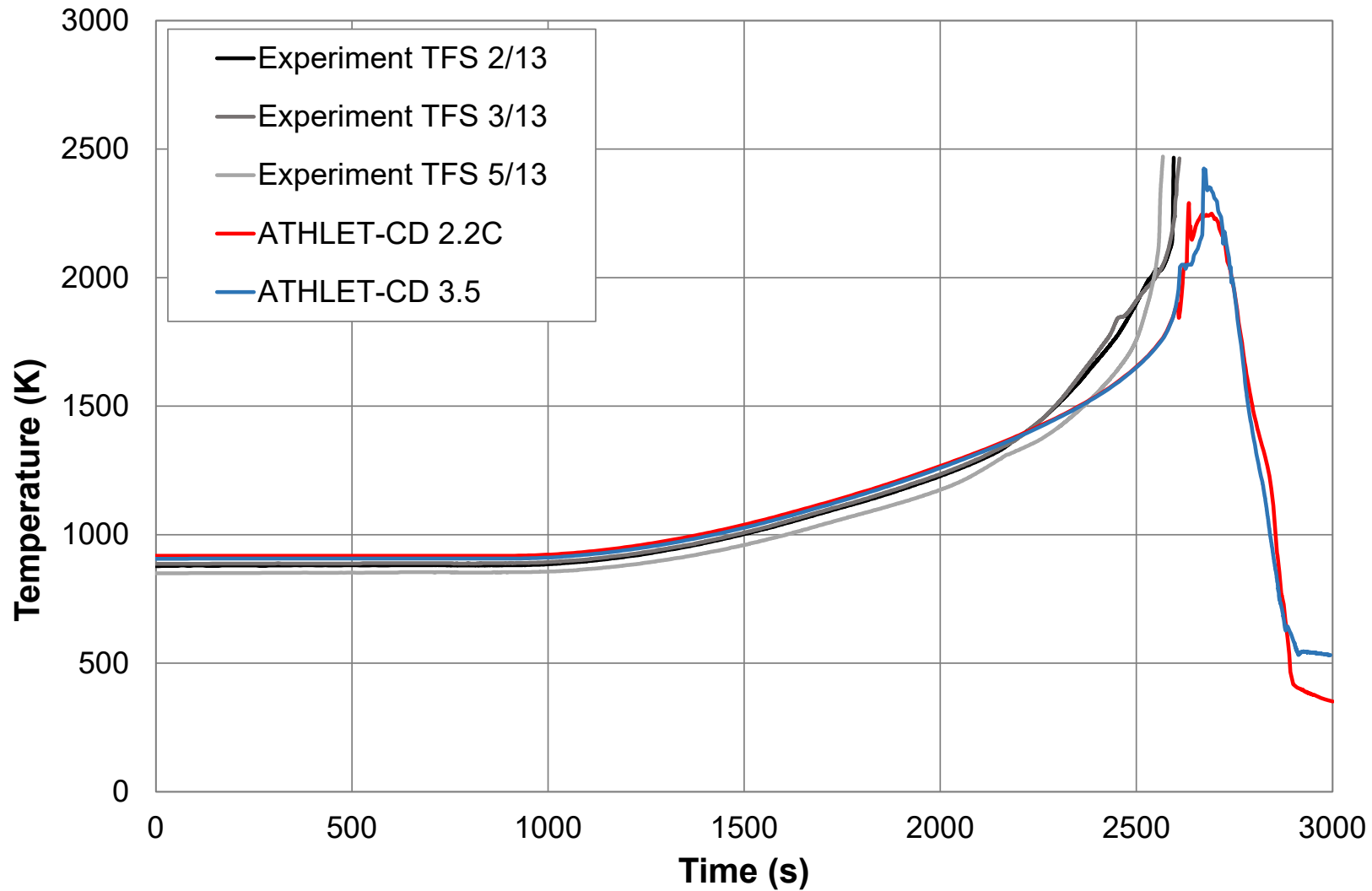
# AC<sup>2</sup>/ATHLET-CD – QUENCH Validation Matrix (II)

Experiment	Calculations done by	Code Version	First Documented
QUENCH-11	GRS, RUB	2.1A, 2.1B, 3.2	2006
QUENCH-12	RUB, KIT		2012
QUENCH-13	RUB	2.2A	2010
QUENCH-15	GRS	3.1A, 3.2	
QUENCH-16	GRS, RUB	2.2C, 3.2, 3.3	2012
QUENCH-17	GRS, RUB	2.2C	2016
QUENCH-18	GRS, RUB	3.1A, 3.2, 3.3	2018
QUENCH-19	GRS	3.2, 3.3.0, 3.3.1	2019
QUENCH-20	GRS	3.3.1	2022

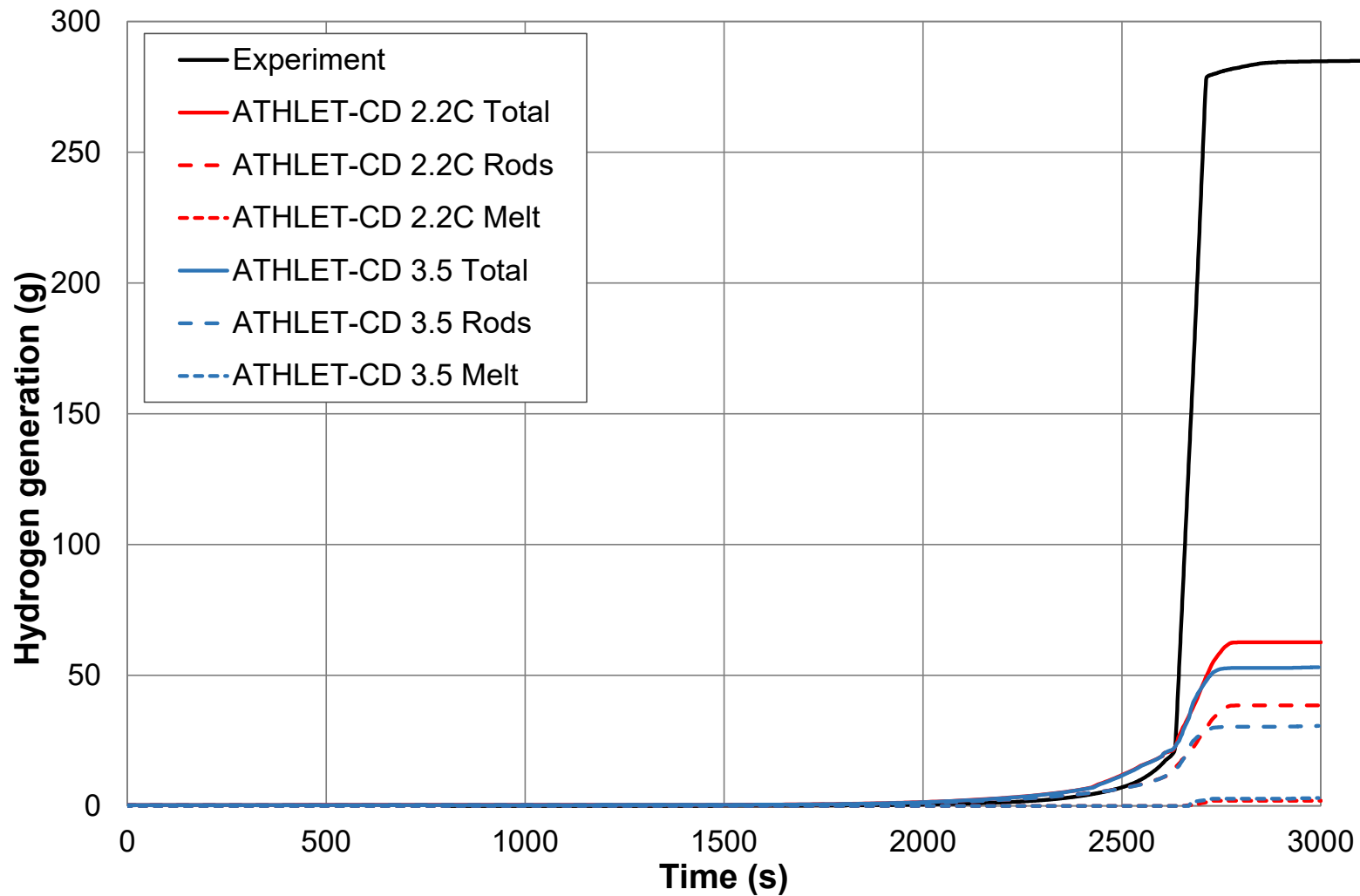
# AC<sup>2</sup>/ATHLET-CD – QUENCH Validation Matrix: Special Test Series

Experiment	Calculations done by	Code Version	First Documented
QUENCH-L0	GRS	3.1A	2016
QUENCH-L1	GRS	3.1A	2016
QUENCH-L2	GRS	3.1A	2015
QUENCH-L3	RUB	3.3	2022
QUENCH-L3HT	RUB	3.2.1, 3.3.0, 3.3.1	2022
QUENCH-ATF-1	GRS, RUB	3.3.0, 3.3.1	2024
QUENCH-ATF-2	GRS, RUB	3.3.1	2025

# QUENCH-03 – Temperatures at 950 mm

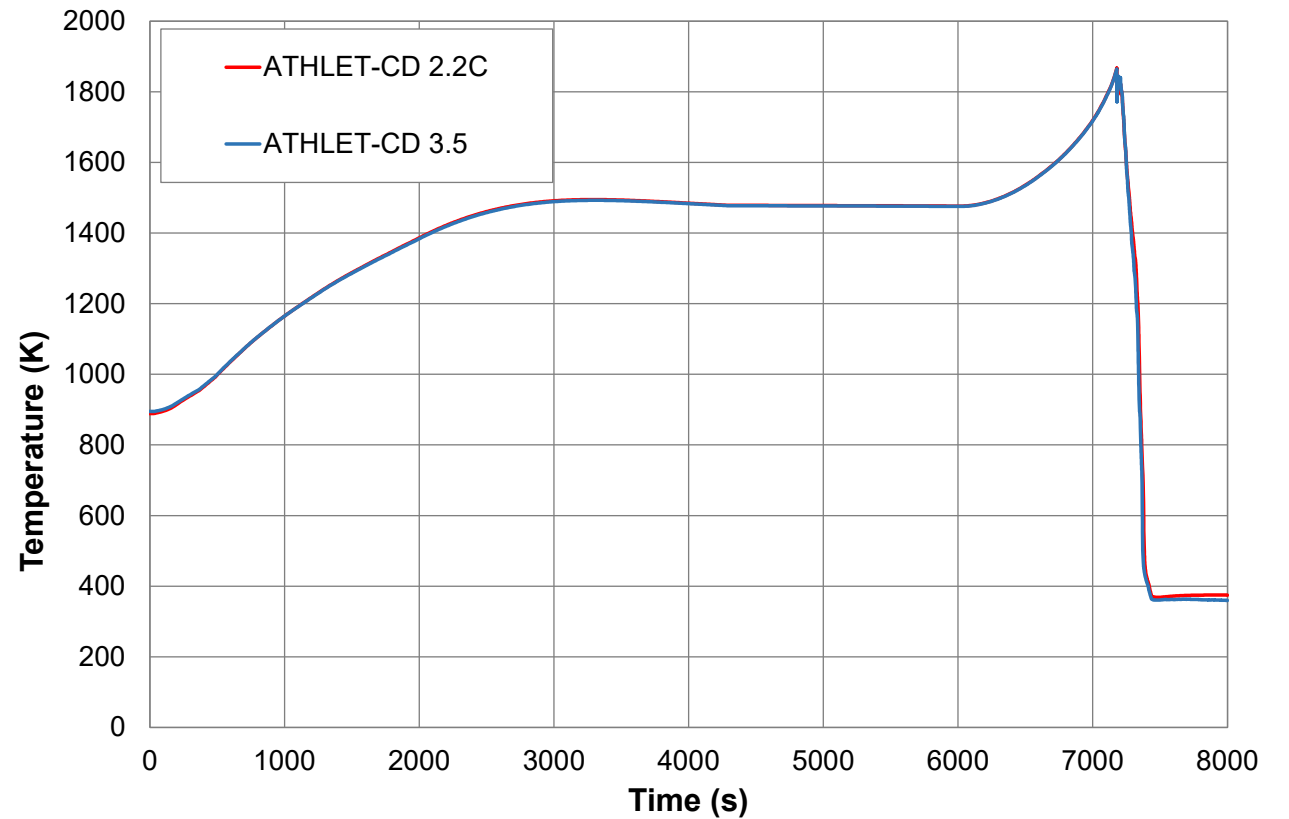
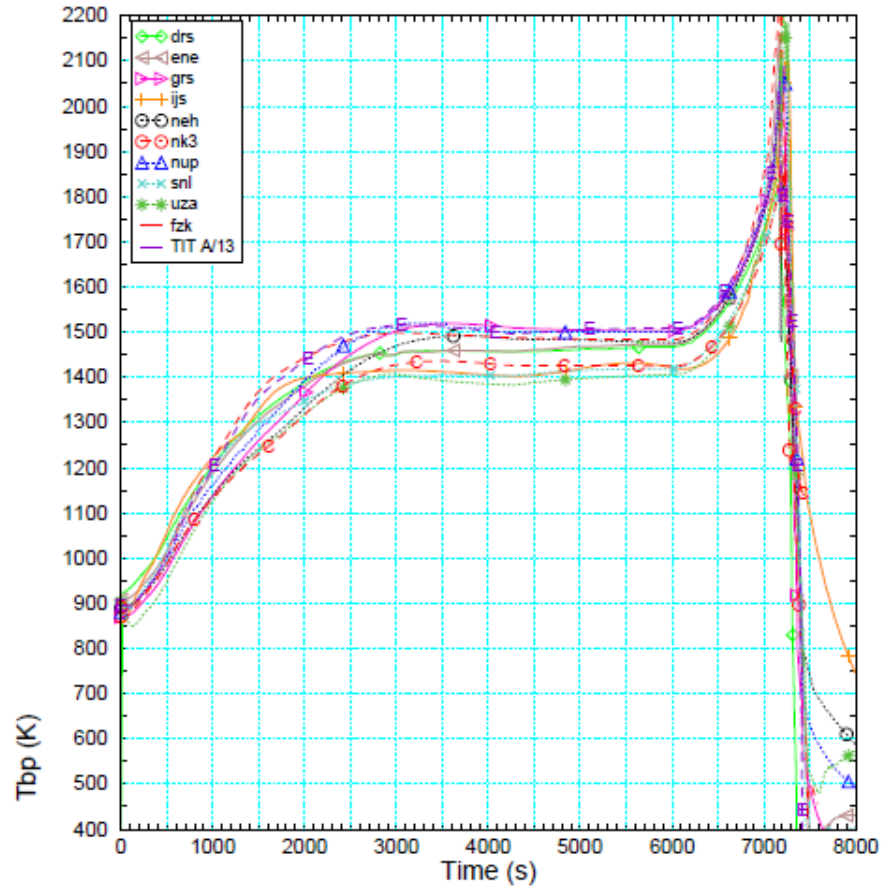


# QUENCH-03 – Hydrogen Generation

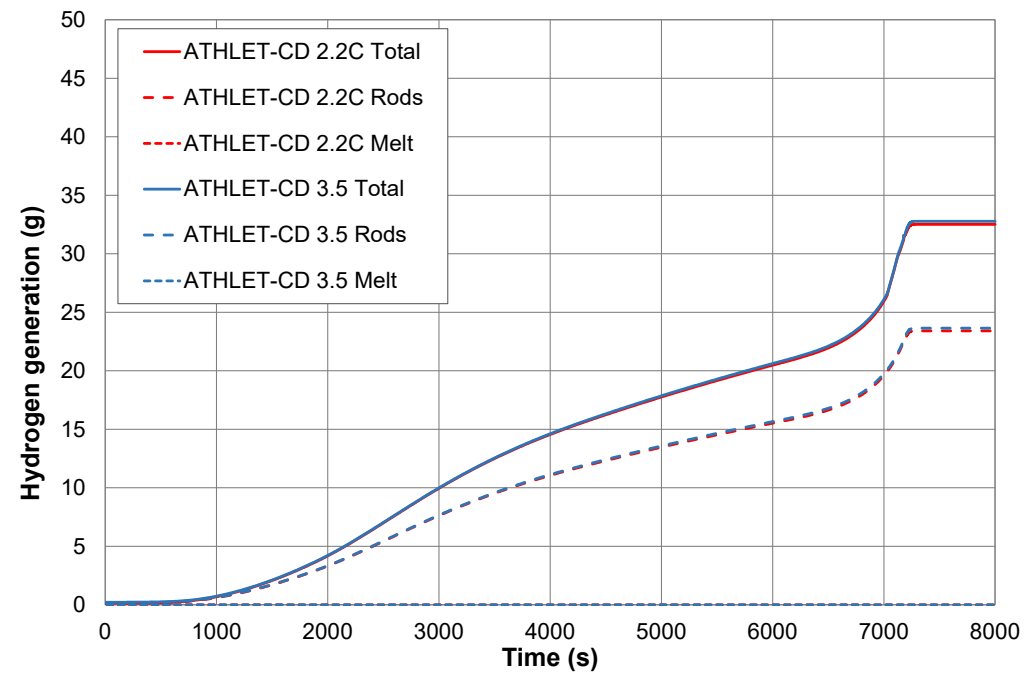
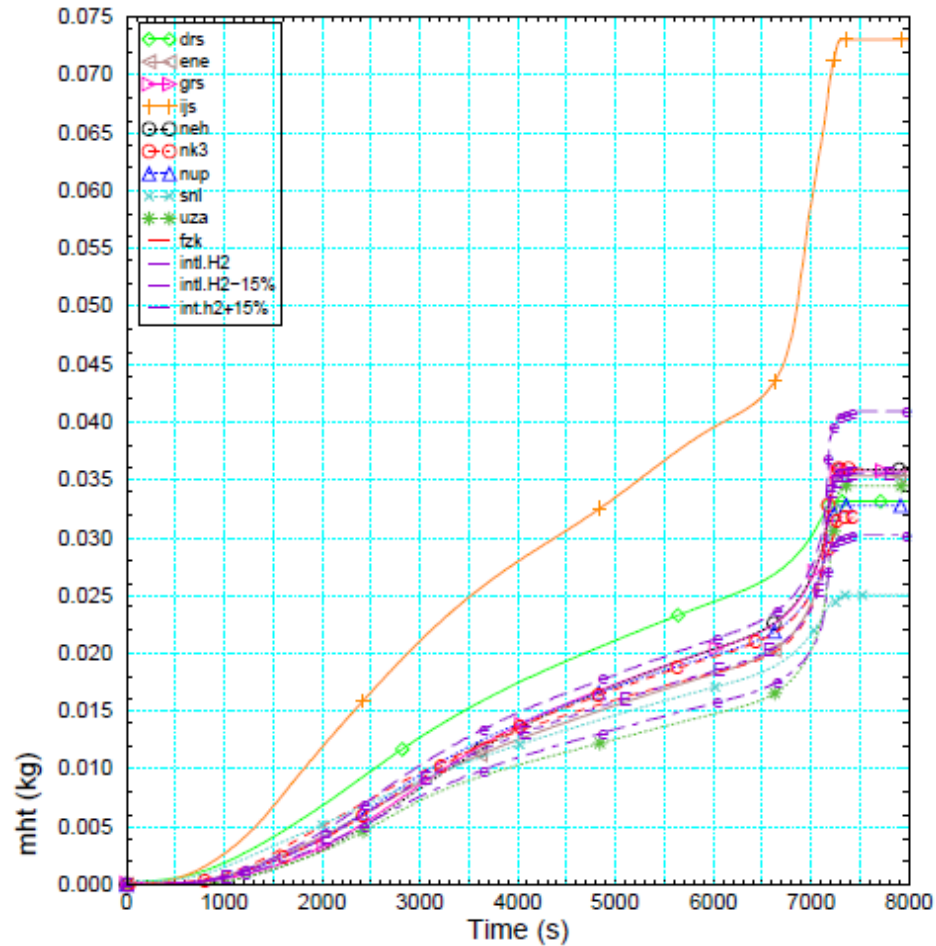




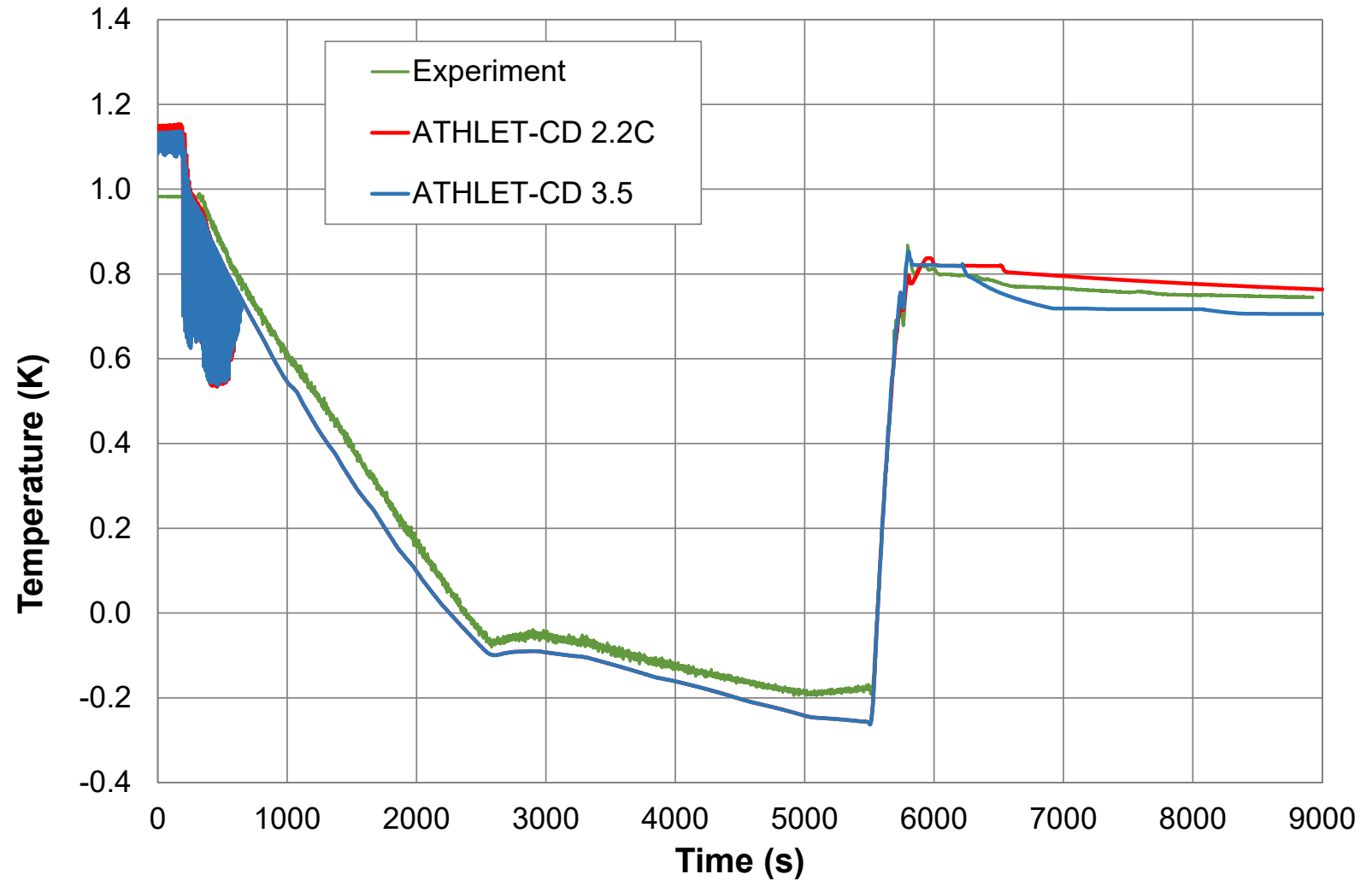
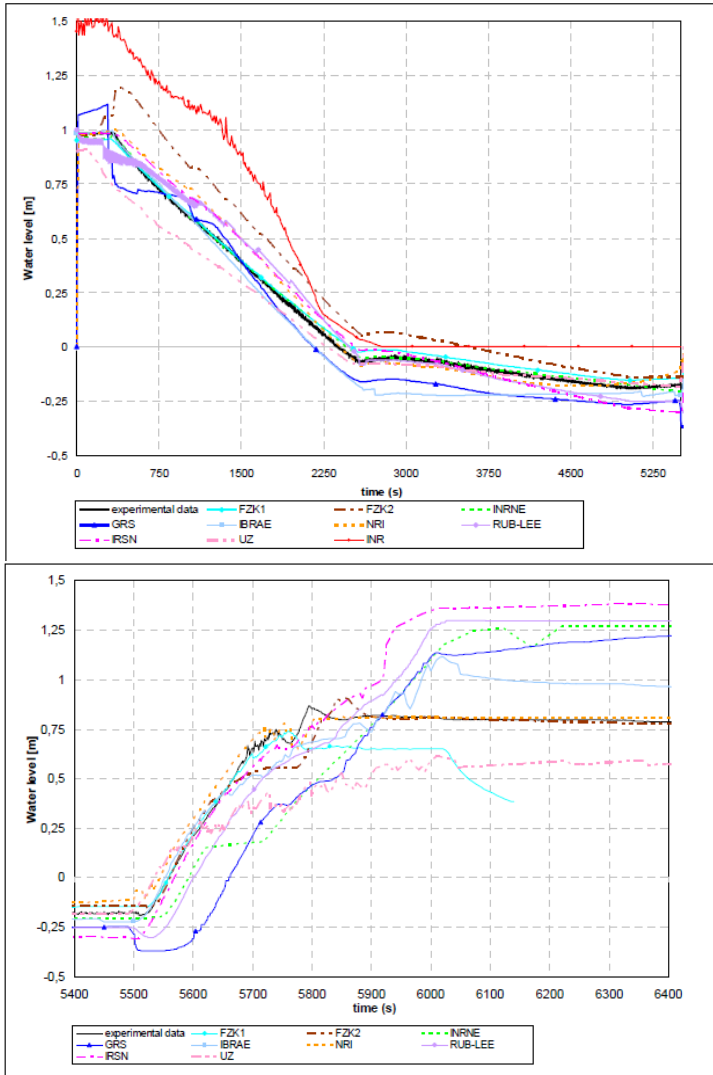
# QUENCH-06 – Temperatures at 950 mm



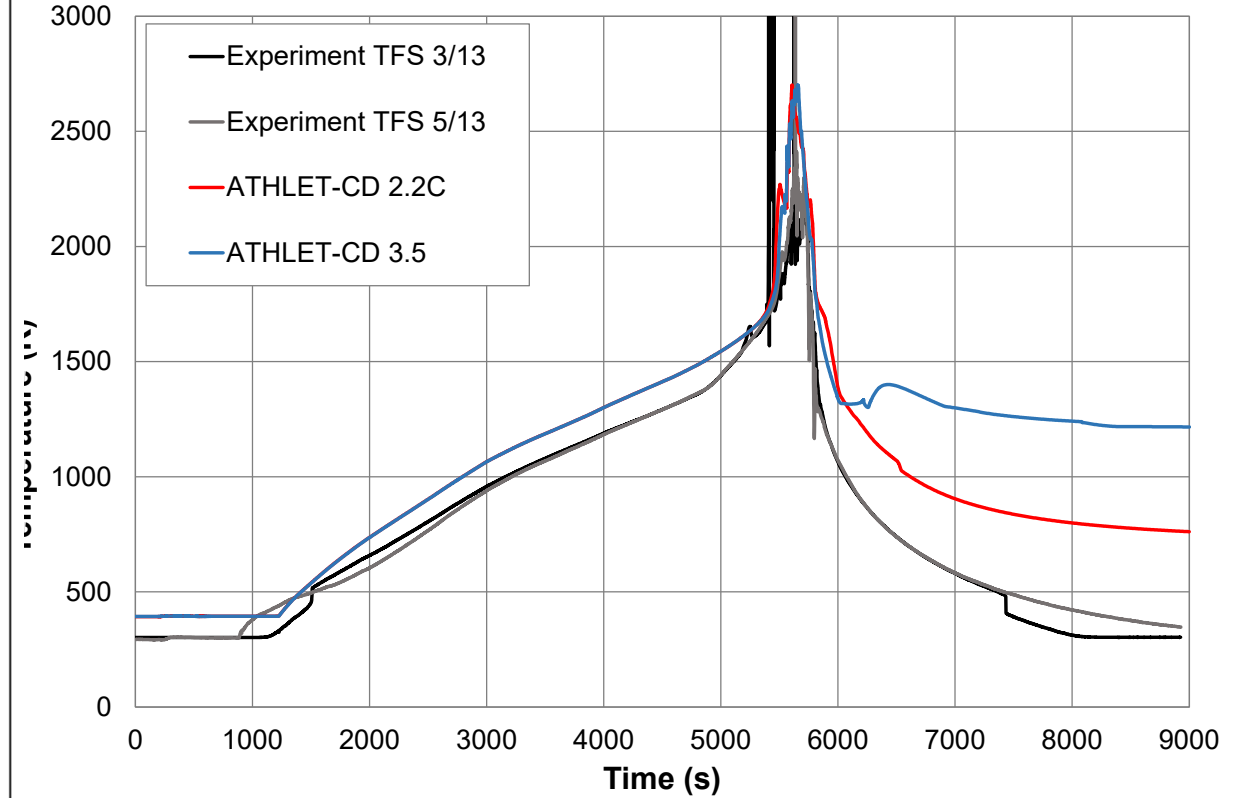
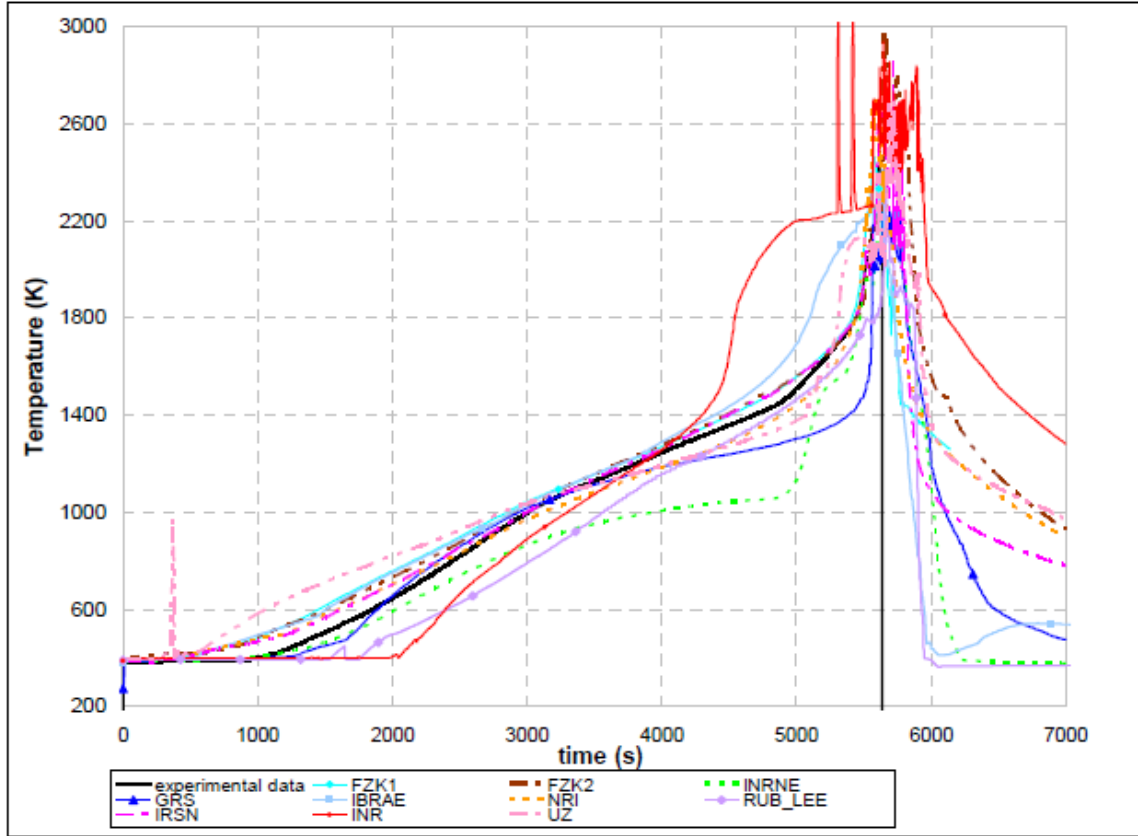
# QUENCH-06 – Hydrogen Generation



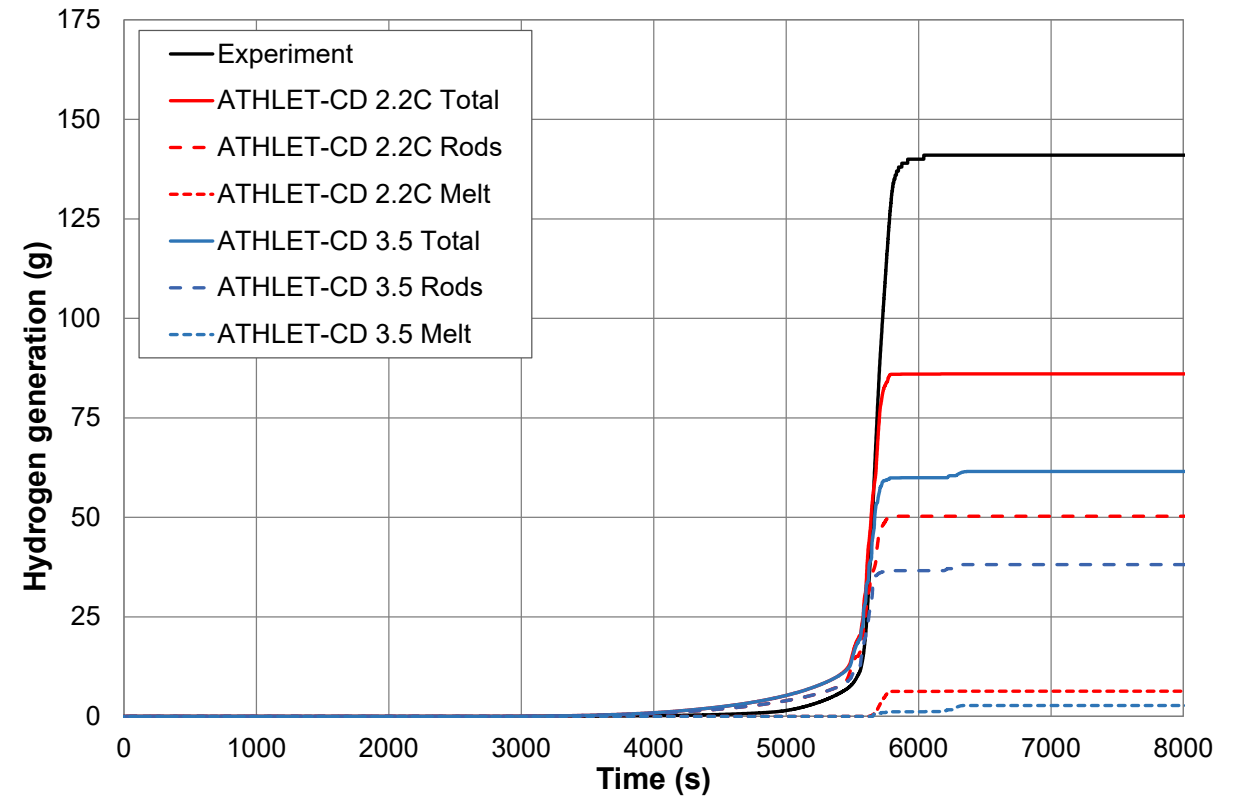
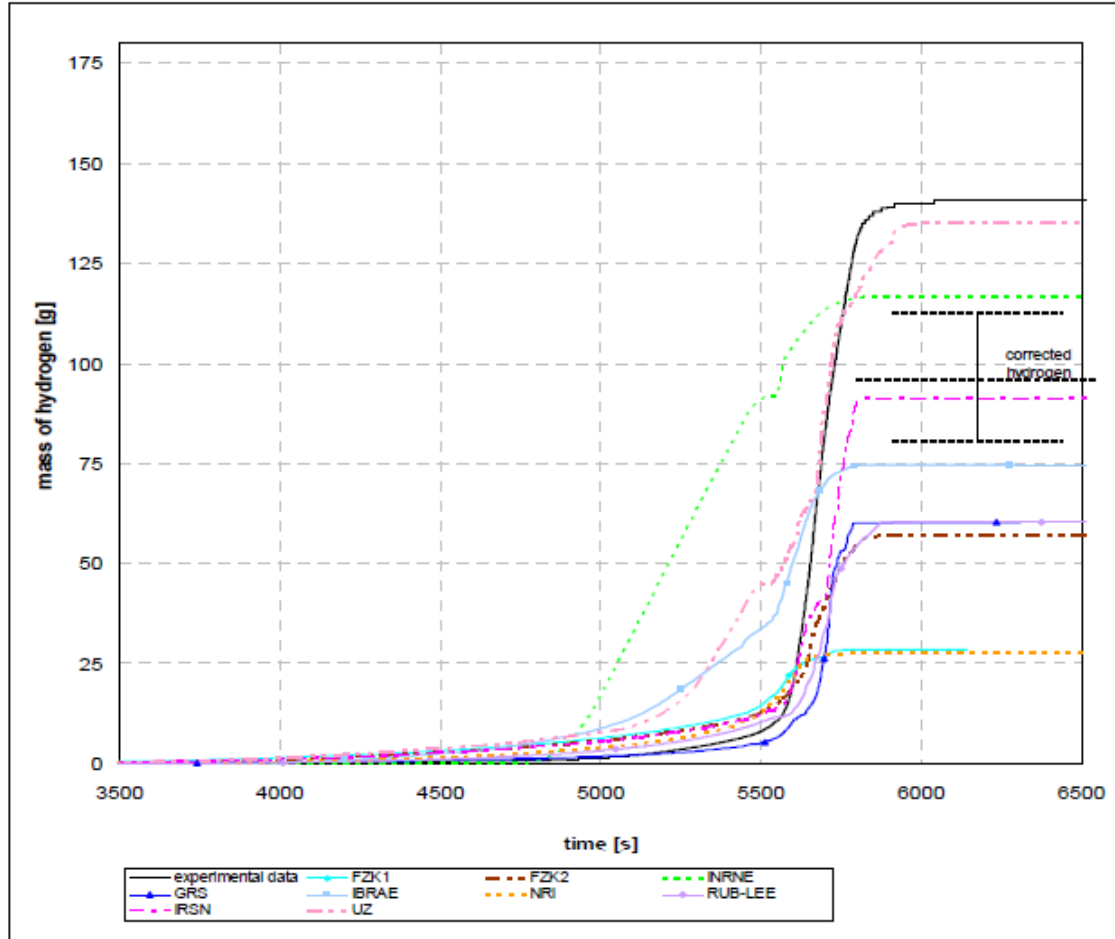
## QUENCH-11 – Water Level



# QUENCH-11 – Temperatures at 950 mm



# QUENCH-11 – Hydrogen Generation



# Conclusion and Outlook

- QUENCH tests are widely used for code validation
- One ISP and several Benchmarks on QUENCH tests were conducted
- Several topics are covered which led also to code improvements to be able to perform calculations
- This wide field of topics provides many data for code validation
- Beside the QUENCH tests for severe accident conditions also a series of LOCA tests was performed which was also used for code validation
- The new topics of QUENCH tests considering ATF rods are challenging for the codes, but this will again force model development and validation efforts
- **Nearly all QUENCH tests are used for AC<sup>2</sup>/ATHLET-CD code validation for app. 30 years and documented since 25 years**
- **The validation against QUENCH tests leads to a significant code improvement and robustness**
- **Hopefully, the data base for code validation will be further enlarged by performing several new QUENCH tests**

# Personal Remark

- First QWS participation in 2005  
Hidden somewhere in the back surrounded by a huge number of famous experts
- Fruitful discussions and collaborations for two decades with Martin, Juri, Mirko and the whole QUENCH team
- My Doctoral Thesis was based on KIT experiments
- Participation in some test conducts with some surprises
- **THANK YOU ALL FOR THE INTERSTING TIME AND GOOD LUCK FOR A SUCCESSFUL FUTURE OF QUENCH (or how it will be called) and a healthy retirement**



# Acknowledgements

The development, validation, qualification and application of AC<sup>2</sup> is funded by



Federal Ministry  
for the Environment, Climate Action,  
Nature Conservation and Nuclear Safety





**Mirco Große**

KIT

## **The SPIZWURZ project - overview and single effect tests**

The SPIZWURZ project is a cooperation between GRS, KIT-INE and KIT-IAM/AWP to investigate the hydrogen re-distribution and hydride re-orientation in cladding tubes under long-term dry storage conditions.

The paper gives first an overview about the project. Later, the measurements of the stress/strain induced by the pellets on the cladding tube of a spent fuel rod stored for more than 35 years as well as of separate effect tests of the parameters influencing hydrogen diffusion and solubility were presented.

The investigations of the spent fuel rod segment show that no significant stress is induced by the fuel on the cladding.

In preparation of the bundle test, the influence of annealing on the tensile properties of the cladding tubes was studied. Annealing at 450°C up to 14 h has only a small influence on the stress – strain curves measured. Annealing at 500°C for one hour reduces the yield stress by more than 25%. It can be concluded that the maximal temperature of the hydrogen loading is 450°C.

Results of the investigations of the hydrogen diffusion in zirconium single crystal depending on their orientation as well as the effect of elastic stress on the hydrogen solubility were presented too. Significant differences in the diffusion rate between the a and the c direction of the hexagonal lattice were found in the measurements at the single crystals. A hydrogen enrichment at the highest elastic stress were detected in a sample with stress gradient. The experimental setup of both studies should be improved to get more reliable results.

An outlook on future investigations and the SPIZWURZ+ project proposal submitted is given at the end of the presentation.

# The SPIZWURZ project - overview and single effect tests

Mirco Grosse, Sarah Weick, Michel Herm

30. Intern. QUENCH Workshop,  
KIT Campus North, 2025/12/18



# Overview

- **SPIZWURZ** = **S**pannungsinduzierte **W**asserstoffumlagerung während Langzeit-**Z**wischenlagerung” (stress induced hydrogen re-distribution during long-term intermediate storage).
- Cooperation between GRS, KIT INE and KIT IAM-AWP
- Duration 06/2020 – 04/2025

Supported by:



Federal Ministry  
for the Environment, Nature Conservation,  
Nuclear Safety and Consumer Protection

FKZ RS1586A/1501609B

based on a decision of  
the German Bundestag



Credit: Audrius Meskauskas

Purpurner Enzian (Spitzwurz)

Purple gentian

# Overview

Hydrogen behaviour in cladding tubes

KIT IAM-AWP

Combination and evaluation

GRS

Stress states between fuel and cladding tube of irradiated fuel rods

KIT-INE

Separate effect tests

Bundle test

Modelling

Pre-calculation bundle test

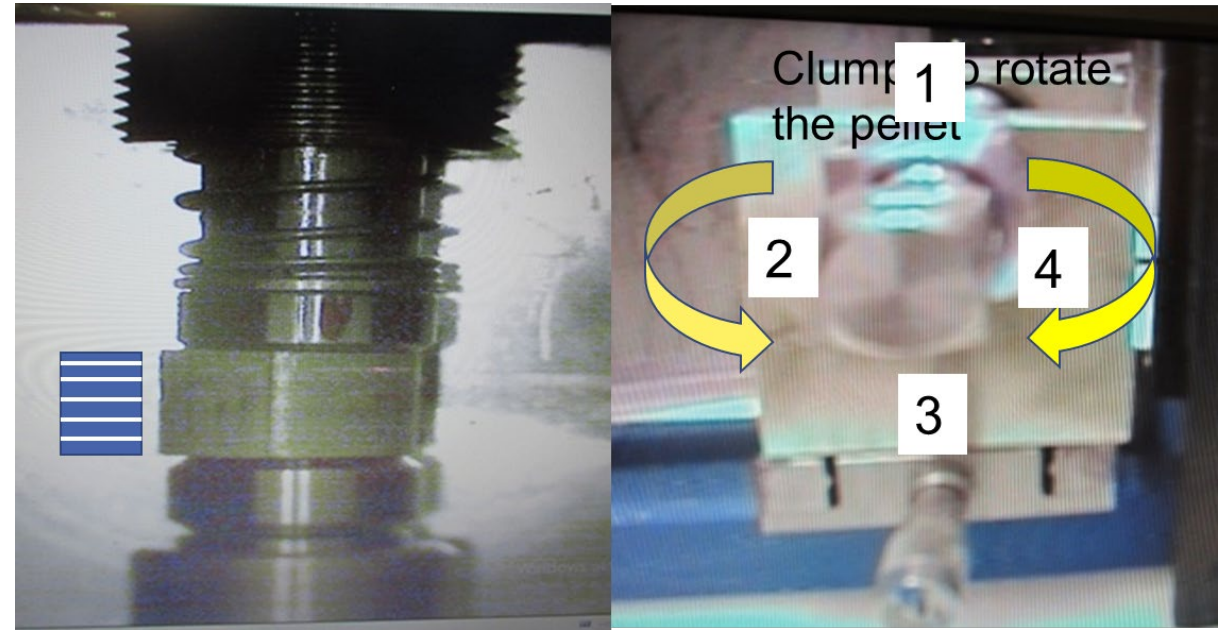
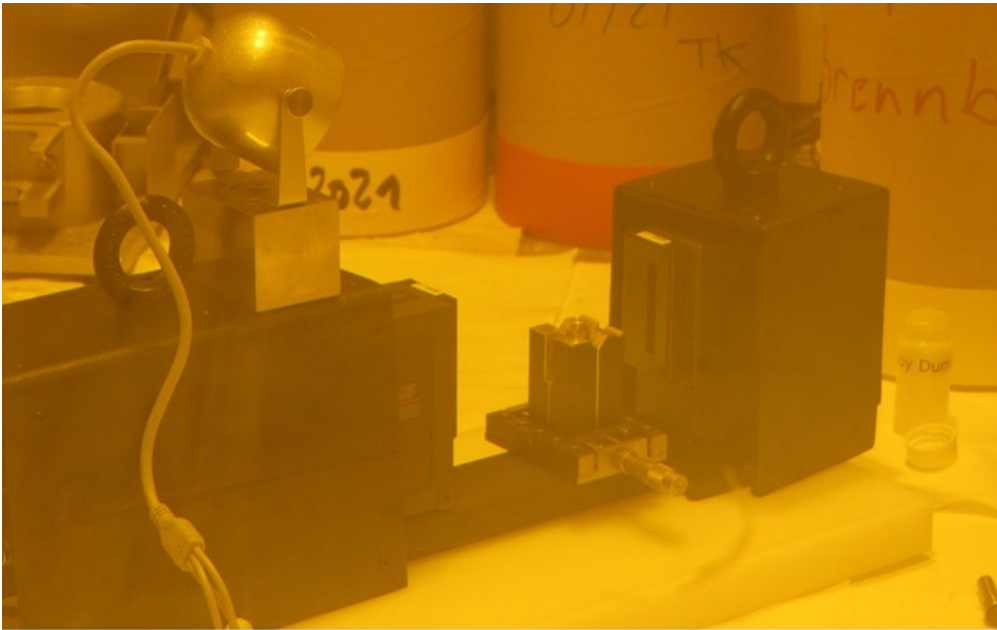
Pre-calculation mech. pellet cladding interaction

Blind benchmark

Open benchmark

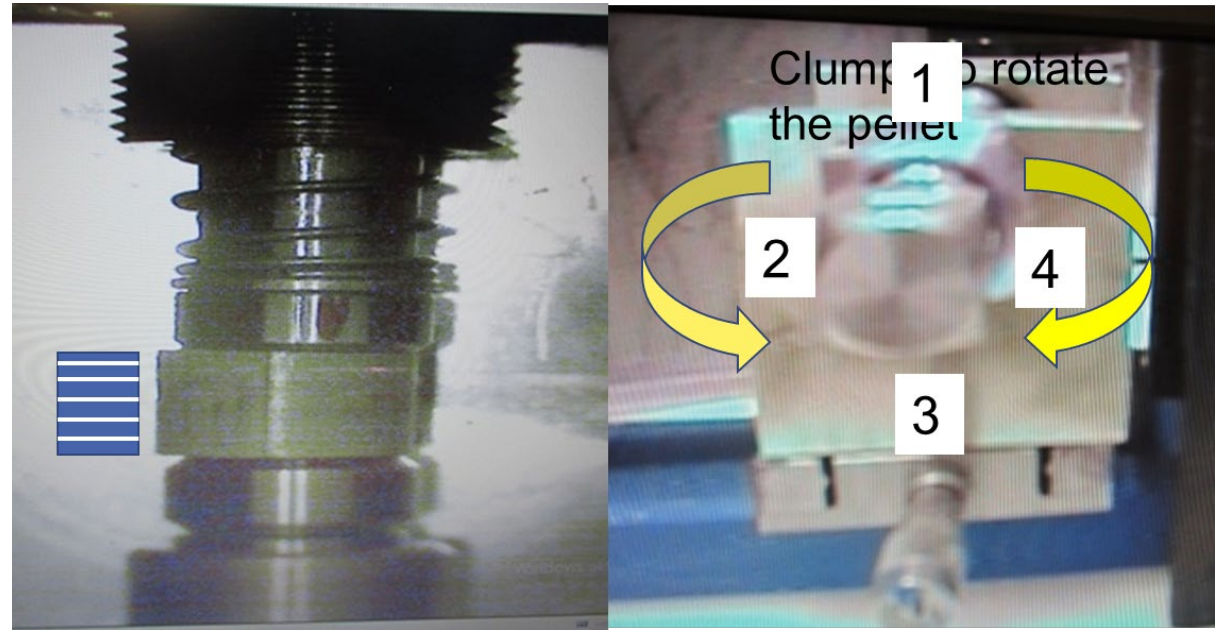
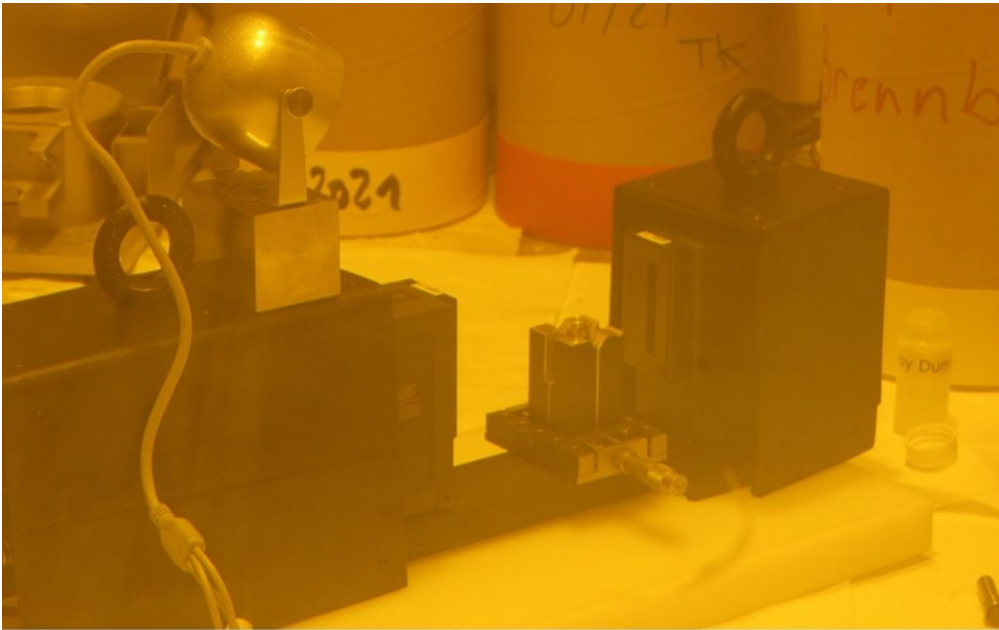
Measurements of the cladding strain with and w/o fuel in an irradiated fuel rod segment

# Stress states between fuel and cladding tube of irradiated fuel rods



- Diameter measurements at 5 axial positions, 8 circumferential positions, 6 measurements per positions
- Chemical removing of the fuel by 50% HNO<sub>3</sub>
- Repeating the diameter measurements

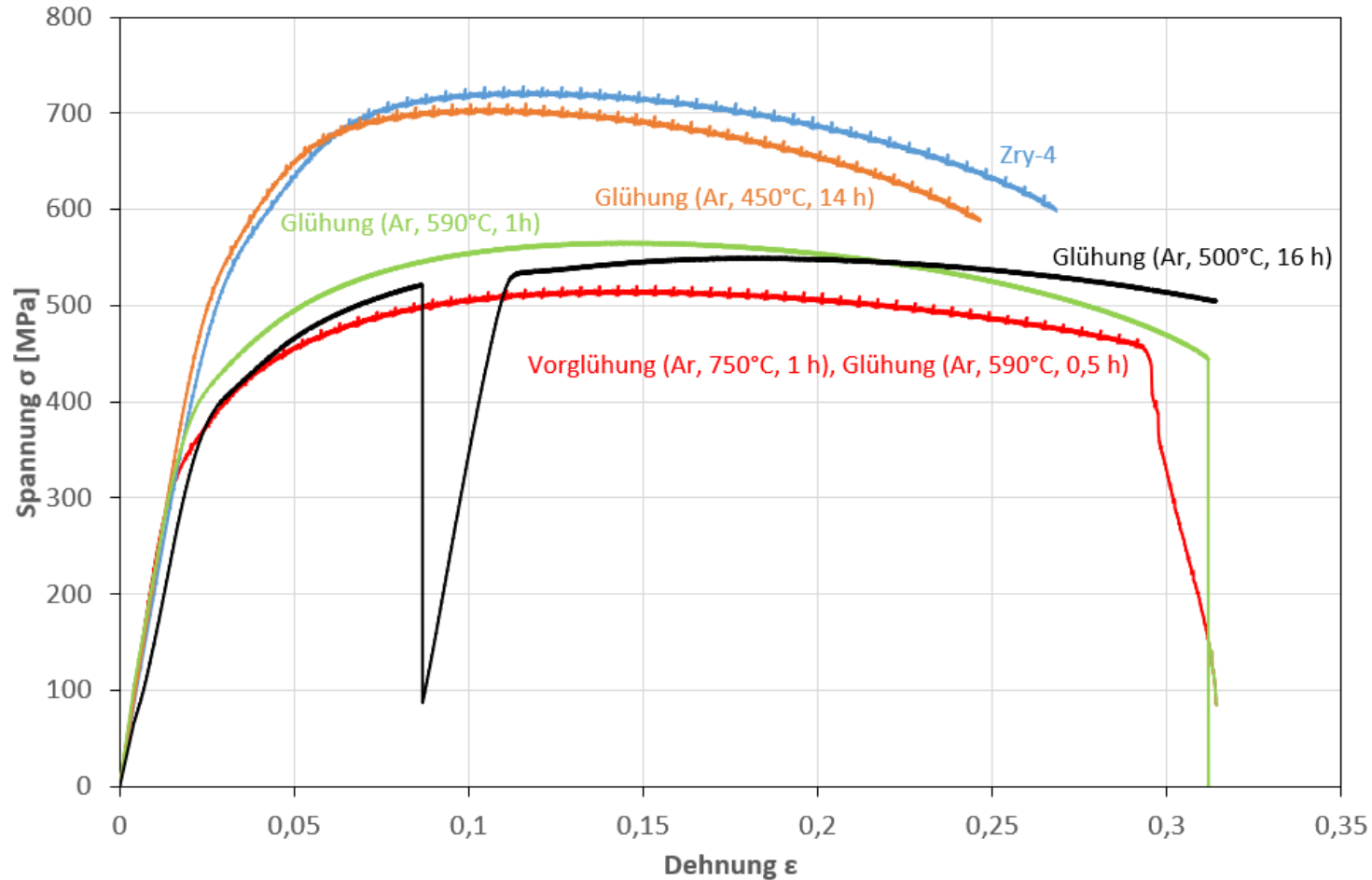
# Stress states between fuel and cladding tube of irradiated fuel rods



Nominal diameter:  $10.750 \pm 0.050$  mm  
Diameter with pellets:  $10.700 \pm 0.003$  mm (slightly oval (30 .. 50  $\mu\text{m}$ ))  
Strain after removing the pellets:  $3.3 \pm 3.1$   $\mu\text{m}$

**The pellets do not induce significant elastic stress/strain to the cladding.**

# Separate effect tests

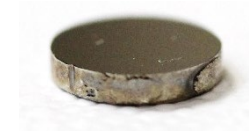


Maximal loading  
temperature: 450°C

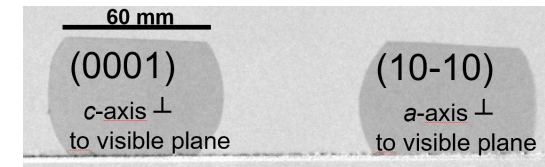
- Stress/strain curves measured at tensile tests at RT to prepare the hydrogen loading of the tubes for the bundle test

# Separate effect tests – Diffusion in Zr single crystals

- Zr single crystals, 6 mm diameter, 1 mm thickness with defined orientation ((0 0 0 1) and (1 0 -1 0) normal to the disc plane)
- Measurements of the circumferential orientation by means of XRD
- Grinding to a more rectangular shape
- Oxidation in Ar/O<sub>2</sub>
- Removing of the oxide layer at one side
- Annealing in H<sub>2</sub>
- Neutron radiography measurements at IMAT (ISIS, RAL, UK)



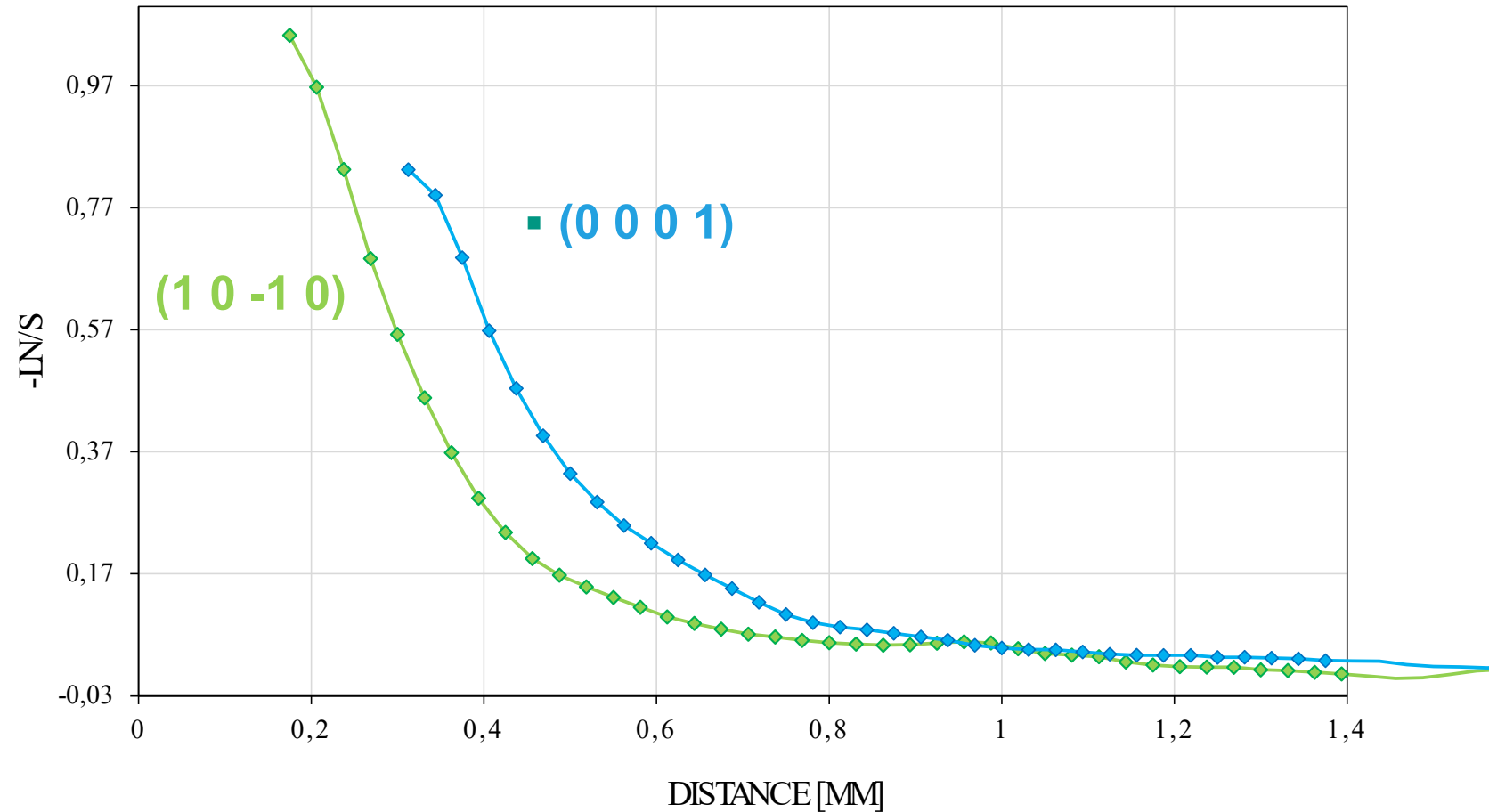
6 mm





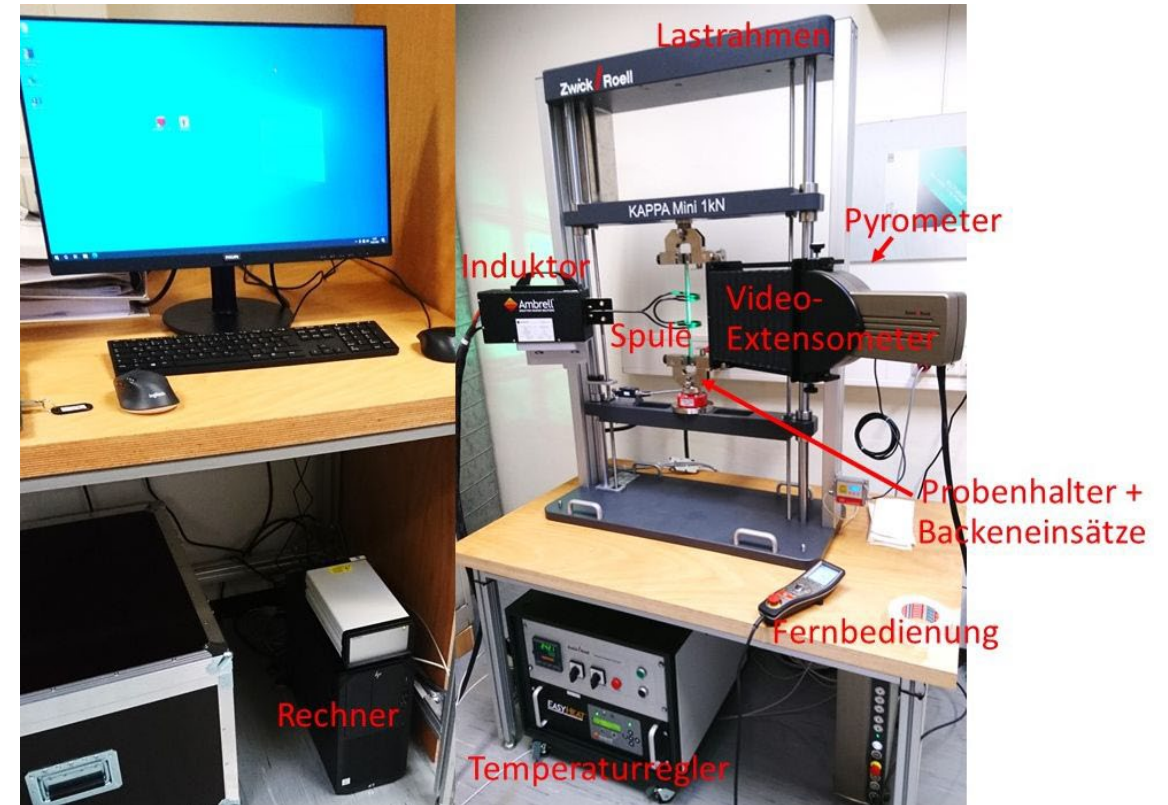
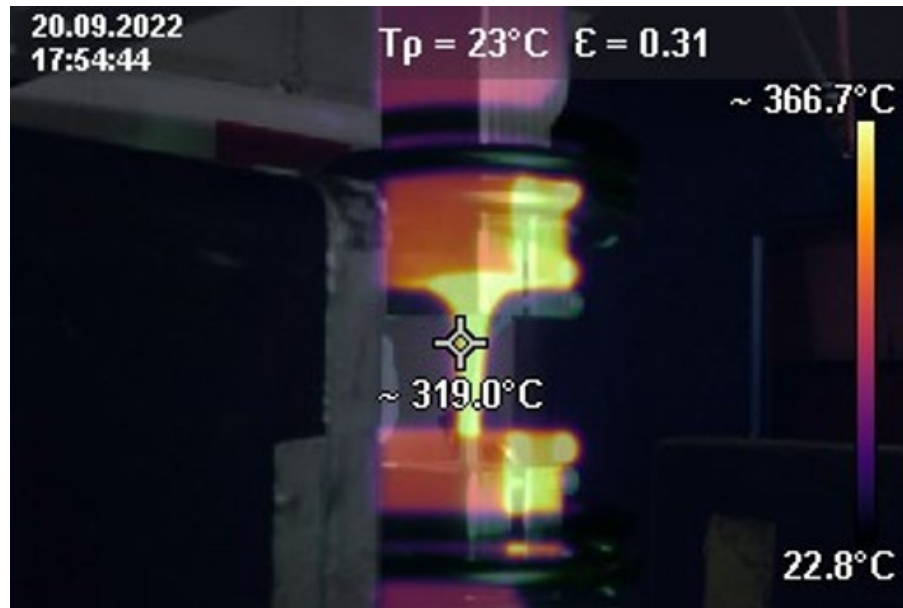
# Separate effect tests – Diffusion in Zr single crystals

- Faster diffusion in the c direction (0 0 0 1) than in the a direction (1 0 -1 0)
- Uncertainties when the hydrogen uptake starts
- In-situ investigations are needed



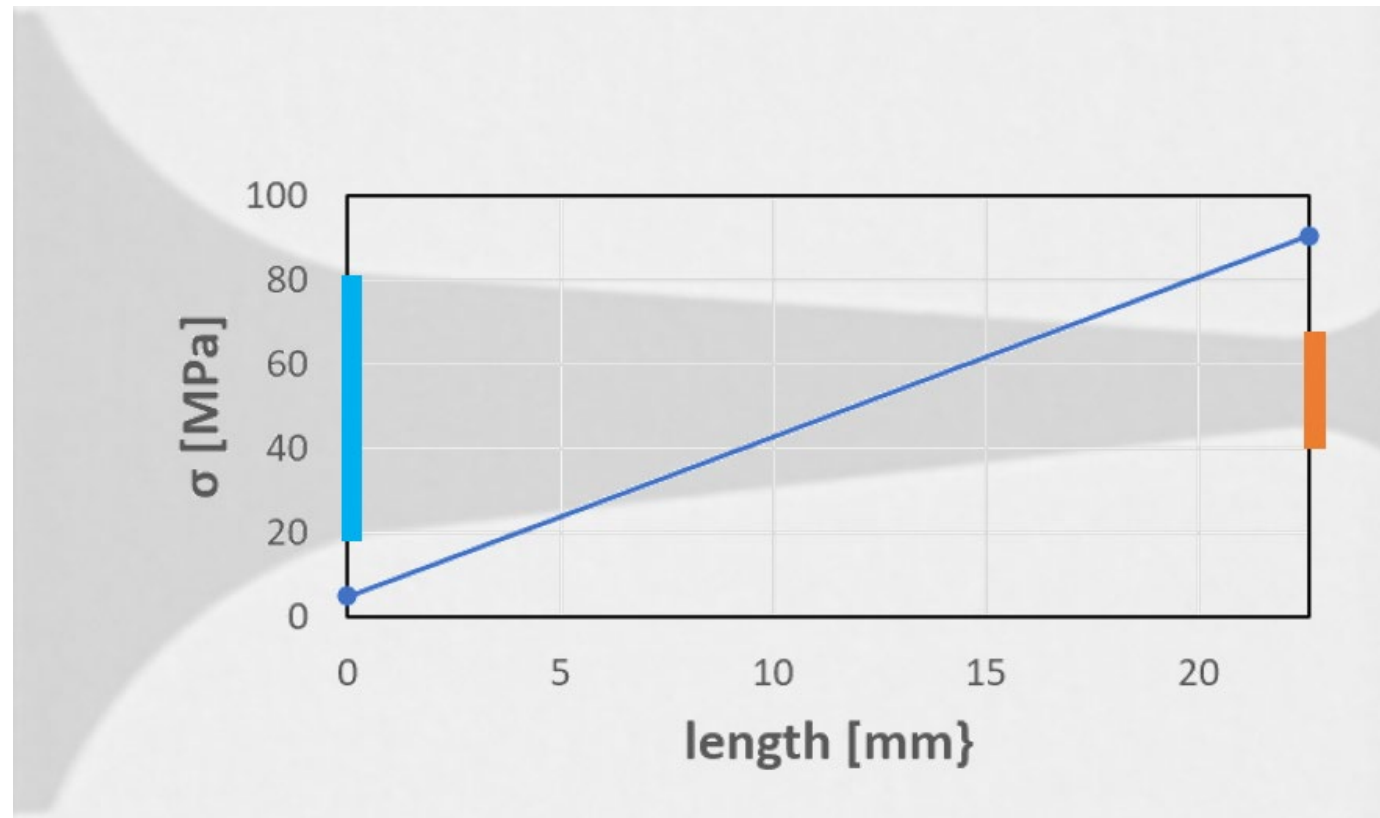
# Seperate effect tests – Influence of elastic stress on the hydrogen solubility

In-situ investigations at ICON (SINQ, PSI) and IMAT (ISIS, RAL) using the ICHAMEL facility



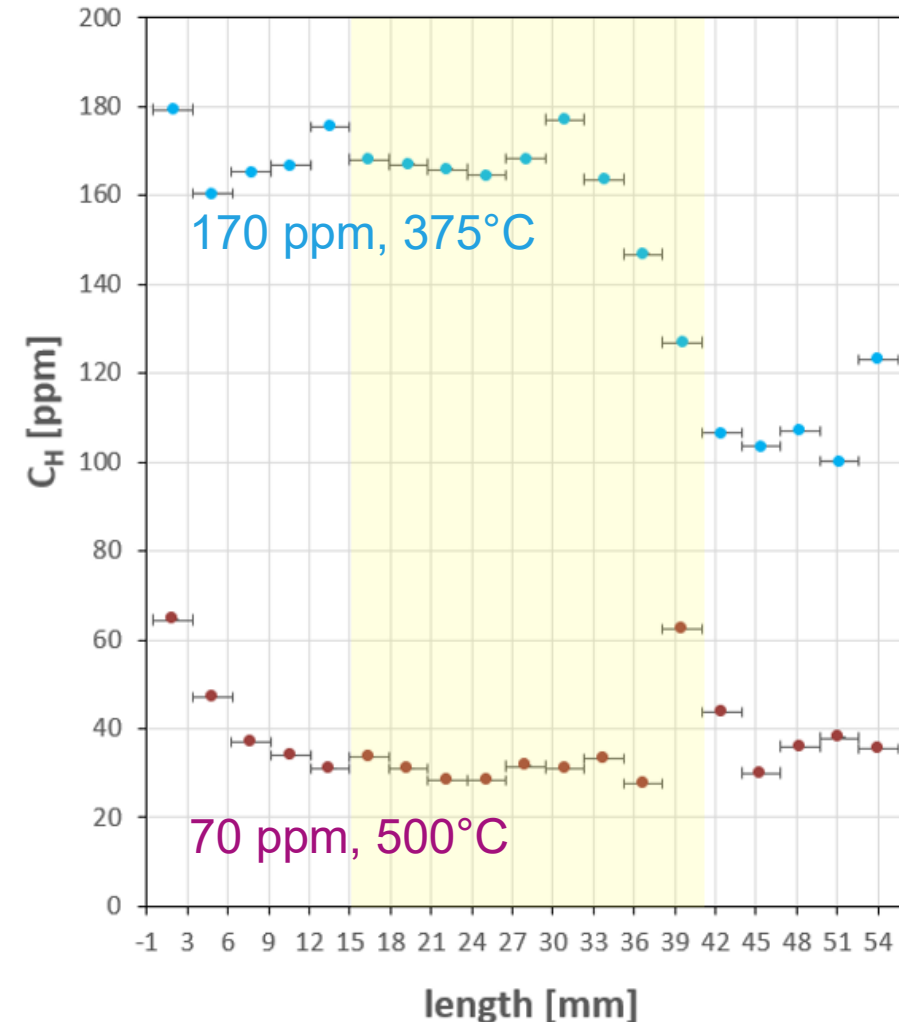
# Separate effect tests – Influence of elastic stress on the hydrogen solubility

Strain distribution along the gauge

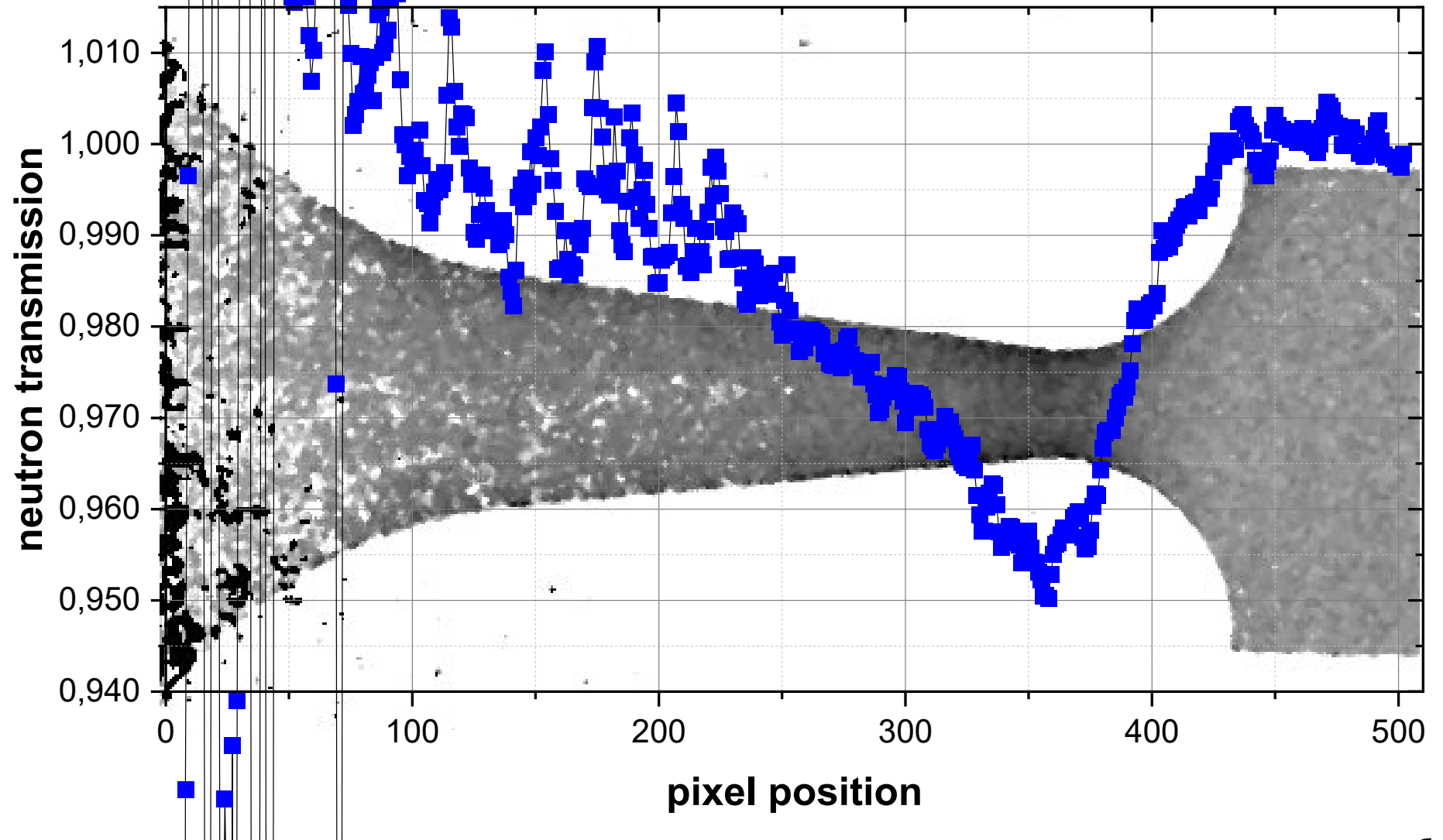


# Seperate effect tests – Influence of elastic stress on the hydrogen solubility

- Commissioning experiments at ICON:
  - Problems with the pyrolytic temperature measurements
  - Outgassing by breaking the oxide layer
  - At 500°C strong creeping until fracture, hydrogen enrichments in the plastic deformed range
- Improvements in the temperature measurements and controlling were needed and performed



# Separate effect tests - Influence of elastic stress on the hydrogen solubility



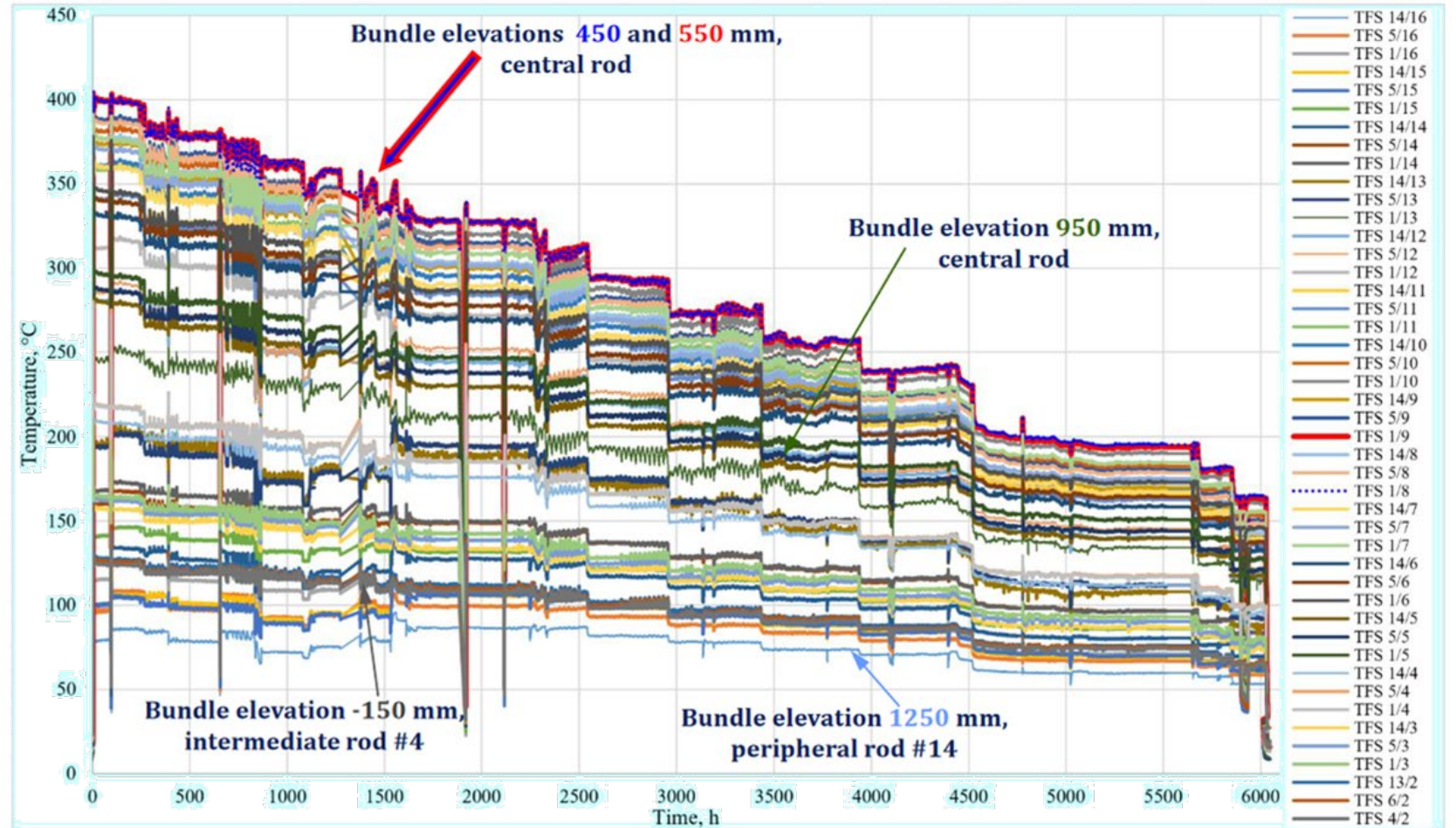
# Bundle test

From May 2023 until  
January 2024 (250 days)

Maximal starting  
temperature: 405°C

Results are already  
published. They are used as  
reference in benchmark  
calculations

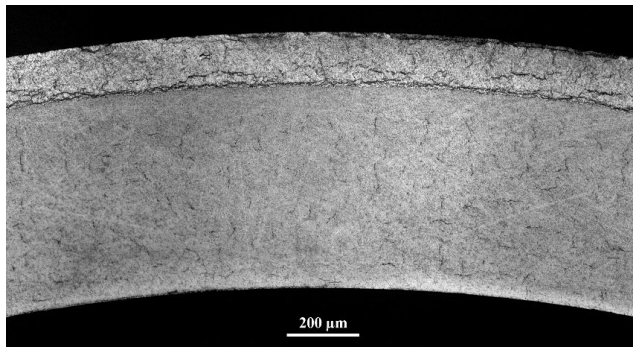
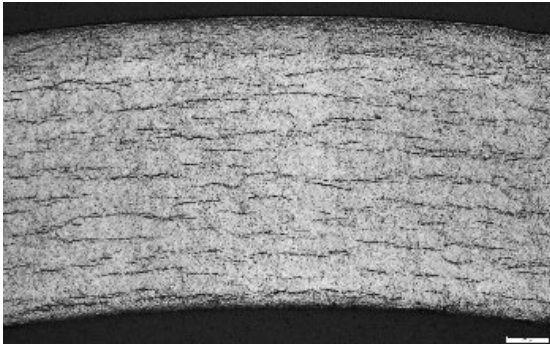
Potentials for improvements



# Bundle test

## Main results:

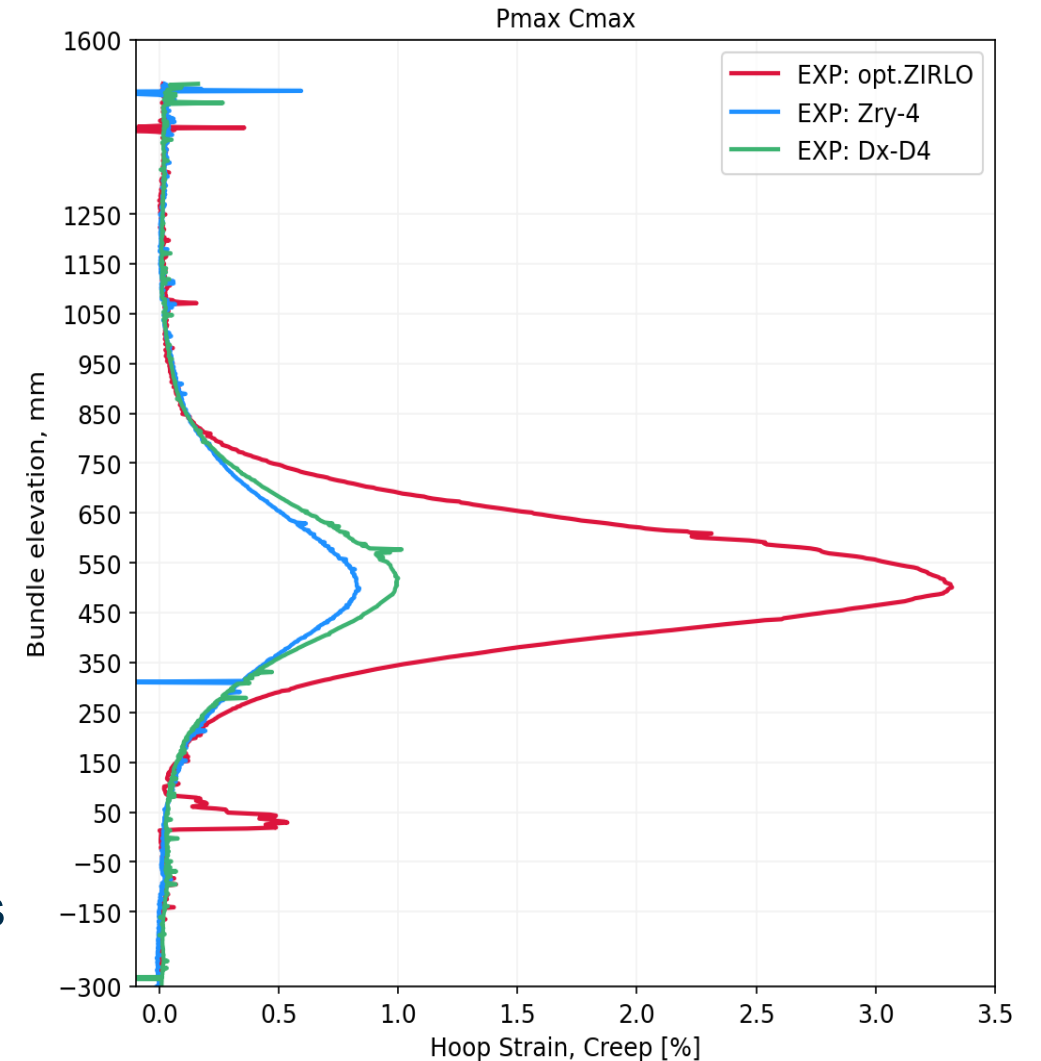
Strong differences in the material behaviour between opt. ZIRLO, Zry-4 and Dx D4 (creep and hydride reorientation)



Opt. ZIRLO: strong creeping (4x stronger than Zry-4 and Dx D4) but nearly no hydride reorientation

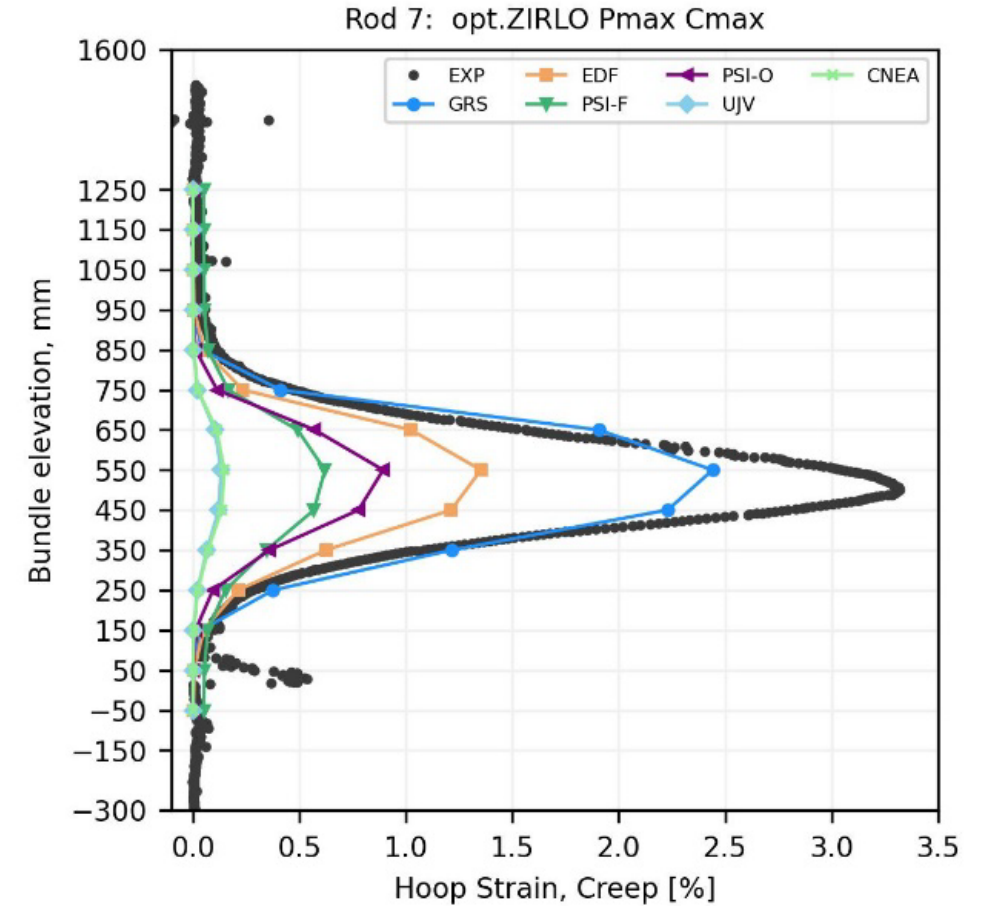
Zry-4: radial and circumferential hydrides in the same order of magnitude

Dx D4: mostly radial hydrides



# Benchmark calculations

- Good agreement between the modelling and the measured creep for Zry-4 and Dx D4
- Not satisfying agreement for opt. ZIRLO
- The codes use models derived from data mostly measured for Zry-4
- Material specific models has to be implemented into the codes





# Outlook

- Proposal for SPIZWURZ+ is submitted. No final decision was made. A feasibility study required is in progress.
- Including other cladding material relevant for Germany (M5, Zry-2, E110) is proposed. Separate effect tests shall be focused on the different behaviour of the materials (creep and hydride reorientation).
- Continuing of the analysis of the SPIZWURZ test.
- Neutron microscopy shall be applied for the determination of the radial hydride fractions.

# Acknowledgement

## Thanks

- to all the KIT colleagues involved in the project: Juri Stuckert, Conrado Rössger, Jürgen Moch, Ursula Peters, Ulrike Stegmaier, Mikhail Kolesnik, ...,
- to the colleagues from GRS and KIT-INE
- to colleagues from BGZ initiating the project

**Thank you for your attention**

# The SPIZWURZ project - overview and single effect tests

Mirco Grosse, Sarah Weick, Michel Herm

30. Intern. QUENCH Workshop,  
KIT Campus North, 2025/12/18





**Juri Stuckert**

KIT

## **Results of the SPIZWURZ bundle test**

The 21-rod SPIZWURZ test bundle with three types of unirradiated claddings (opt. ZIRLO, Zry-4, DX-D4) was used to conduct a long-term integral experiment, approximately simulating dry storage conditions. A variety of parameters typical of an integrated test allowed for the acquisition of a large amount of experimental data necessary for verifying the corresponding computer codes. The claddings were preliminarily hydrogenated to concentrations of 100 and 300 wppm in a specially designed HOKI tubular furnace, distributed as uniformly as possible over a 1.3 m length. Hydrogenation was carried out at 450 °C by sequentially feeding fixed masses of hydrogen through a specially treated inner surface of the claddings. It was noted that the rate of hydrogenation of the opt. ZIRLO claddings is 1.5 times lower than for the Zry-4 claddings. After the hydrogen loading of the cladding tubes, the axial distribution of hydrogen was determined by laser scanning profilometry calibrated by hot gas extraction.

During the experiment, two values of internal rod pressure were used: 106 and 146 bar, which were maintained constant throughout the experiment (250 days). The peak cladding temperature decreased in steps of  $\approx 15$  K from 400 to 165 °C (average cooling rate  $\approx 0.9$  K/day). The maximal cooling rate during each temperature step was 6 K/h, step duration was about 10 h.

The post-test laser scanner measurements of the outer cladding diameter showed significant creep: radial deformation values are between 0.2 and 3.3% (diameter increase and the corresponding wall thinning). The largest creep of 3.3% was measured for opt. ZIRLO claddings hydrogenated to 300 wppm. The corresponding maximum creep value was 0.93% for Zry-4 and 1% for DX-D4. A clearly visible dependence of the degree of creep on the hydrogen concentration is observed for the opt. ZIRLO claddings: the creep of claddings hydrogenated to 300 wppm is 1.2-1.5 times higher than that of claddings hydrogenated to 100 wppm. A number of claddings show radially asymmetric wall thinning, which can be associated with the radial shift of the pellets from the central axis of the rod and the corresponding asymmetric heat supply along the circumference of the cladding.

The metallographic investigations revealed a uniform distribution of hydrides throughout the entire cladding circumference for all three cladding types used. In the DX-D4 claddings, hydrogen primarily diffused toward the outer liner. The degree of hydride reorientation was significantly higher in the Zry-4 claddings compared to the opt. ZIRLO claddings.

The difference in the behavior of the Zry-4 and opt. ZIRLO may be due, in part, to their different grain microstructures. Opt. ZIRLO claddings have a finer grain size than Zry-4. Moreover, although the temperatures during hydrogenation (450 °C) and the experiment itself (max. 400 °C) were relatively low, EBSD measurements showed grain growth from approx. 6  $\mu\text{m}$  for the initial state to post-test 16  $\mu\text{m}$  for Zry-4 (12  $\mu\text{m}$  after hydrogenation), and from initial 3  $\mu\text{m}$  to post-test 4.3  $\mu\text{m}$  for opt. ZIRLO.

## Results of the SPIZWURZ bundle test

J. Stuckert, M. Große, J. Moch, C. Rössger, U. Peters, T. Y. Lin, S. Weick

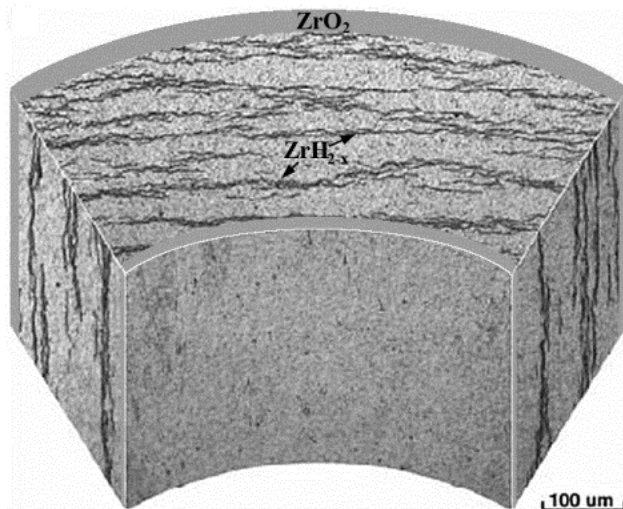
Institute for Applied Materials; Program NUSAFE



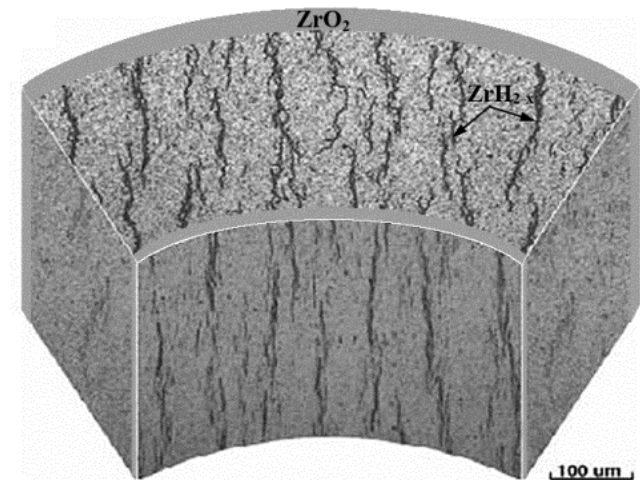
## Goal of bundle test:

investigation of behavior of hydrides during the long-time dry storage of spent fuel with

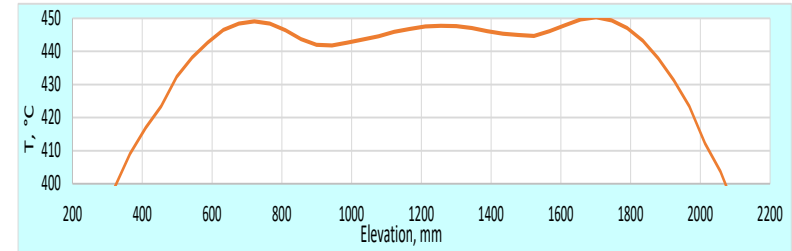
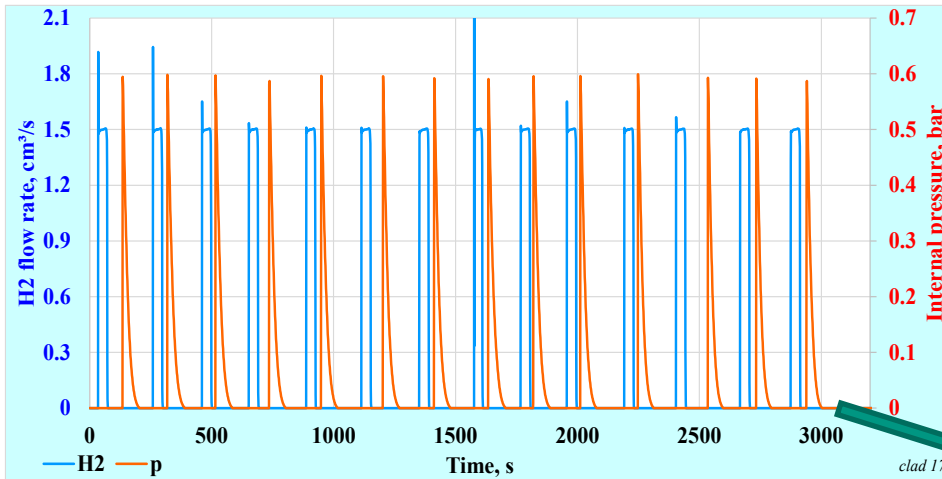
- *different cladding materials (Zry-4, opt. ZIRLO, DUPLEX)*
- *different cladding inner pressures (140, 100 bar)*
- *different hydrogen contents (100, 300 wppm)*
- *different temperature histories (due to axial T profile in the bundle)*



long time cool-down:  
 reorientation of  
 hydrides



# Hydrogenation of each cladding in extended pulse mode to prevent rapid formation of hydrides near to the inner cladding surface



HOKI oven with axial temperature profile:  
 $T \approx 450 \text{ }^\circ\text{C}$  along the length of  $\approx 1250 \text{ mm}$

after pulse filling followed **homogenization** stage at  $450 \text{ }^\circ\text{C}$  during 4 h and then almost linear cooldown to  $50 \text{ }^\circ\text{C}$  during 12 h

pulse filling of the internal cladding volume after special treatment of the inner cladding surface and evacuation of the cladding tube:  
 repeated depressurization of inner cladding volume due to  $\text{H}_2$  absorption

1) stepwise hydriding of cladding to 300 wppm H

**14 injections** with  $p_{max} = 0.6 \text{ bar}$  →

$$\text{total } m_{\text{H}_2} = 14 \times \left( \frac{\mu p_{max} V_{hot}}{RT_{hot}} + \frac{\mu p_{max} V_{cold}}{RT_{cold}} \right) = 0.05 \text{ g}$$

$$M_{clad \ 125 \text{ cm}} = 170 \text{ g} \quad C_H = 0.05/170 \approx 300 \text{ wppm}$$

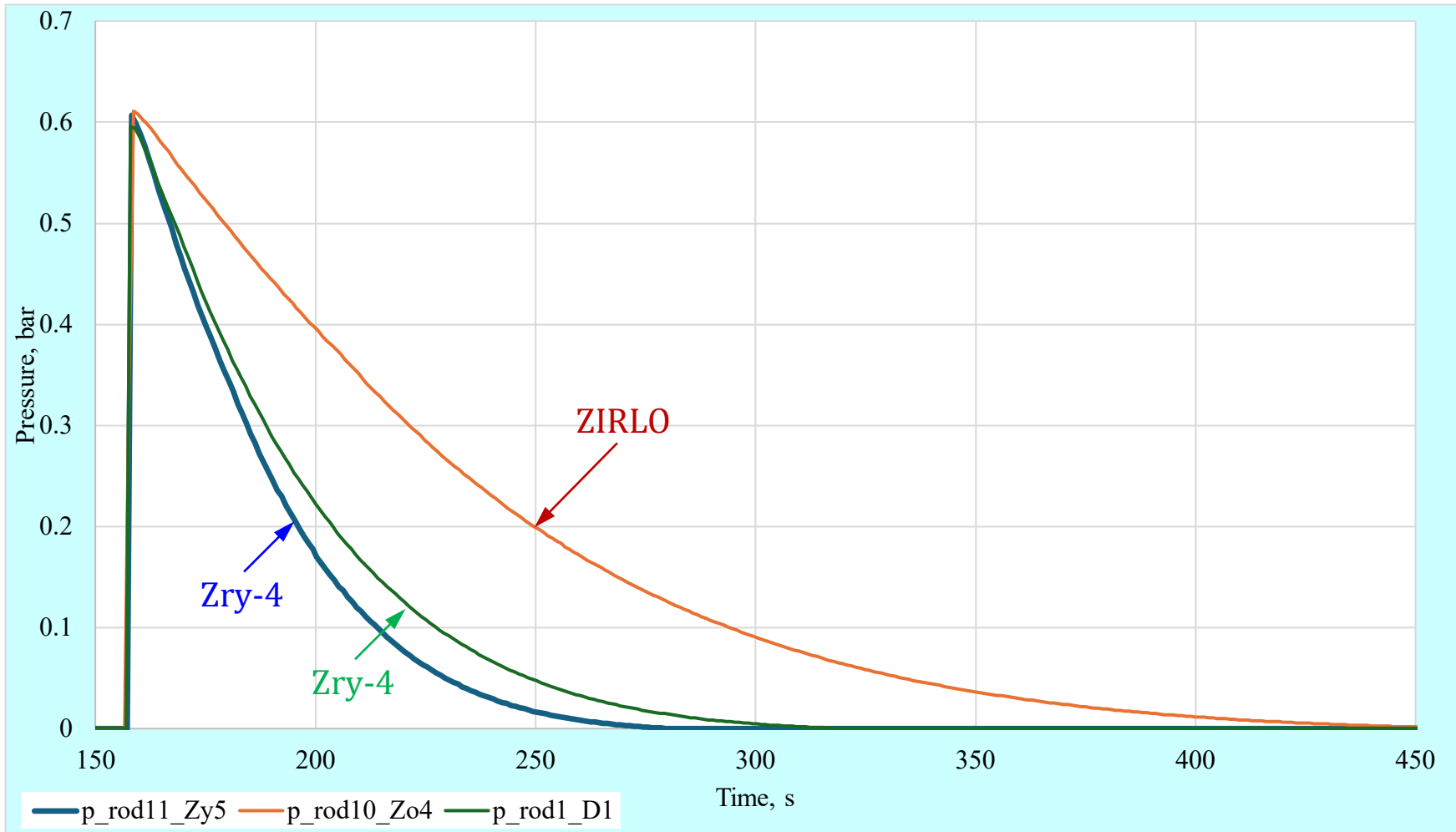
2) stepwise hydriding of cladding to 100 wppm H

**5 injections** with  $p_{max} = 0.6 \text{ bar}$  →

$$\text{total } m_{\text{H}_2} = 5 \times \left( \frac{\mu p_{max} V_{hot}}{RT_{hot}} + \frac{\mu p_{max} V_{cold}}{RT_{cold}} \right) = 0.0179 \text{ g}$$

$$M_{clad \ 125 \text{ cm}} = 170 \text{ g} \quad C_H = 0.0179/170 \approx 100 \text{ wppm}$$

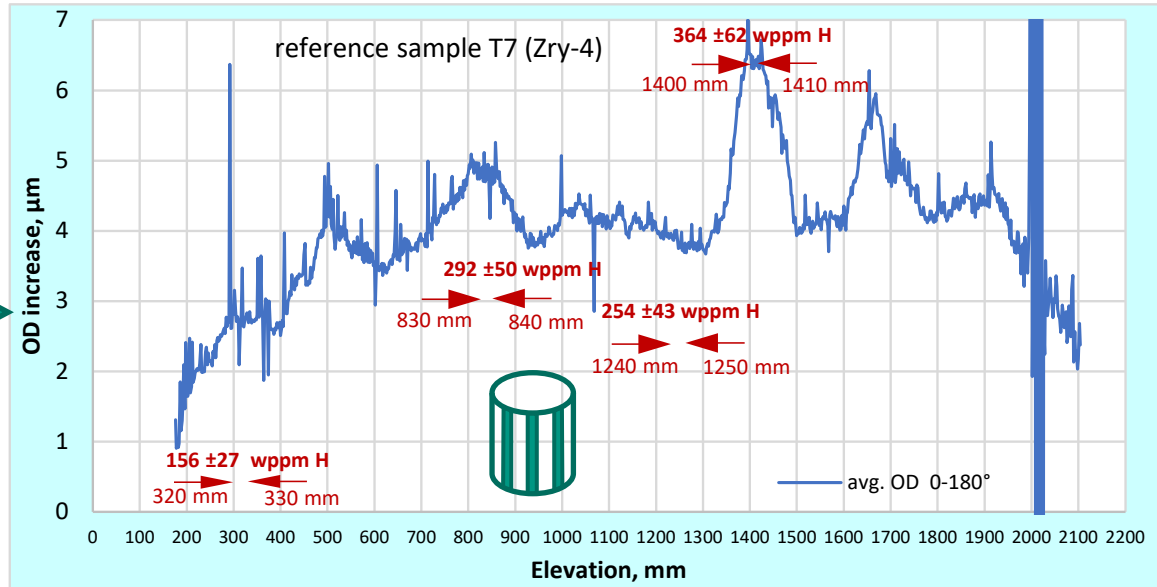
# Hydrogenation duration (1 cycle) for different claddings materials



Slower charging of ZIRLO in comparison to Zry-4 (difference in diffusion coefficients?)



# Determination of axial distribution of hydrogen concentration by increase of circumferential strain at each elevation

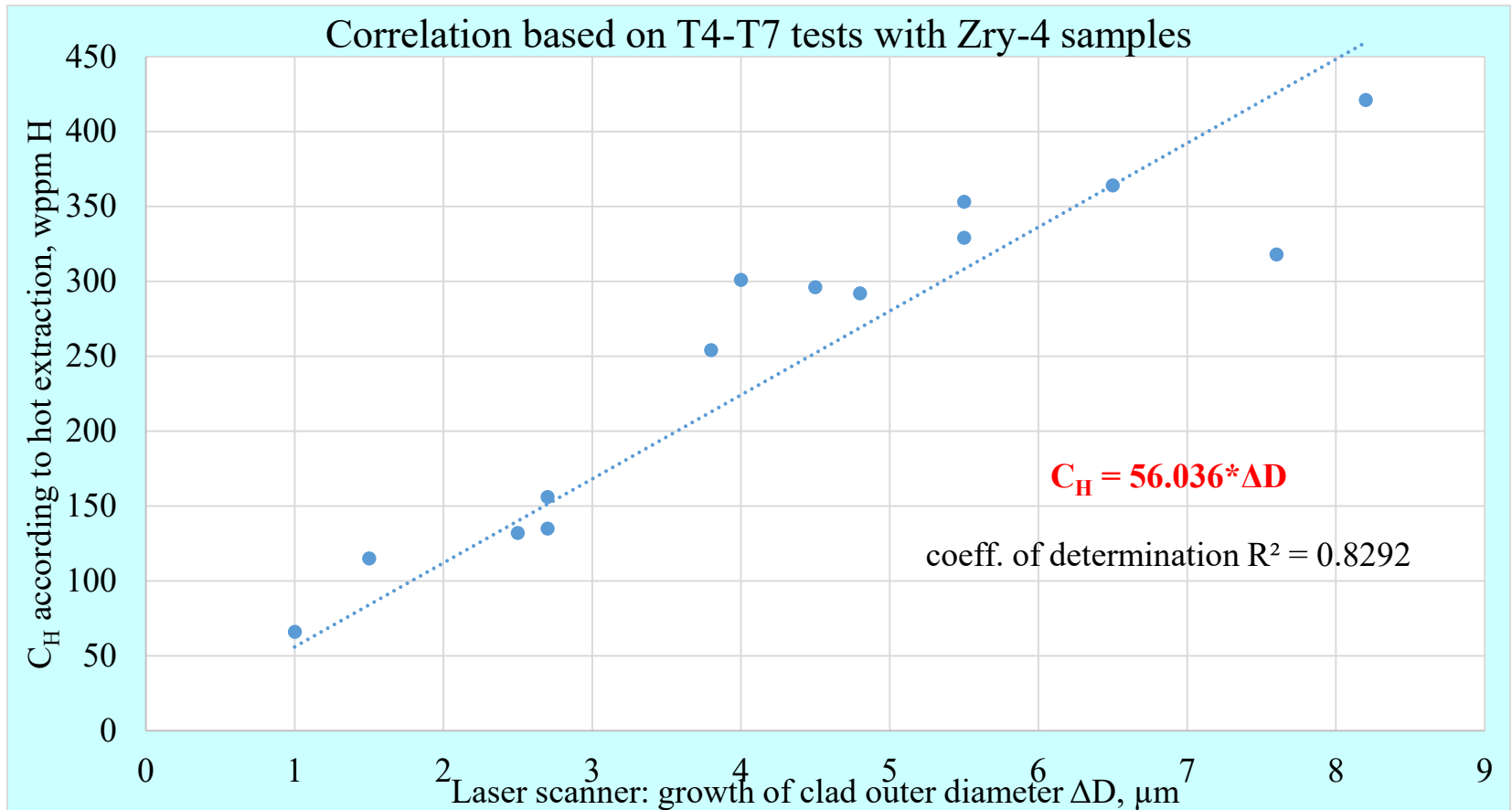


axial profile of cladding diameter increase (laser scanner)  
 and corresponded hydrogen concentrations  
 (hot extraction from 3 lamellas 10x1 mm)

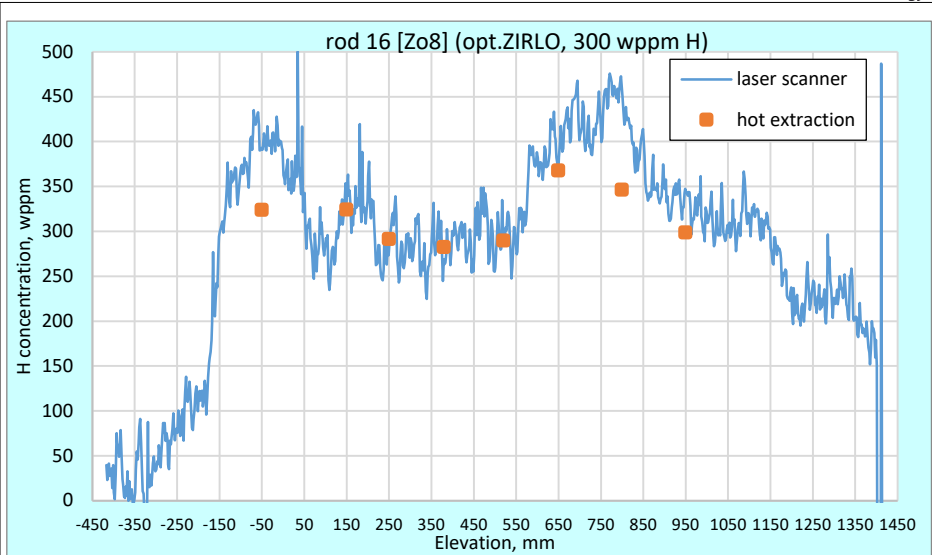
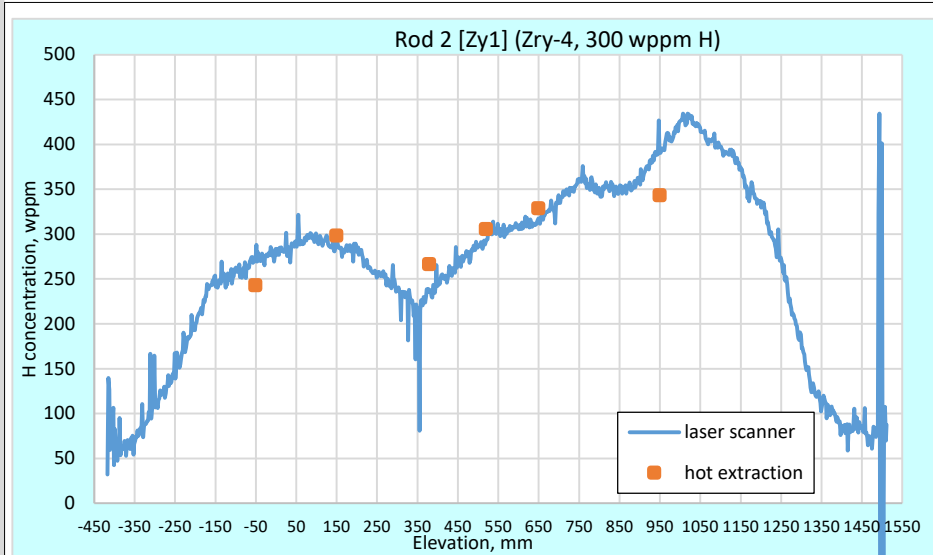
profilometry of clads with laser scanner  
**steps: 3° tangential, 2 mm axial**  
 (thermal expansion ±0.3 μm for ±5 °C)

# Correlation between hydrogen content and increase of averaged cladding diameter

sample	ref. T4			ref. T5			ref. T6				ref. T7			
	axial position, mm	750	1250	1650	750	1250	1650	405	755	1155	1455	325	835	1245
<b>OD increase, <math>\mu\text{m}</math> (laser scanner)</b>	<b>7.6</b>	<b>4</b>	<b>5.5</b>	<b>8.2</b>	<b>5.5</b>	<b>4.5</b>	<b>1</b>	<b>2.5</b>	<b>2.7</b>	<b>1.5</b>	<b>2.7</b>	<b>4.8</b>	<b>3.8</b>	<b>6.5</b>
<b>hot extraction, wppm</b>	<b>318</b>	<b>301</b>	<b>329</b>	<b>421</b>	<b>353</b>	<b>296</b>	<b>66</b>	<b>132</b>	<b>135</b>	<b>115</b>	<b>156</b>	<b>292</b>	<b>254</b>	<b>364</b>
$\pm$ wppm	48	45	49	105	88	74	17	33	34	29	27	50	43	62
SD				25	3	2	27	2	1	5	4	13	6	3

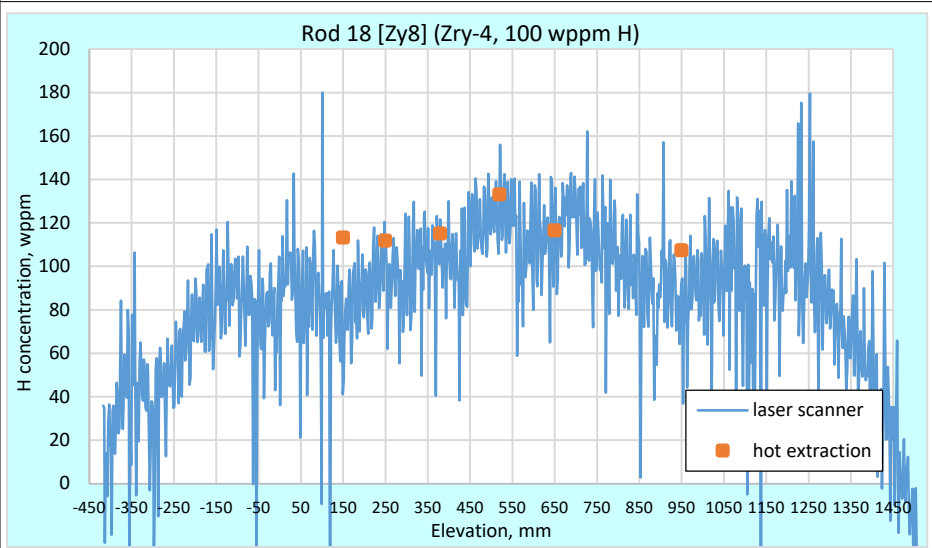
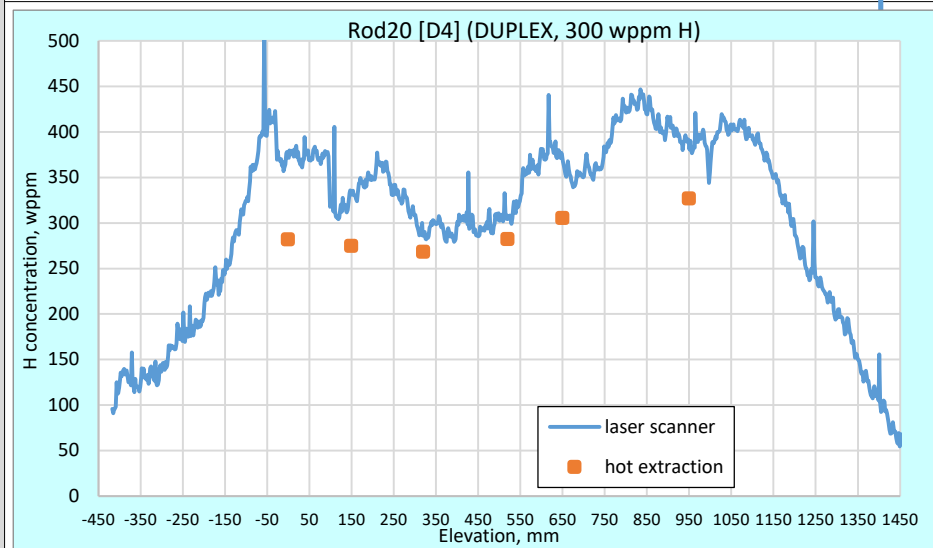


# Axial hydrogen distribution for claddings: comparison of laser scanner data and post-test hot extraction



**Zry-4, 300 wppm**

**opt. ZIRLO, 300 wppm**

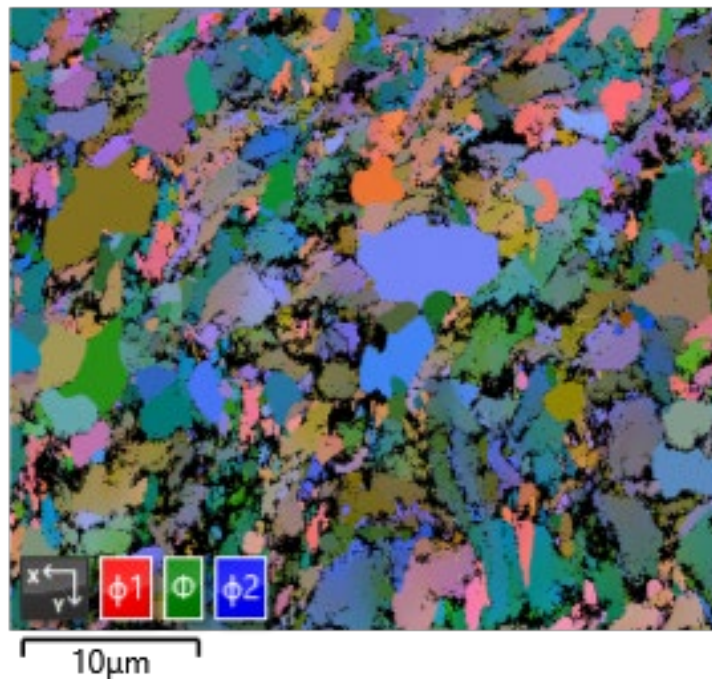


**DX-D4, 300 wppm**

**Zry-4, 100 wppm**

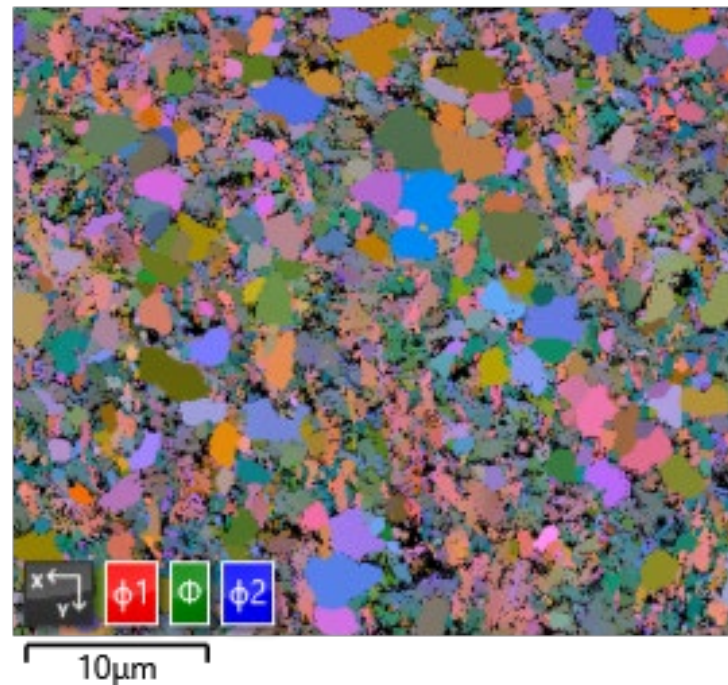
# Microstructure of as-received claddings: EBSD analysis

Euler Color 1



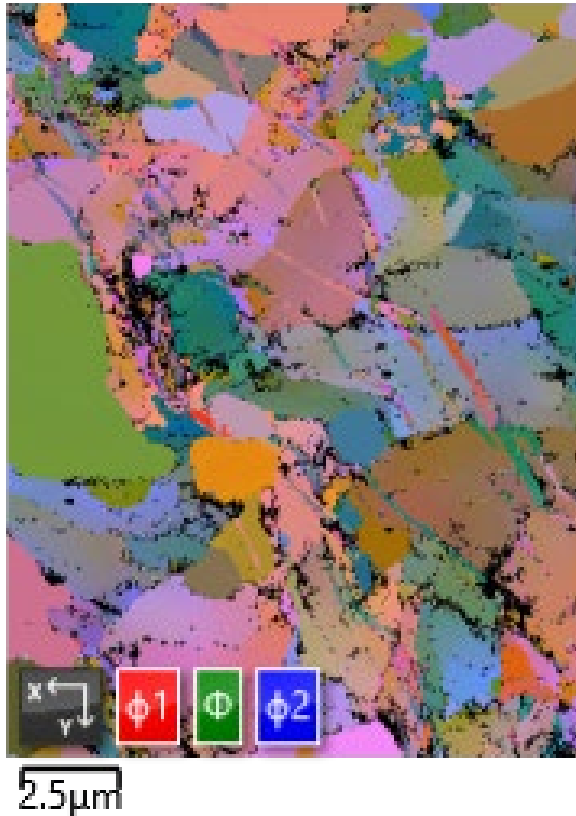
cold-worked and stress-relieved (CWSR) **Zry-4**:  
 avg. grain area: weight mean **5.74  $\mu\text{m}^2$**   
 (biaxial grains  $\bar{D} \approx 3.6 \mu\text{m}$ ,  $\bar{d} \approx 2.0 \mu\text{m}$ )

Euler Color 2

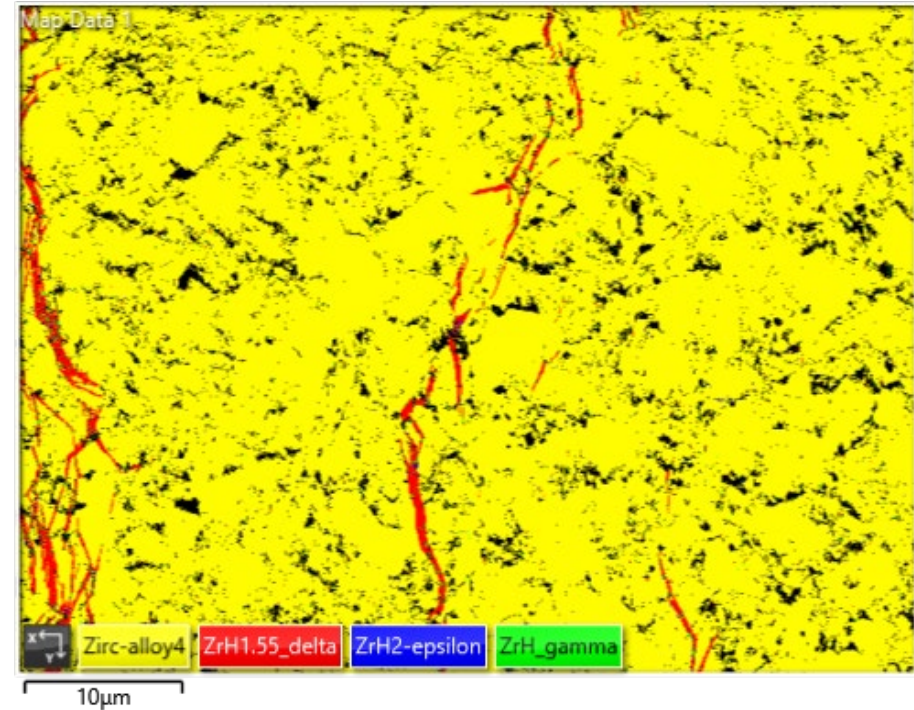


partially recrystallized (PRXA) **opt. ZIRLO**:  
 avg. grain area: weight mean **2.92  $\mu\text{m}^2$**   
 ( $\bar{D} \approx 2 \mu\text{m}$ )

Euler Color 1



EBSD Layered Image 1

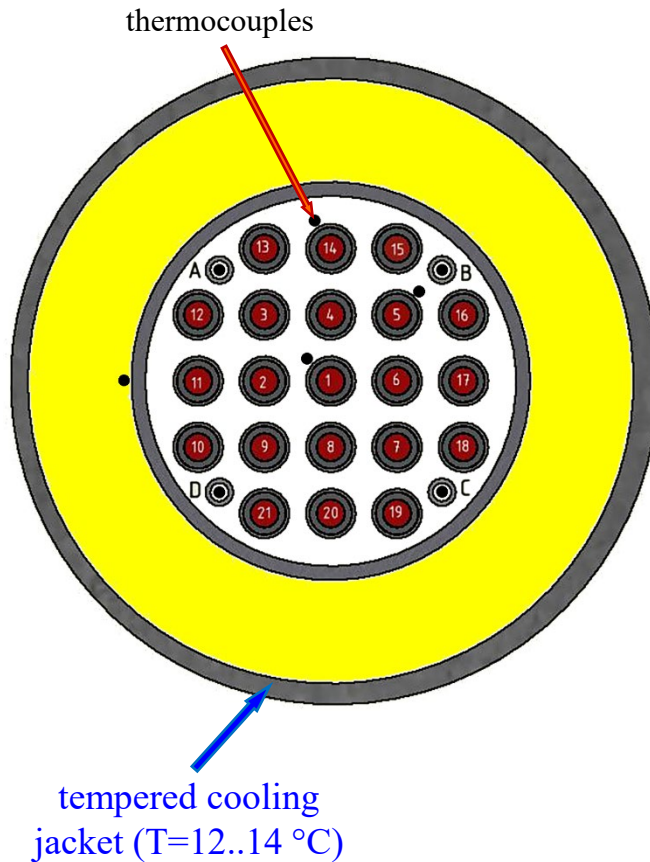
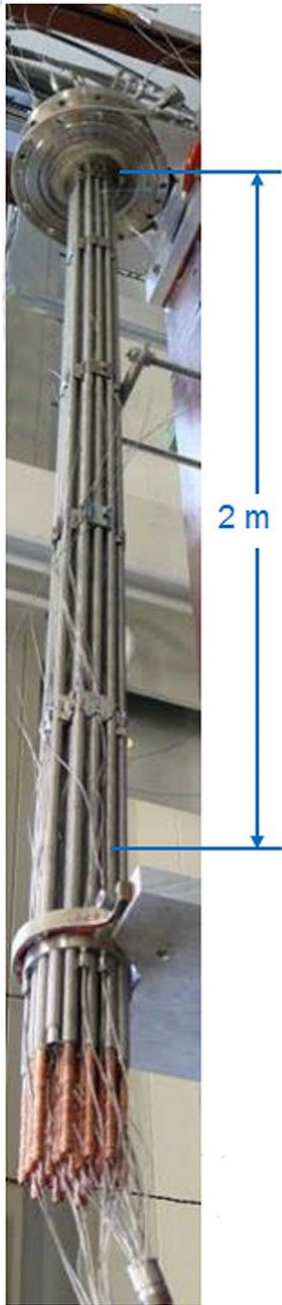


CWSR Zry-4 hydrogenated at 450 °C (total heat treatment  $\approx$  1 day):  
 avg. grain area weight mean **12.79  $\mu\text{m}^2$**   
 (biaxial grains  $\bar{D} \approx 4.9 \mu\text{m}$ ,  $\bar{d} \approx 3.3 \mu\text{m}$ )

Zry-4:  
 inter- and intra-granular  $\delta$ -hydrides with avg. length of  $\approx 10 \mu\text{m}$  and  
 width  $\approx 0.3 \dots 0.6 \mu\text{m}$ ; radial distance between hydrides  $\approx 20 \mu\text{m}$

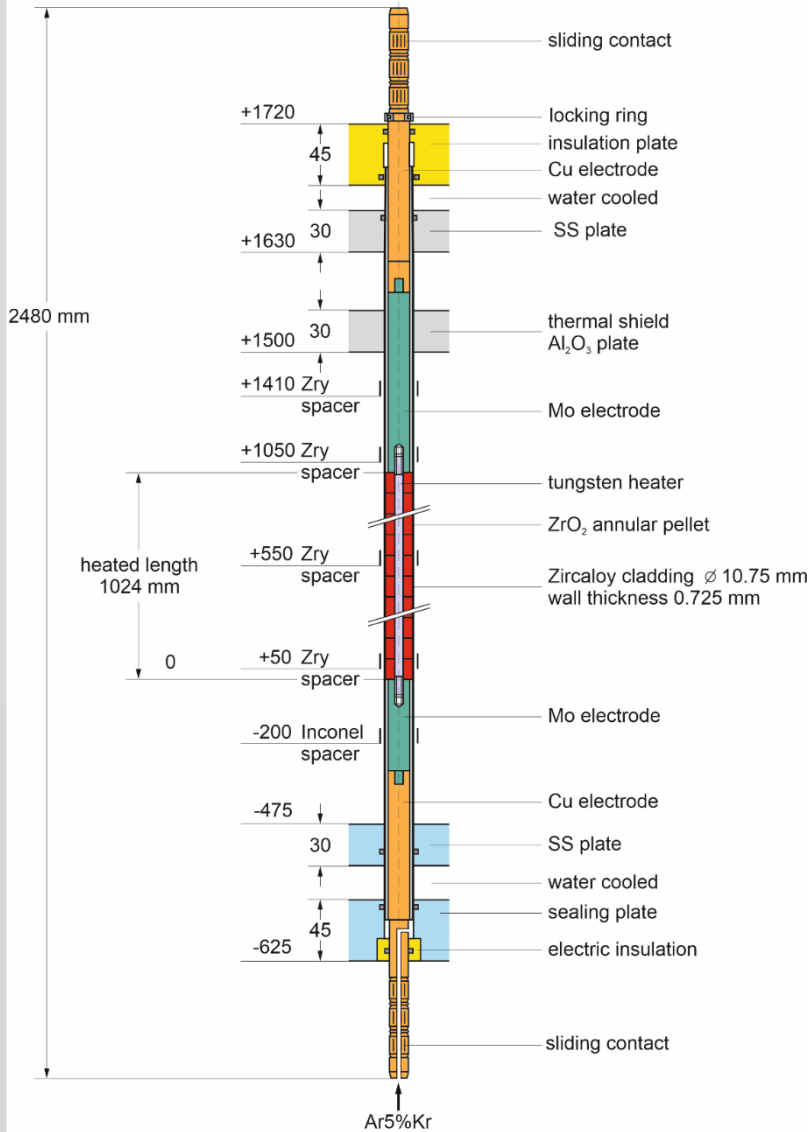
**doubling of the grain area** in comparison to as-received cladding

# SPIZWURZ bundle



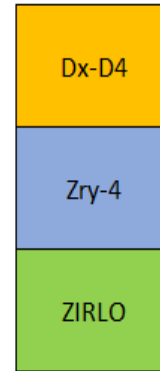
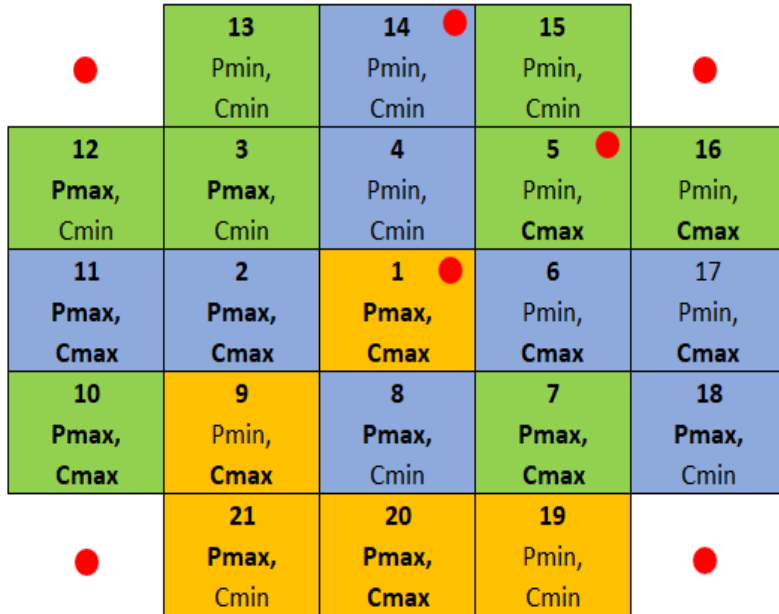
Bundle size		21 heated rods
Pitch		14.3 mm
Corner rod (4)	material	Zircaloy-4
	instrumented (A, B, C, D)	tube $\varnothing$ 6x0.5 (bottom: -1140 mm)
Grid spacer	material	Zircaloy-4
	length	42 mm
	sheet thickness	0.5 mm
	elevation of lower edge	Zry: -100, 150, 550, 1050, 1410 mm
Shroud	material	Zirconium 702 (flange: Zry-4)
	wall thickness	3.17 mm
	outside diameter	86.0 mm
	length (extension)	1600 mm (-300 mm to 1300 mm)
Shroud insulation	material	ZrO <sub>2</sub> fiber
	insulation thickness	~ 36 mm
	elevation	-300 to ~1000 mm
Cooling jacket	Material: inner/outer	Inconel 600 (2.4816) / SS (1.4571)
	inner tube	$\varnothing$ 158.3 / 168.3 mm
	outer tube	$\varnothing$ 181.7 / 193.7 mm
Thermocouples	at cladding surfaces	rods 1, 5, 9; totally 3x15=45
	inside corner rods	one at each elevation 2-16, totally 15
	at shroud outer surface	one at each elevation 3-15, totally 13

# Heated rod



<b>Cladding OD / ID</b>		<b>10.75 / 9.3 mm</b>
<b>Cladding thickness</b>		<b>0.725 mm</b>
<b>Cladding length</b>	<b>(position in the bundle)</b>	<b>2278 mm (between -593 and 1685 mm)</b>
<b>Rod length</b>	<b>(elevations)</b>	<b>2480 mm (-690 to 1790 mm)</b>
<b>Internal rod pressure; gas</b>		<b>5.5 MPa abs.; Kr</b>
<b>Material of middle heater</b>		<b>Tungsten (W)</b>
	<b>surface roughness</b>	<b>Ra=1.6 <math>\mu</math>m</b>
<b>Tungsten heater length</b>		<b>1024 mm (between 0 and 1024 mm)</b>
<b>Tungsten heater diameter</b>		<b>4.6 mm</b>
<b>Annular pellet</b>	<b>material</b>	<b>ZrO<sub>2</sub>;Y<sub>2</sub>O<sub>3</sub>-stabilized</b>
	<b>dimensions</b>	<b><math>\varnothing</math> 9.15/4.75 mm; L=11 mm</b>
	<b>surface roughness</b>	<b>Ra=0.3 <math>\mu</math>m</b>
<b>Pellet stack</b>		<b>0 mm to ~1020 mm</b>
<b>Molybdenum heaters and copper electrodes</b>	<b>length of upper part</b>	<b>766 mm (576 Mo, 190 mm Cu)</b>
	<b>length of lower part</b>	<b>690 mm (300 Mo, 390 mm Cu)</b>
	<b>outer diameter:</b>	
	<b>prior to coating</b>	<b>8.6 mm</b>
	<b>after coating with ZrO<sub>2</sub></b>	<b>9.0 mm</b>
	<b>coat. surface roughness</b>	<b>Ra=6-12 <math>\mu</math>m</b>
	<b>borehole of Cu-electrodes</b>	<b>diameter 2 mm, length 96 mm</b>
<b>Gas volume inside the rod</b>	<b>heated</b>	<b>15 cm<sup>3</sup></b>
<b>Gas volume outside the rod</b>	<b>not heated (room T)</b>	<b>20 cm<sup>3</sup></b>

# Bundle composition



● Thermocouples

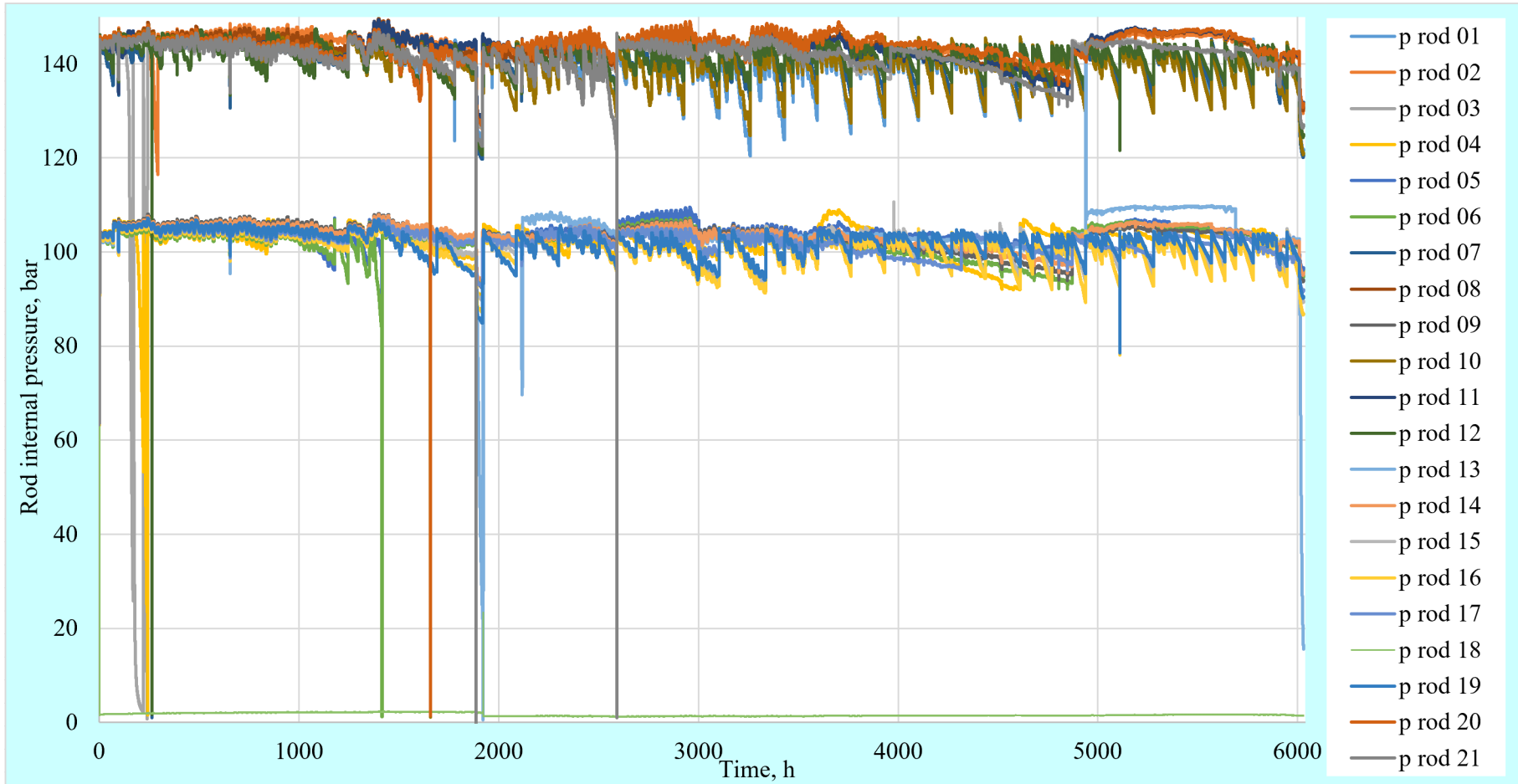
hydrogen content in cladding  
 Cmax = 300 wppm H  
 Cmin = 100 wppm H

pressure inside the rod  
 Pmax = 146 bar  
 Pmin = 106 bar

number	rod	alloy	H conc., wppm	mark
D1	1	<b>DUPLEX</b>	<b>300</b>	D1
Zry0212	2	<b>Zry-4</b>	<b>300</b>	Zy1
Zo049	3	<b>ZIRLO</b>	<b>100</b>	Zo1
Zy31	4	<b>Zry-4</b>	<b>100</b>	Zy2
Zo087	5	<b>ZIRLO</b>	<b>300</b>	Zo2
Zy85	6	<b>Zry-4</b>	<b>300</b>	Zy3
Zo156	7	<b>ZIRLO</b>	<b>300</b>	Zo3
Zry197	8	<b>Zry-4</b>	<b>100</b>	Zy4
D2	9	<b>DUPLEX</b>	<b>300</b>	D2
Zo165	10	<b>ZIRLO</b>	<b>300</b>	Zo4
Zry199	11	<b>Zry-4</b>	<b>300</b>	Zy5
Zo220	12	<b>ZIRLO</b>	<b>100</b>	Zo5
Zo221	13	<b>ZIRLO</b>	<b>100</b>	Zo6
Zy914	14	<b>Zry-4</b>	<b>100</b>	Zy6
Zo332	15	<b>ZIRLO</b>	<b>100</b>	Zo7
Zo351	16	<b>ZIRLO</b>	<b>300</b>	Zo8
Zry1021	17	<b>Zry-4</b>	<b>300</b>	Zy7
	18	<b>Zry-4</b>	<b>100</b>	Zy8
D3	19	<b>DUPLEX</b>	<b>100</b>	D3
D4	20	<b>DUPLEX</b>	<b>300</b>	D4
D5	21	<b>DUPLEX</b>	<b>100</b>	D5

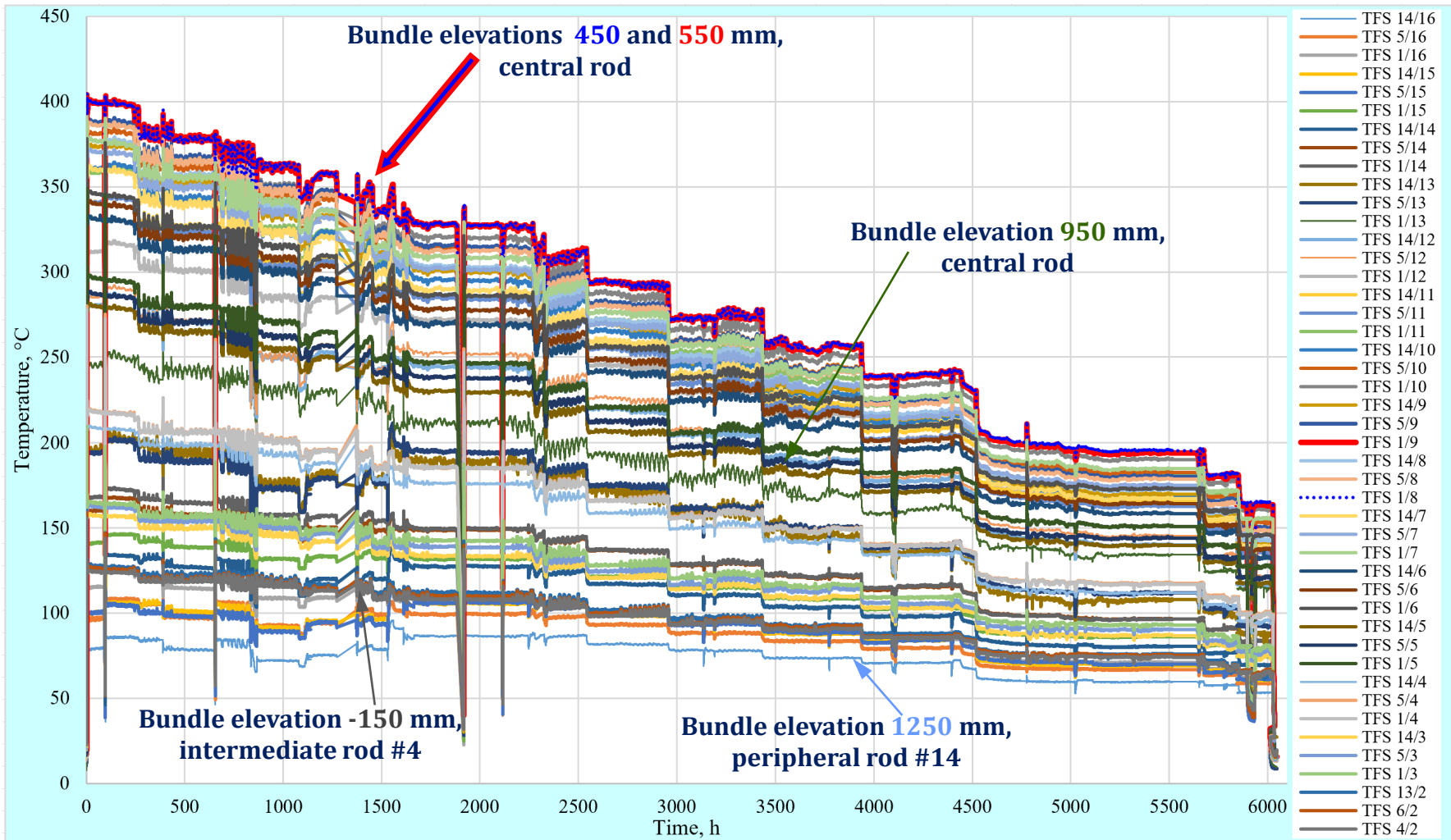


# Pressures inside the rods between 12.05.2023 and 18.01.2024



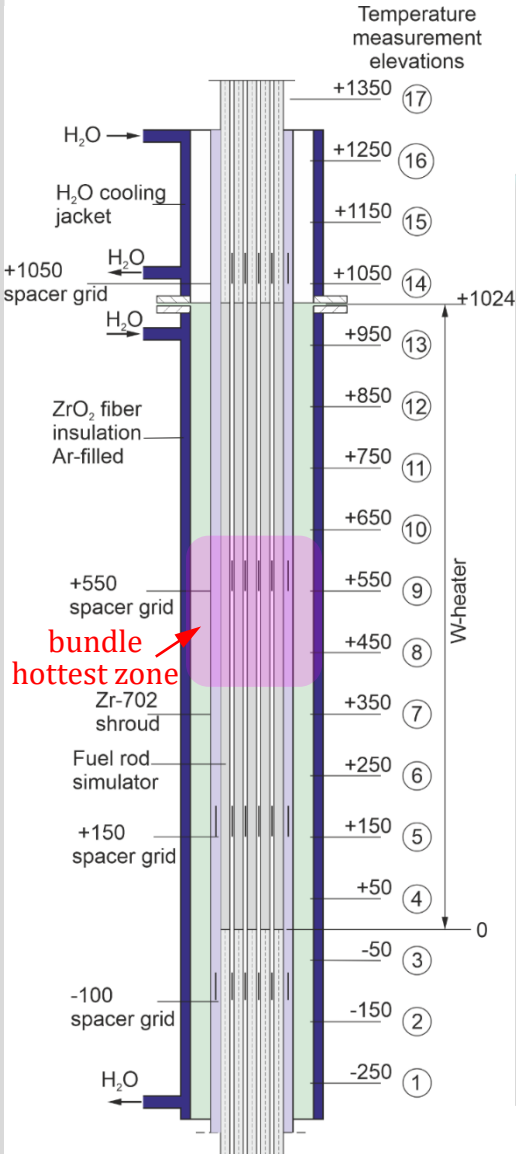
- two pressurization levels of **106 and 146 bar**
- daily refill of 7 rods with Ar+O<sub>2</sub> due to small leakages
- short depressurizations of 6 rods due to change of sealing rings

# Reading of cladding surface thermocouples (TFS) between 12.05.23 and 18.01.24

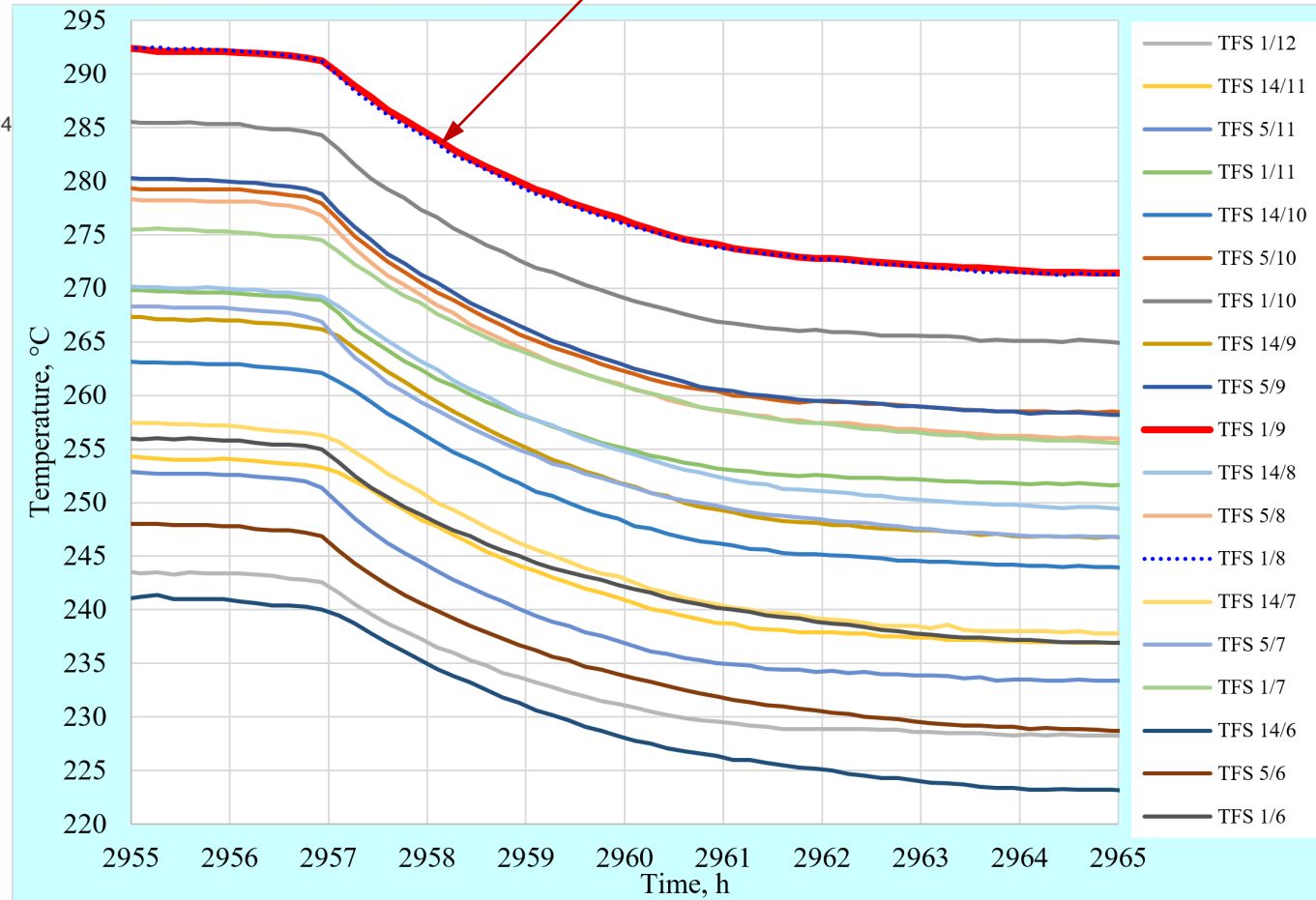


- peak cladding temperature decreased in steps with 15 K decrement and average duration of 400 h, average cooling rate 0.9 K/day
- periodic daily temperature fluctuations  $\approx \pm 1.5$  K for each thermocouple
- 4 el. power breakdowns

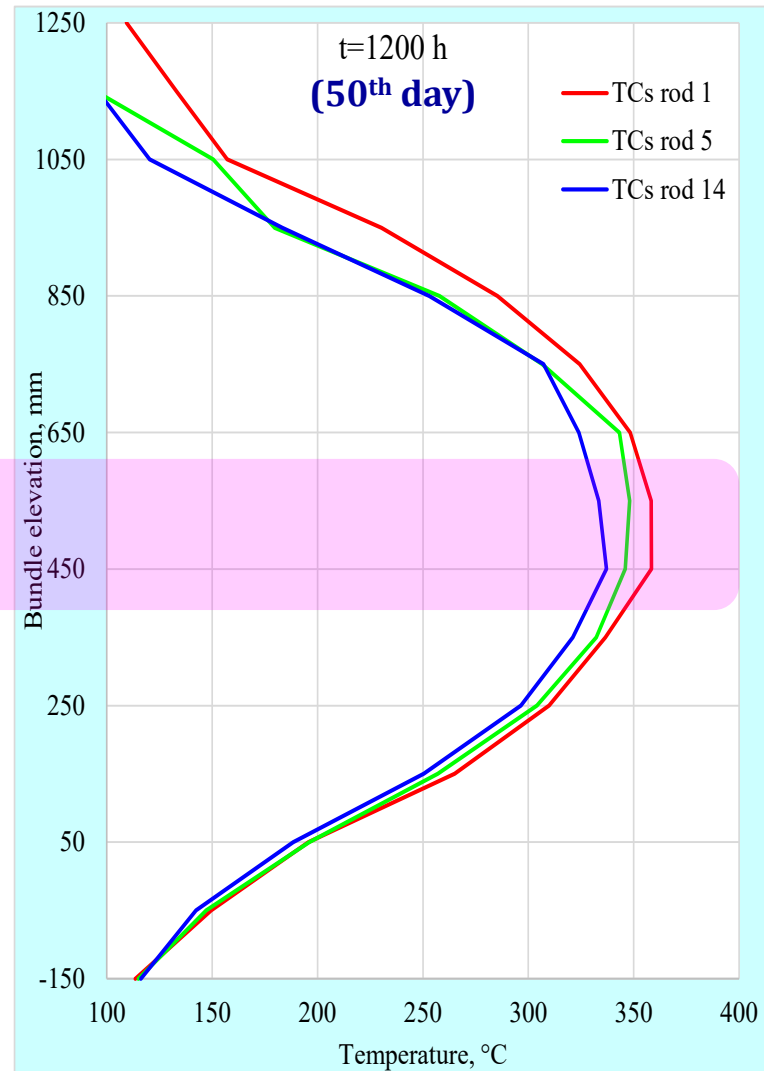
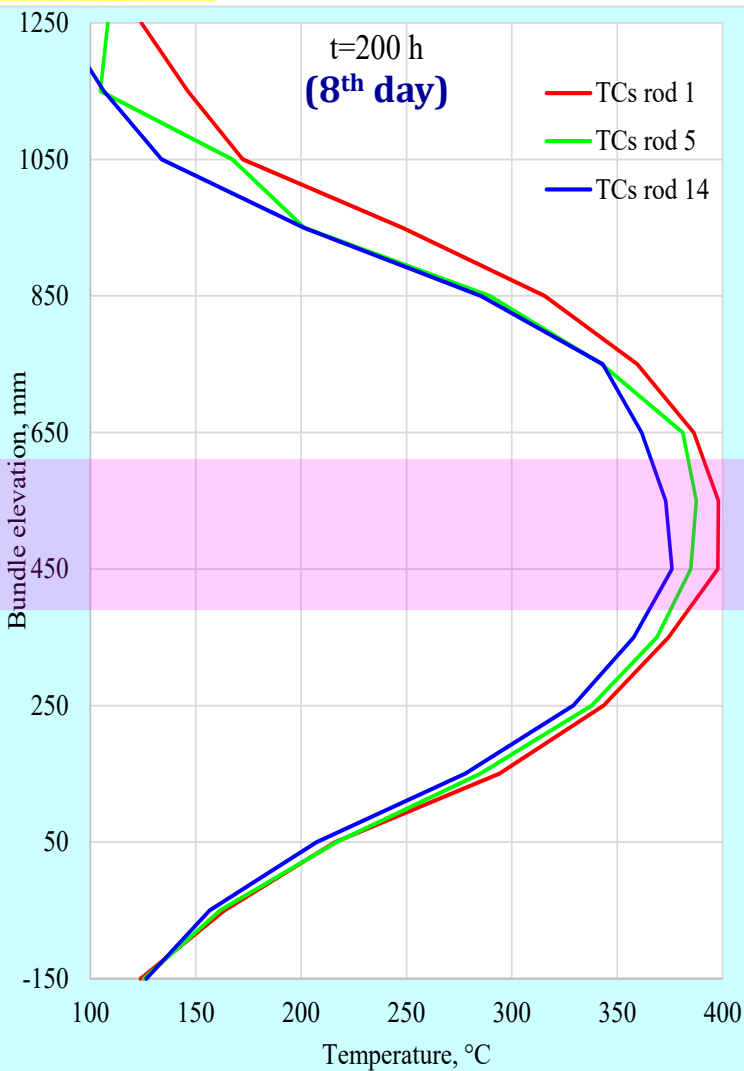
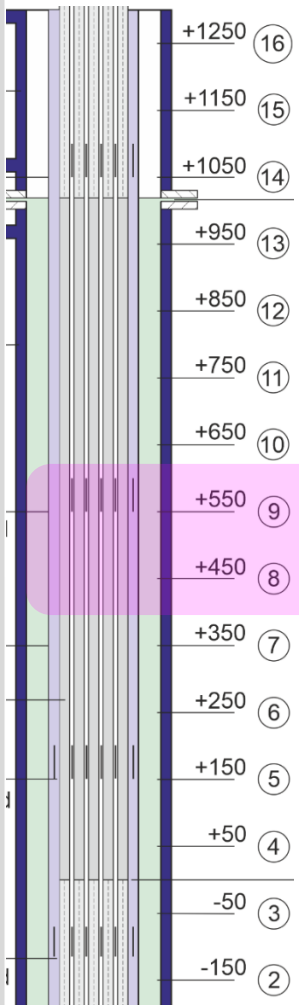
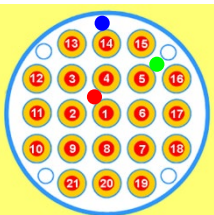
# Smooth temperature decrease on the time of the power step reduction

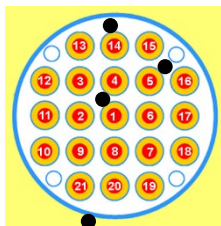


cooling rate decreased from 6 K/h ( $1.7 \cdot 10^{-3}$  K/s) to 0 K/s during 10 h

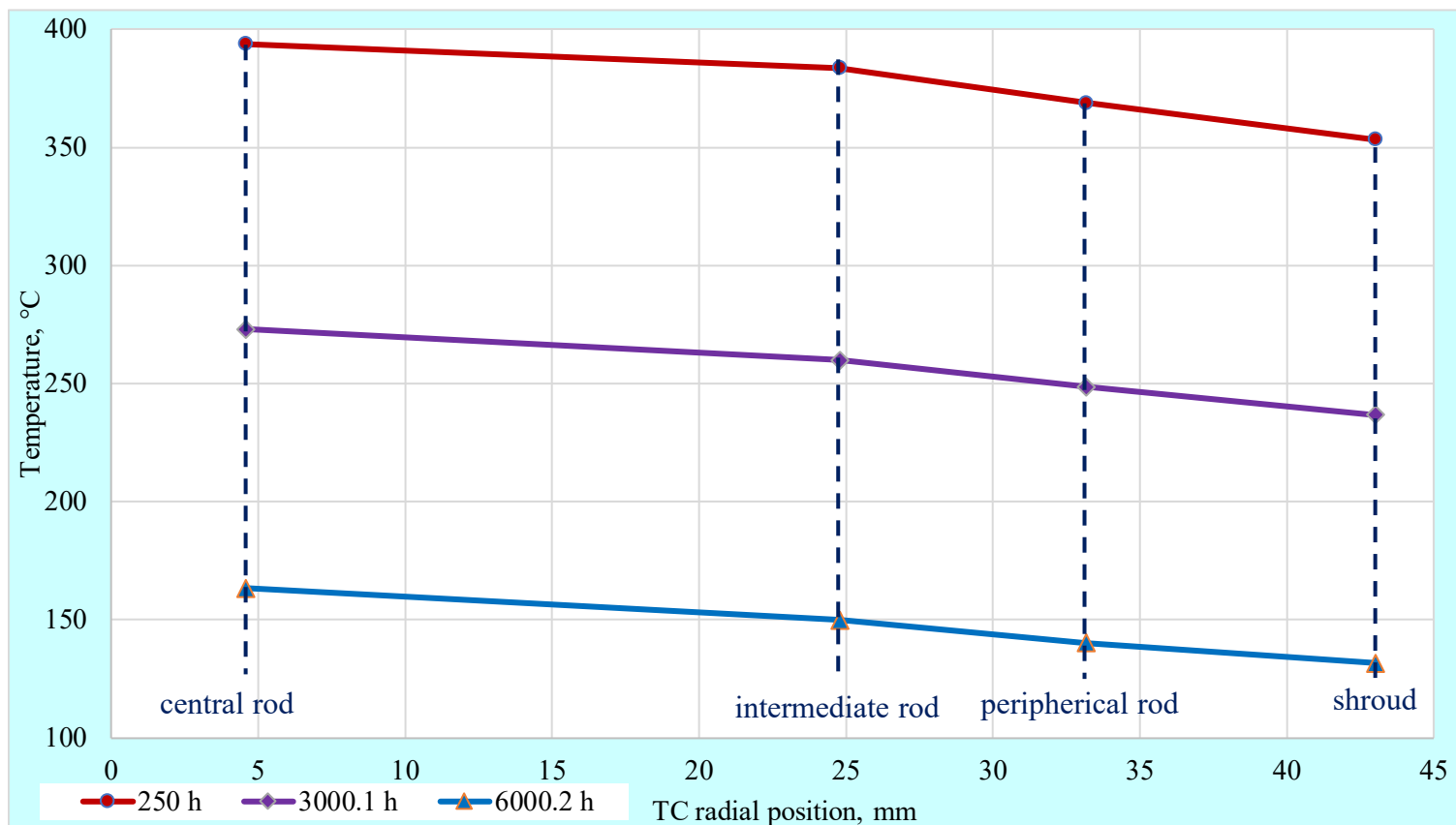


# Axial temperature distribution for three rod groups



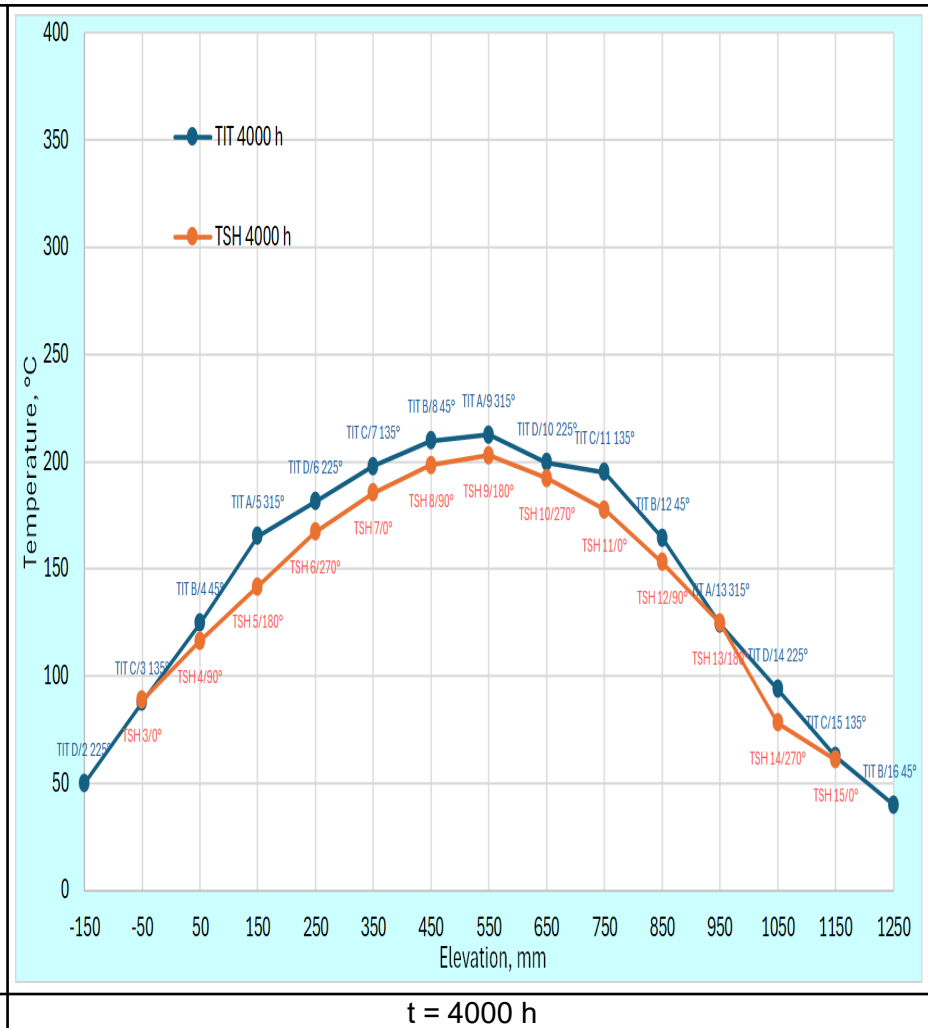
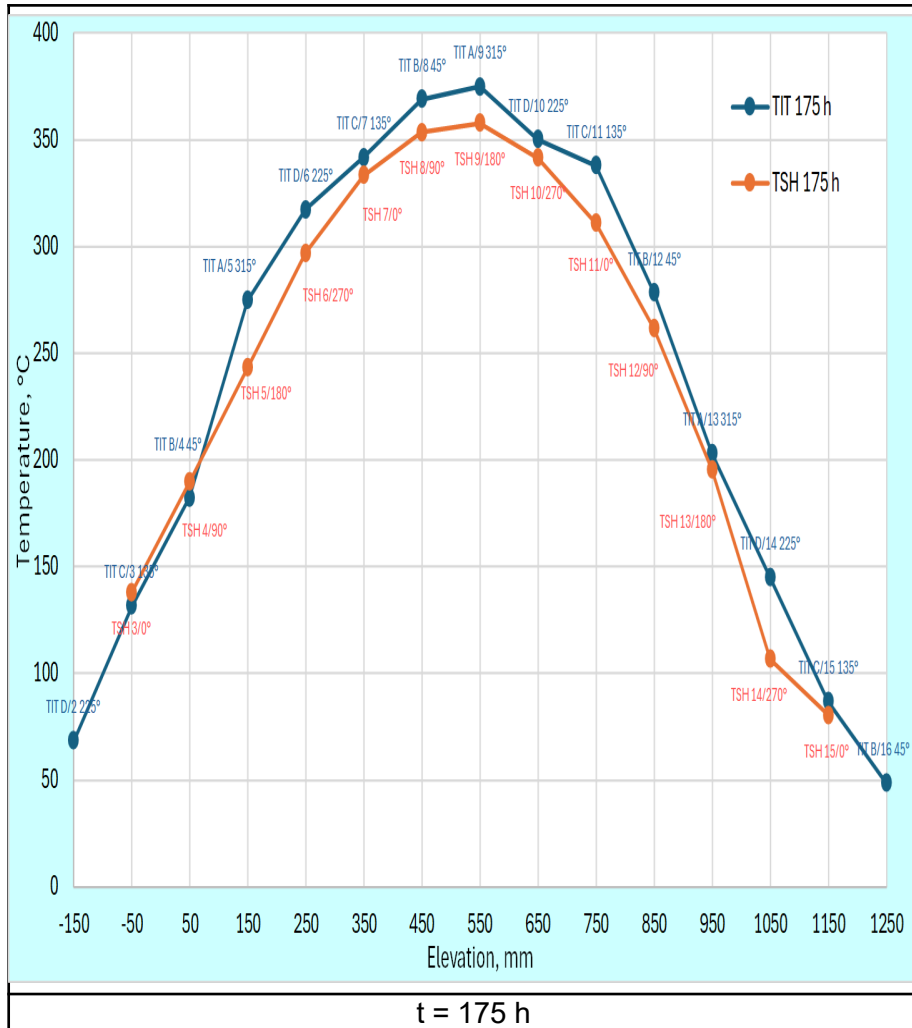


# Radial temperature distribution



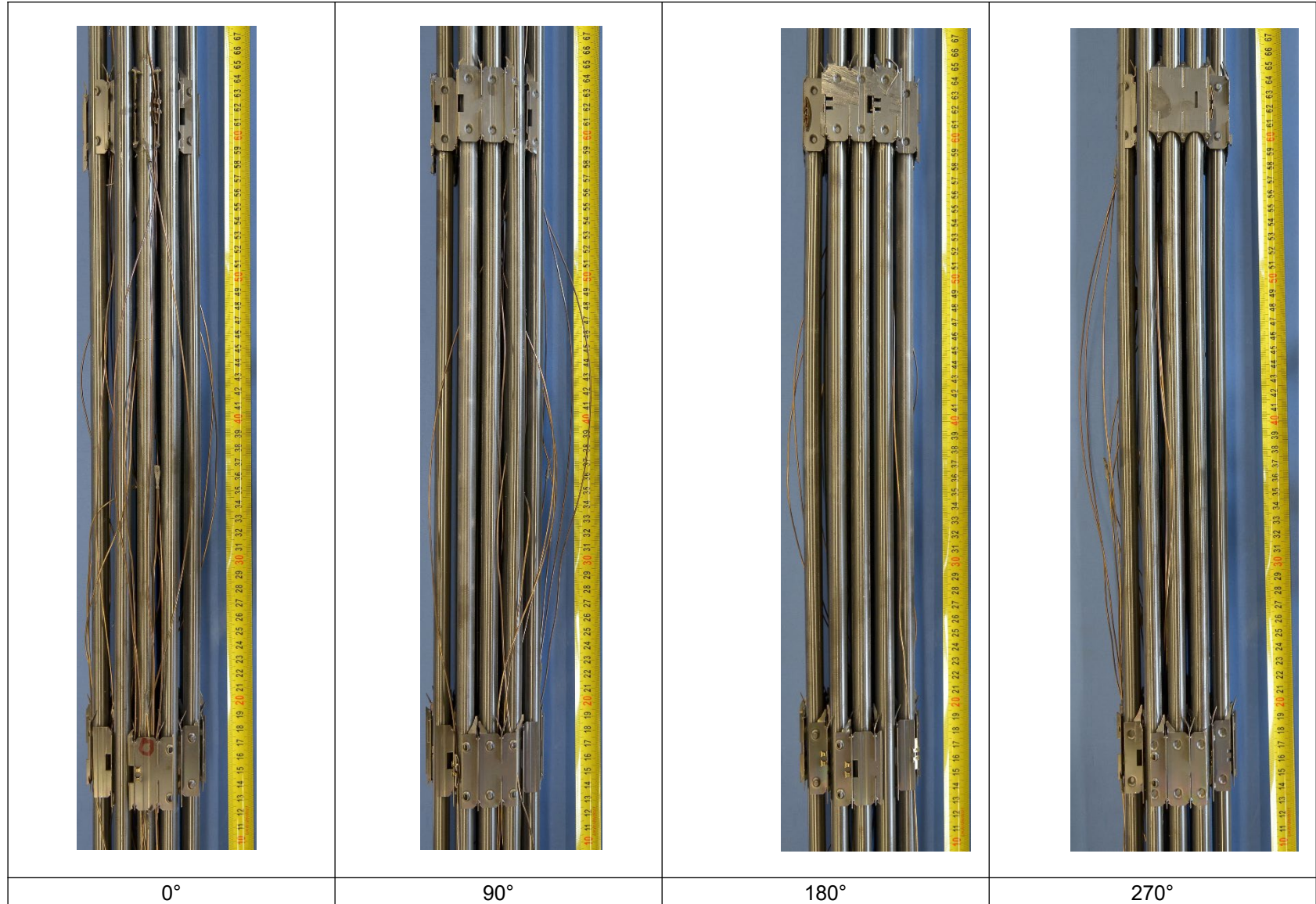
**The radial temperature gradient: 40 K (test start), 30 K (test end)**

# Indirect estimation of radial symmetry in bundle: comparison of corner rods and shroud temperatures



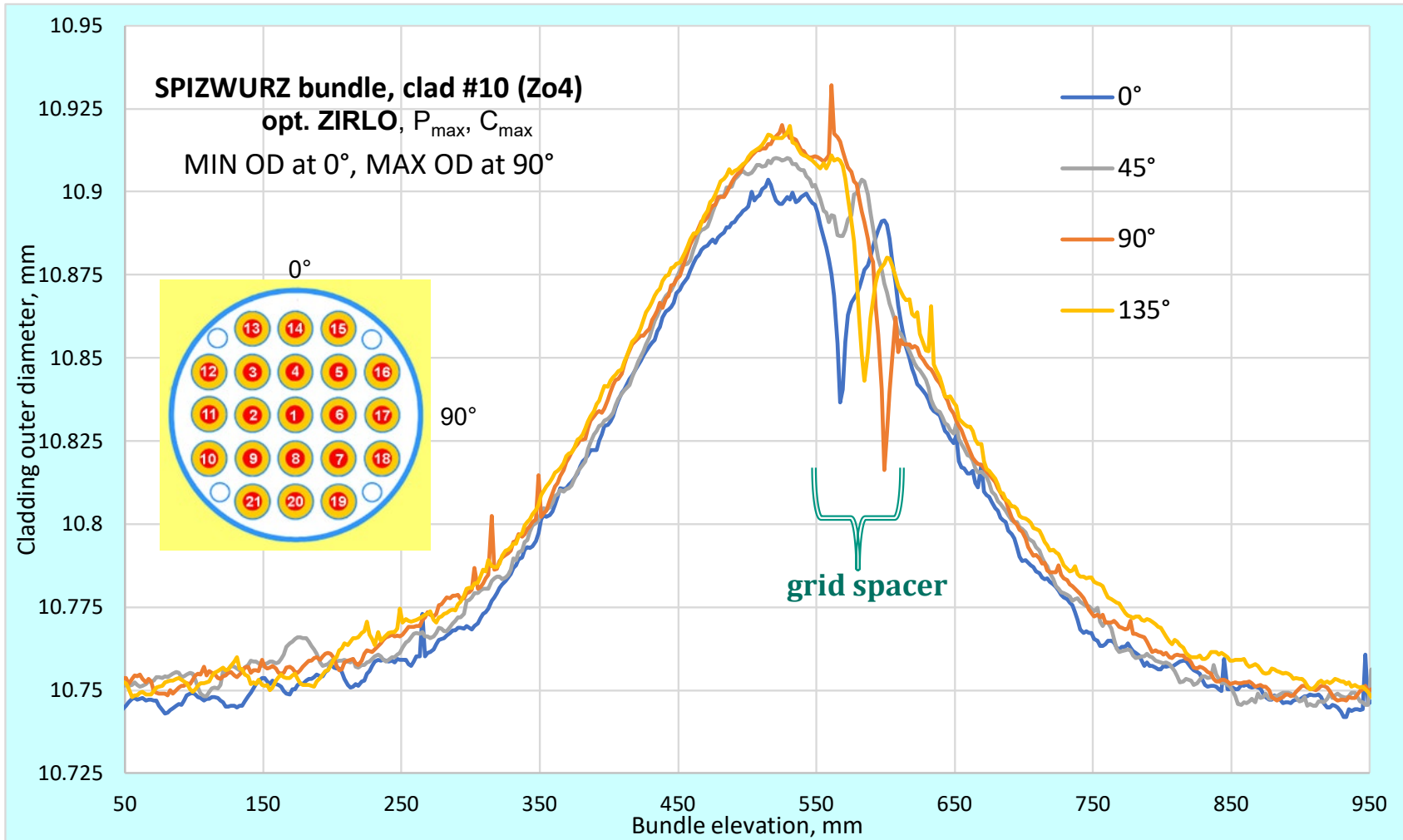
**The circumferential temperature scatter is  $\pm 8$  °C at the beginning of the test and  $\pm 5$  °C before the end of the test**

# SPIZWURZ bundle: post-test view between two middle grid spacers



# Results of creep measurements with the laser scanner:

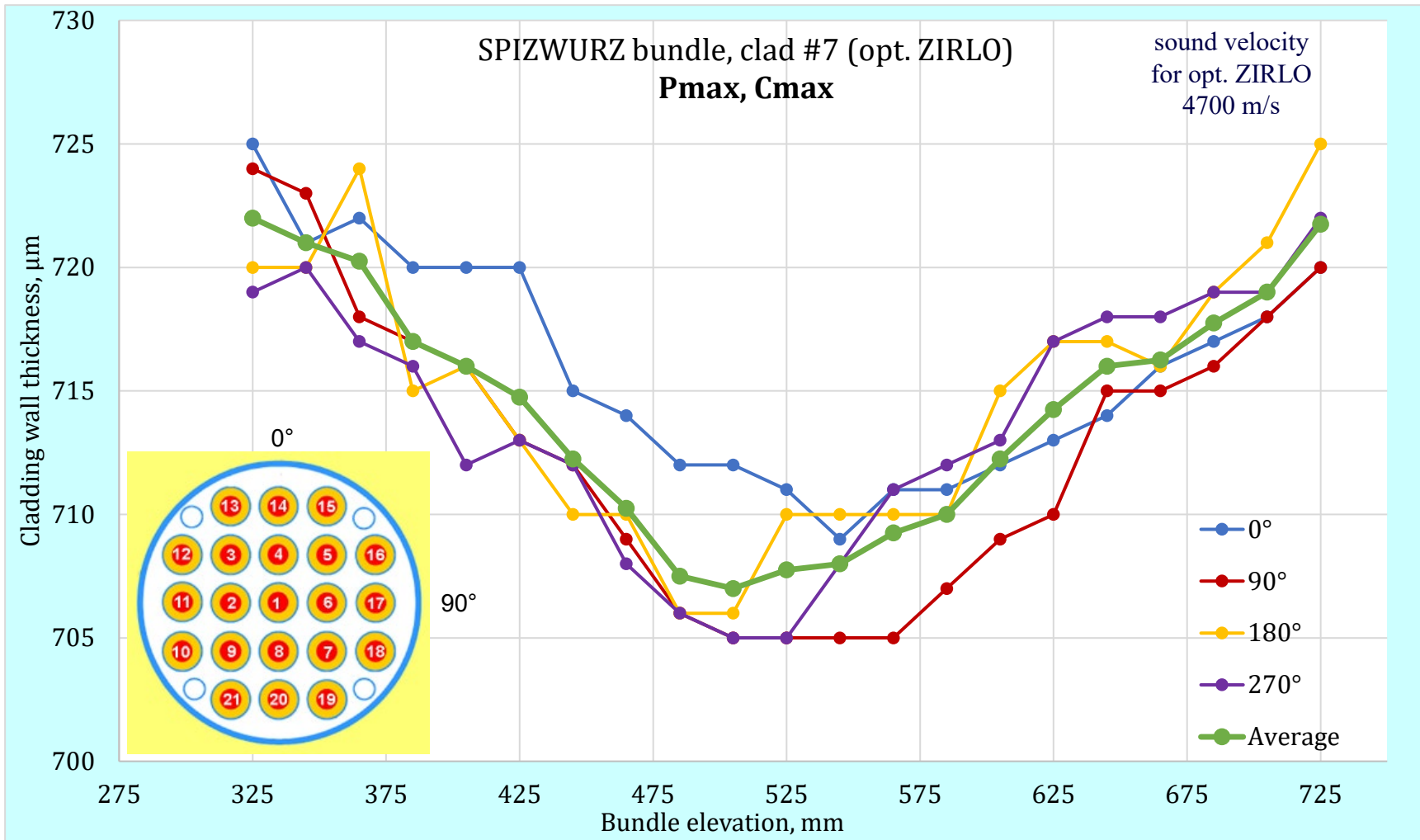
- 1) small ovality of cladding (comparison of scanning at 4 angles);
- 2) influence of grid spacer springs (creep limitation)



Max cladding ovality  $OD_{max} - OD_{min} = 20 \mu\text{m}$  at 520 mm (hottest bundle elevation);  
 average ovality along the cladding is  $8 \mu\text{m}$ , what is comparable with delivered ovality of  $5 \mu\text{m}$

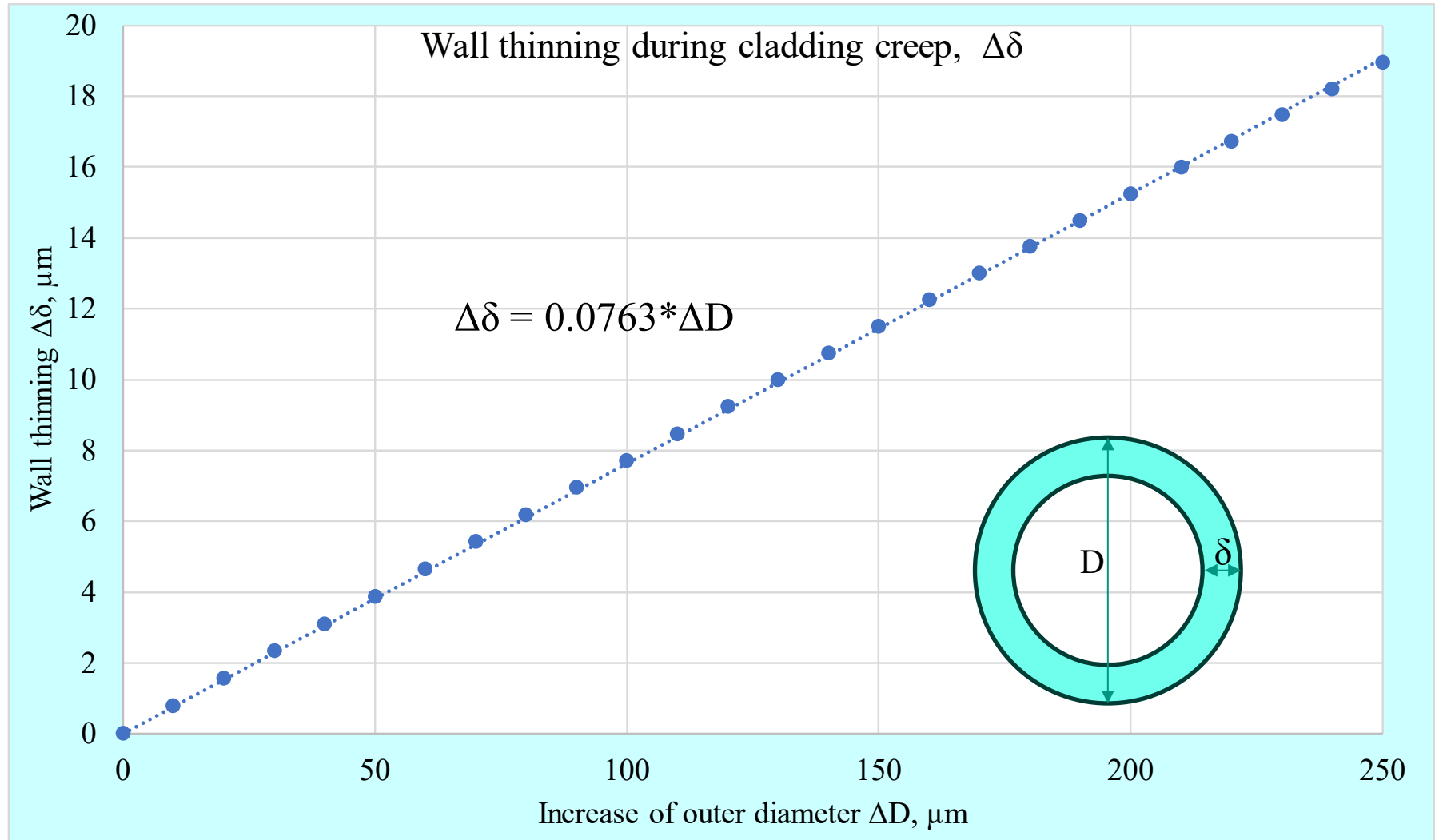


# Ultrasound measurements of wall thickness along four cladding sides: not symmetrical wall thinning at each bundle elevation

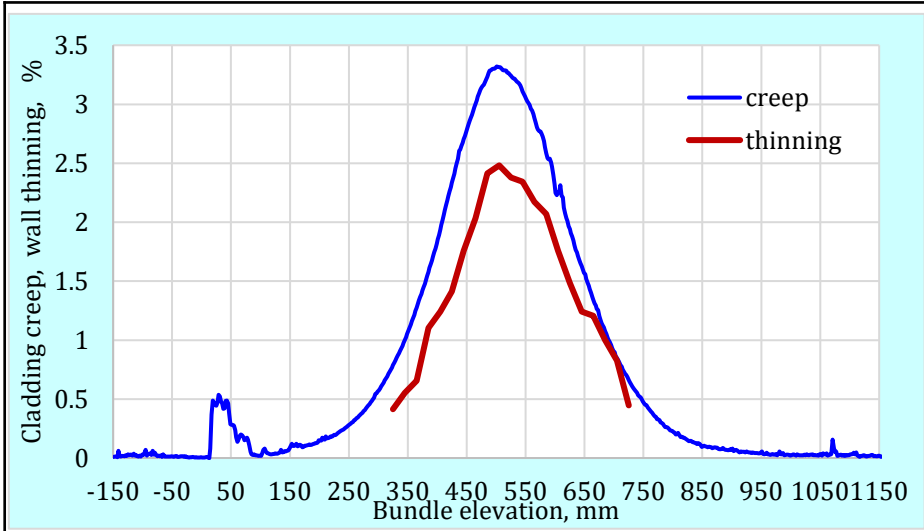


The probable reason of the asymmetrical thinning could be a shift of the pellets from the midline

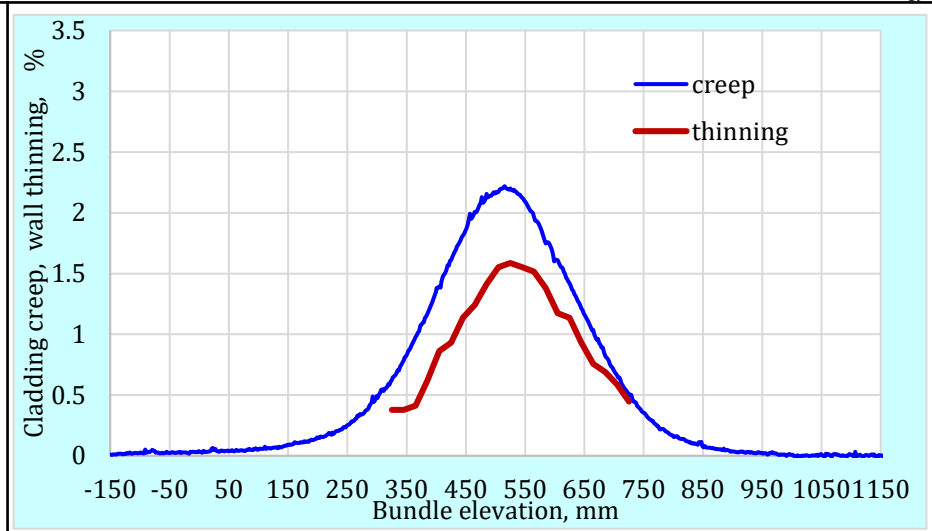
# 2D wall thinning during cladding creep (cross-section area change): calculated dependence of thinning on the increase in outer diameter



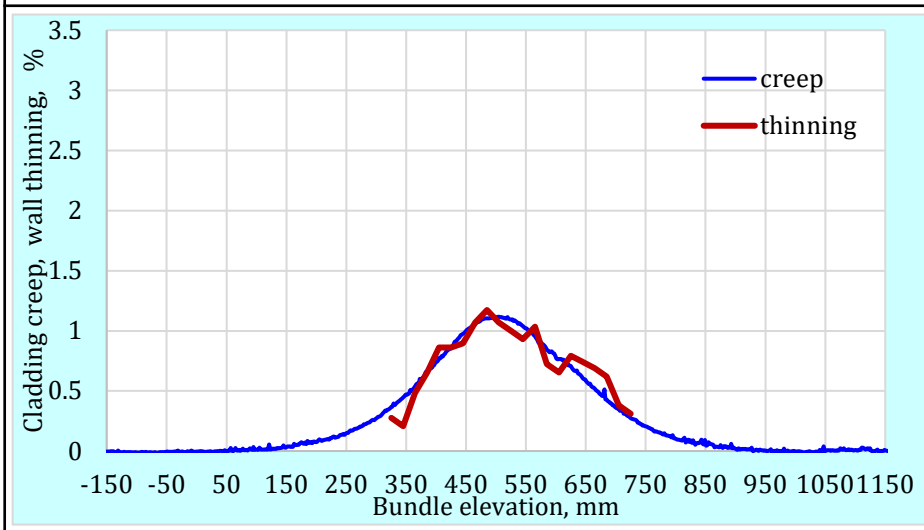
# opt. ZIRLO: cladding creep, wall thinning



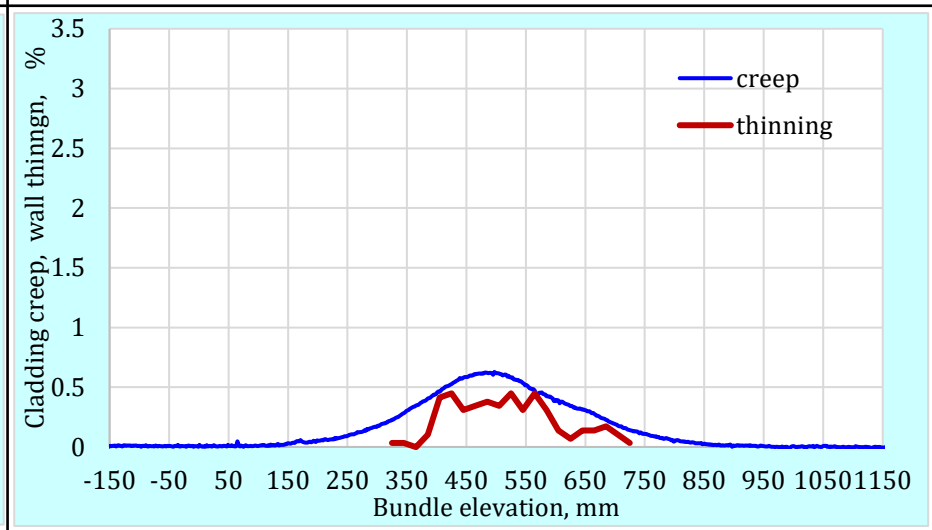
cladding 7: opt. ZIRLO, Pmax, Cmax



cladding 3: opt. ZIRLO, Pmax, Cmin

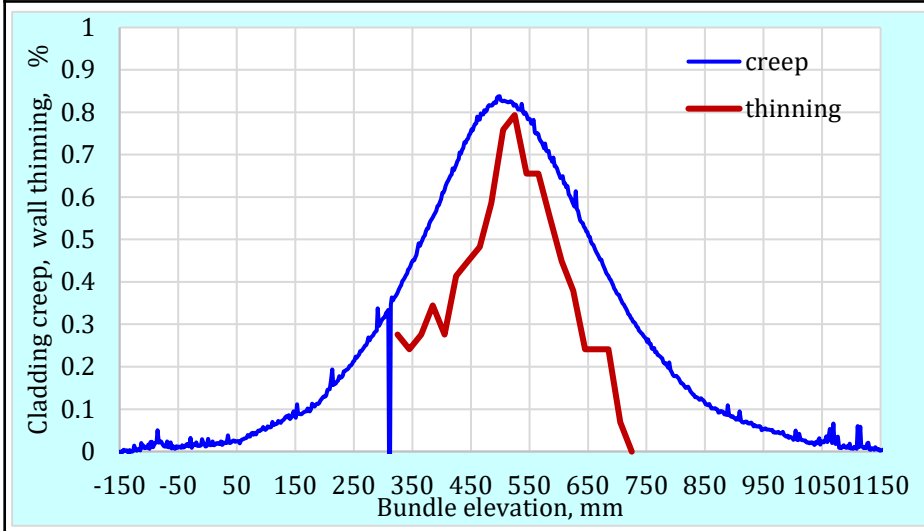


cladding 5: opt. ZIRLO, Pmin, Cmax

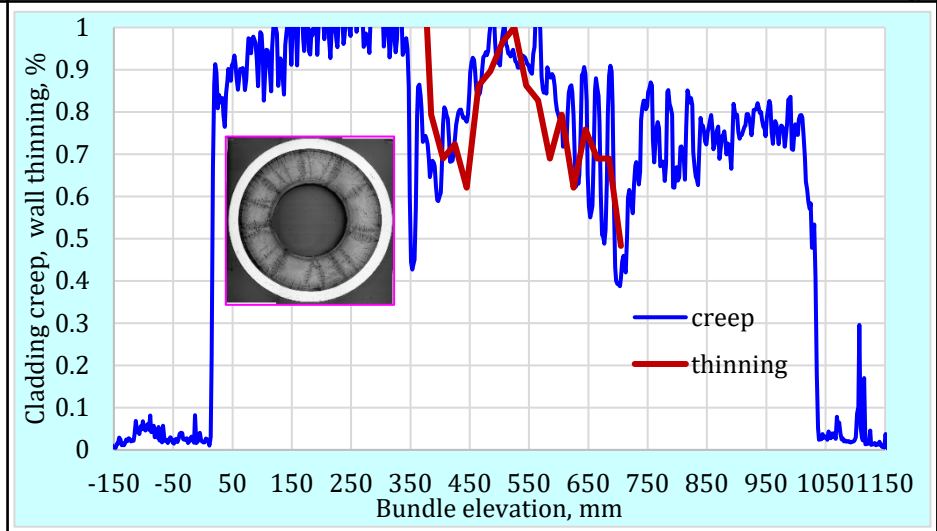


cladding 13: opt. ZIRLO, Pmin, Cmin

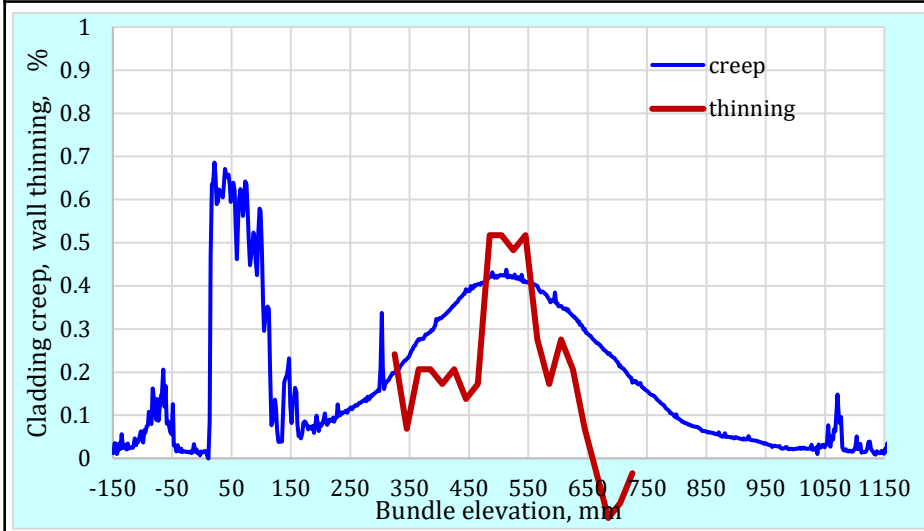
# Zry-4: cladding creep, wall thinning



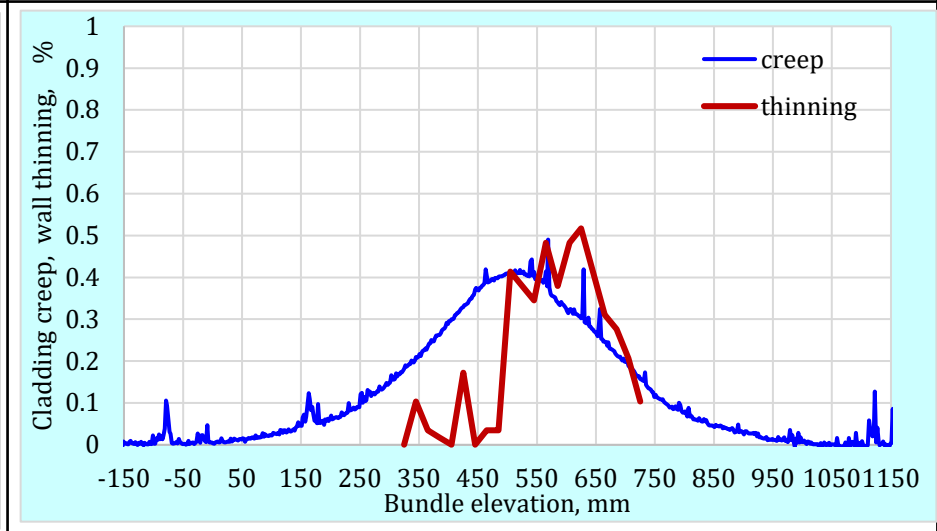
cladding 2: Zry-4, Pmax, Cmax



cladding 8: Zry-4, Pmax, Cmin;  
contact of the cladding with the extended pellet

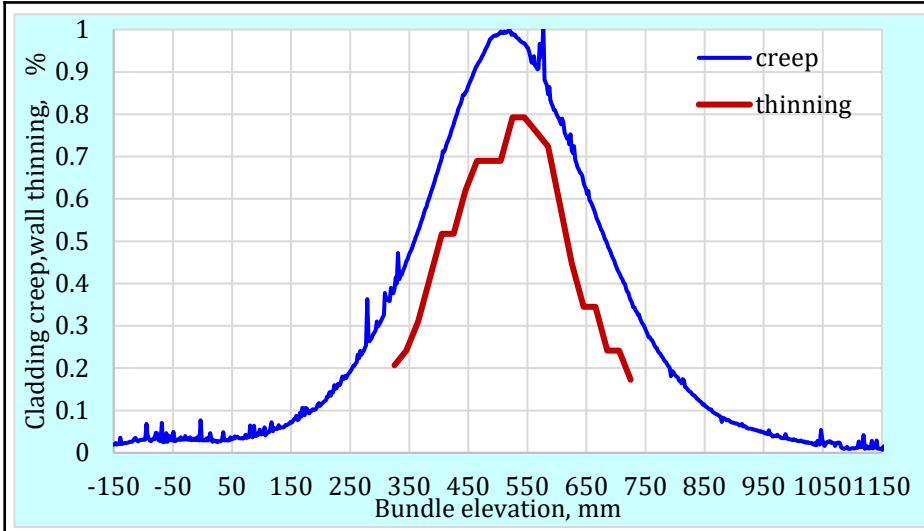


cladding 6: Zry-4, Pmin, Cmax

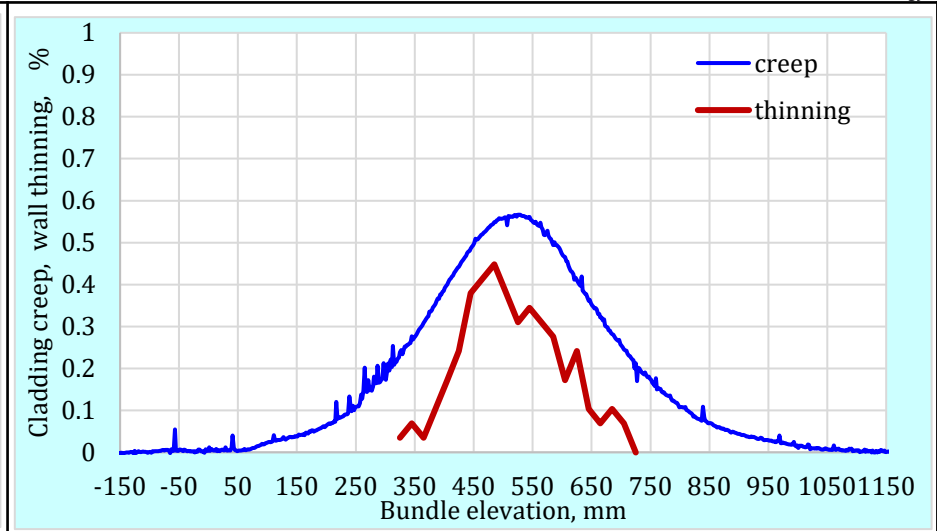


cladding 4: Zry-4, Pmin, Cmin

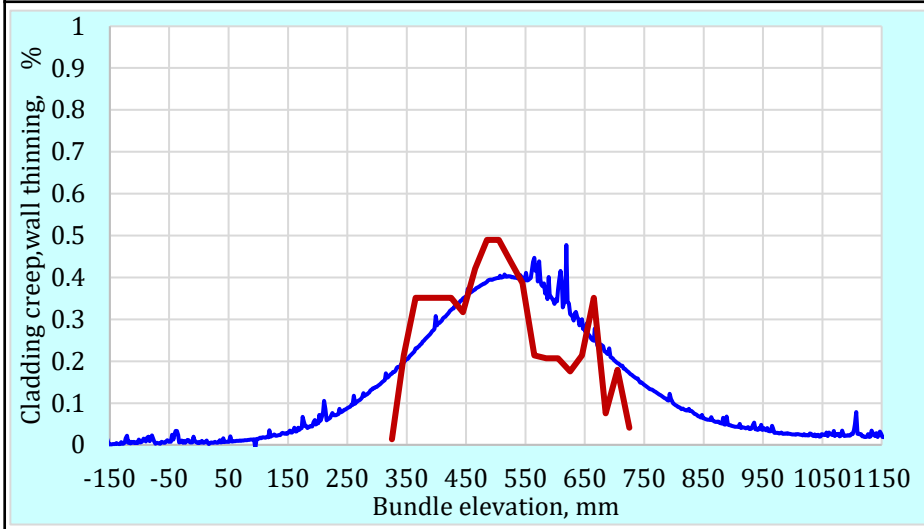
# DX-D4 claddings: cladding creep, wall thinning



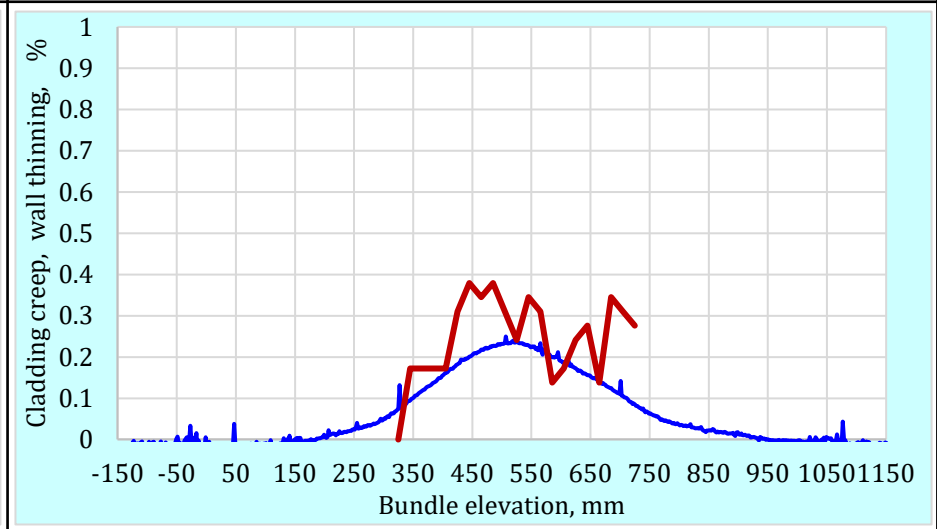
cladding 1: DX-D4, Pmax, Cmax



cladding 21: DX-D4, Pmax, Cmin



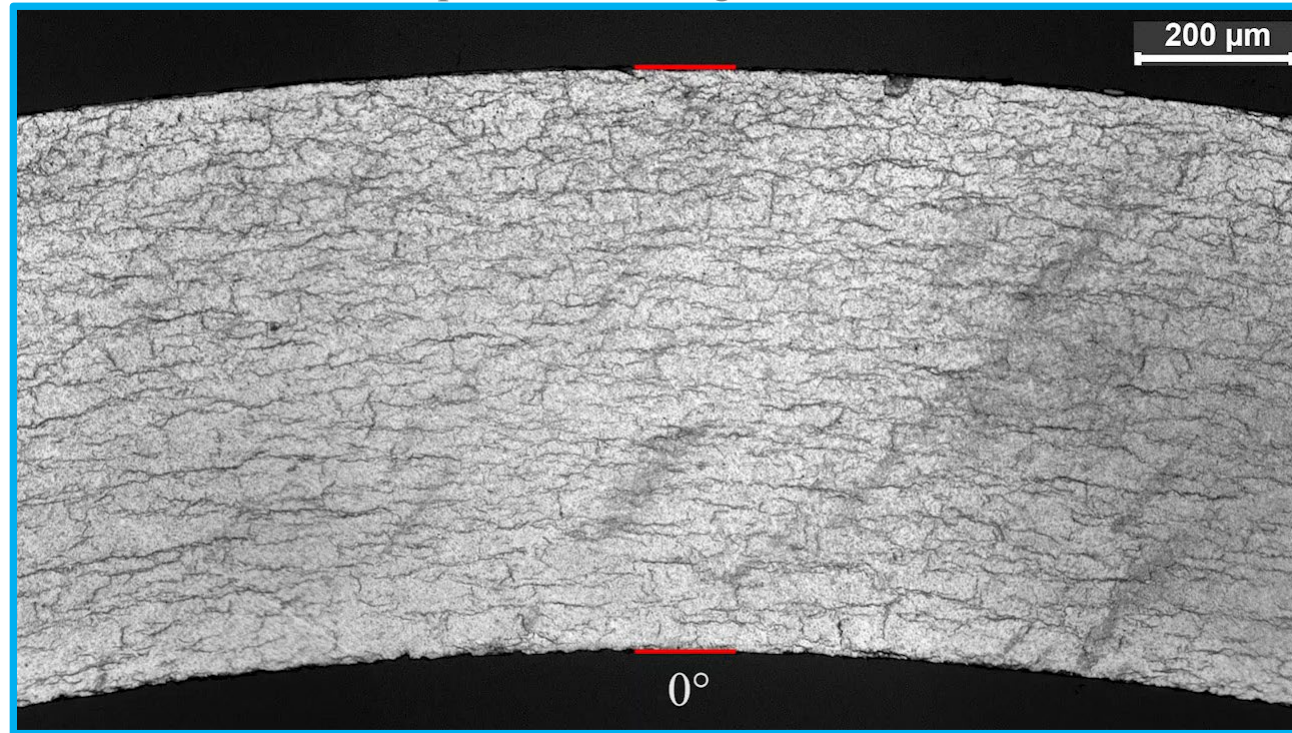
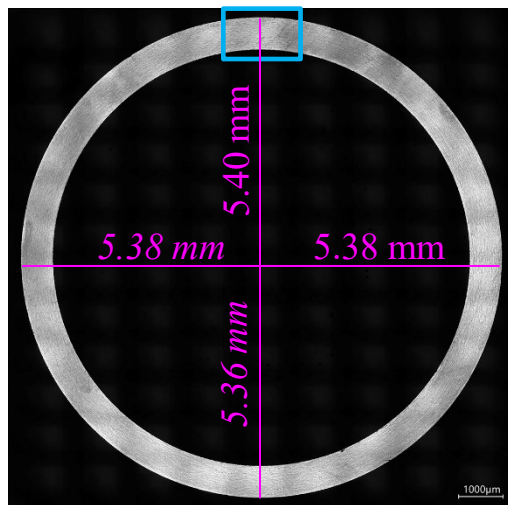
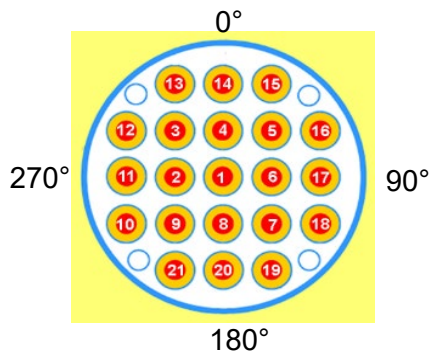
cladding 9: DX-D4, Pmin, Cmax



cladding 13: opt. ZIRLO, Pmin, Cmin

# Post-test clad #11 (Zry-4, 146 bar, 300 wppm H), elevation 520 mm: metallographic observation of hydrides and cladding thinning

Link to movie: <https://www.doi.org/10.5445/IR/1000189500>

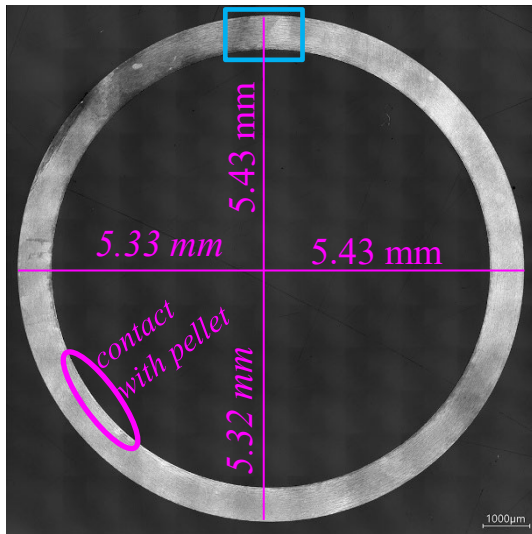
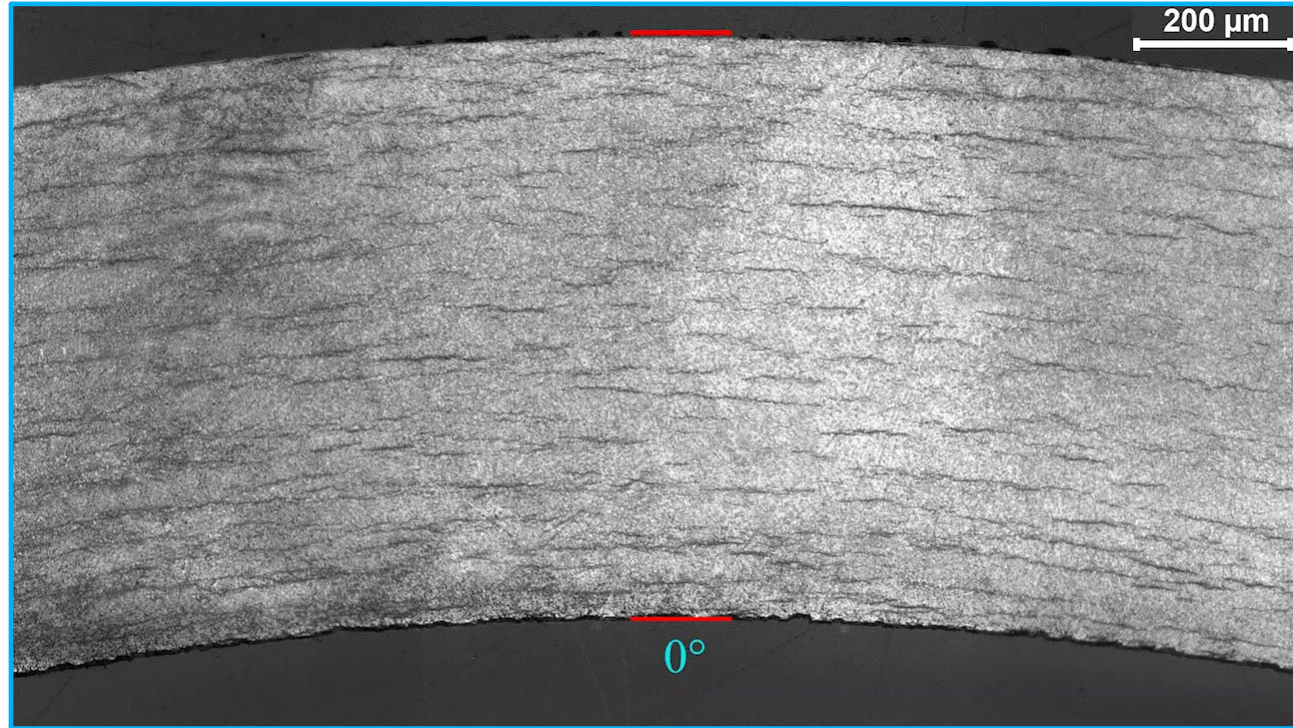
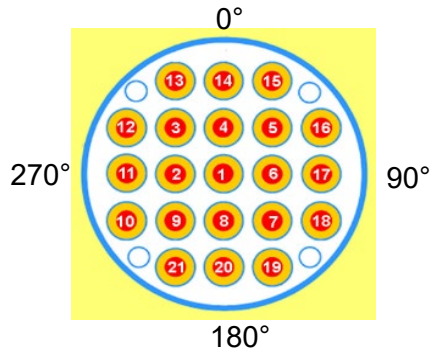


- Circumferential homogeneity of hydrides appearance;
- Not very radial symmetry for the wall thinning:

angle	wall thickness, $\mu\text{m}$
0°	721
90°	718
180°	711
225°	708
270°	710

# Post-test clad #10 (opt. ZIRLO, 146 bar, 300 wppm H), elevation 320 mm: metallographic observation of hydrides and cladding thinning

Link to movie: <https://www.doi.org/10.5445/IR/1000189571>



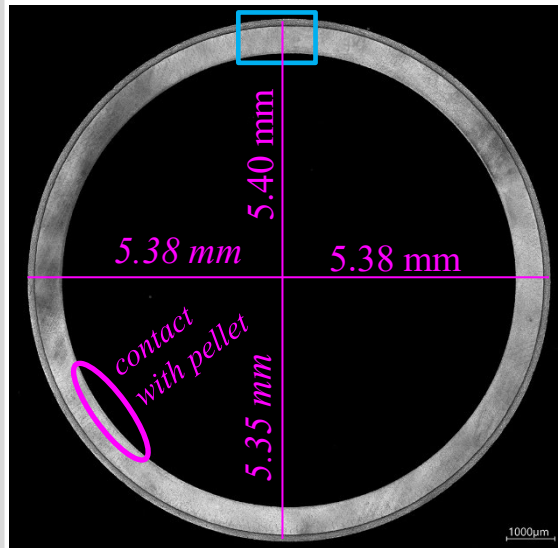
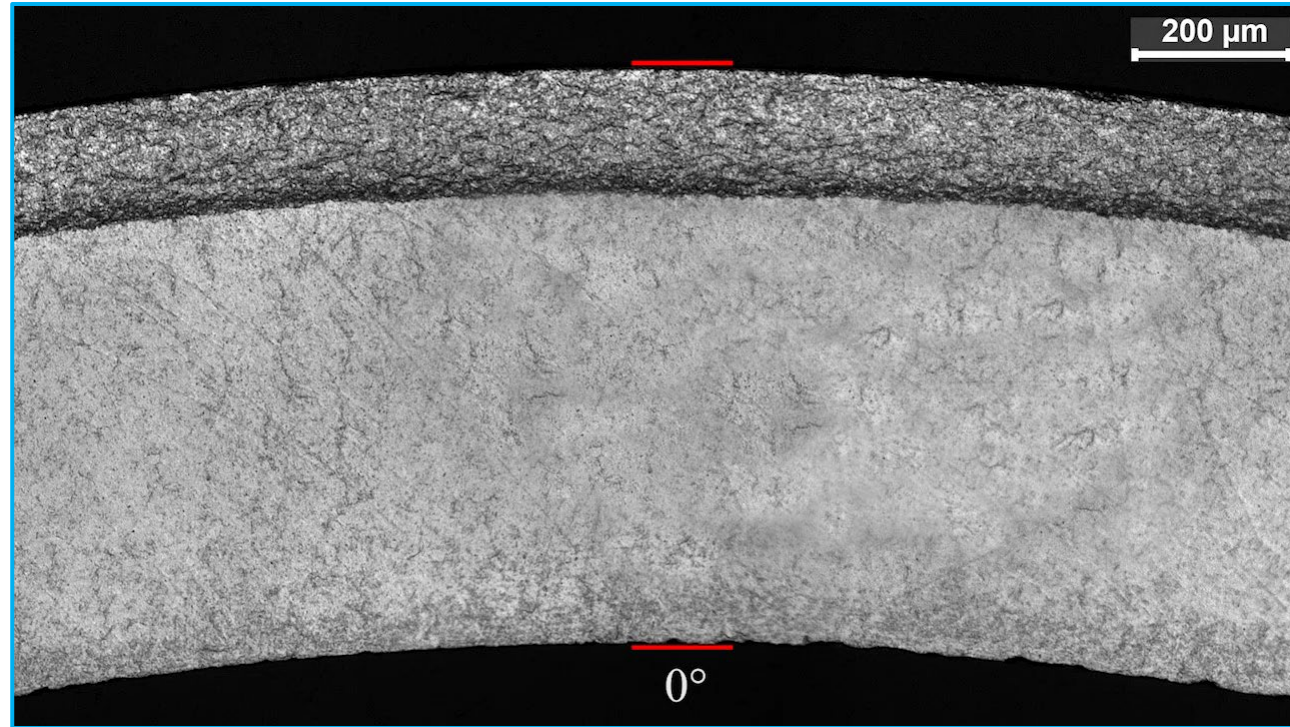
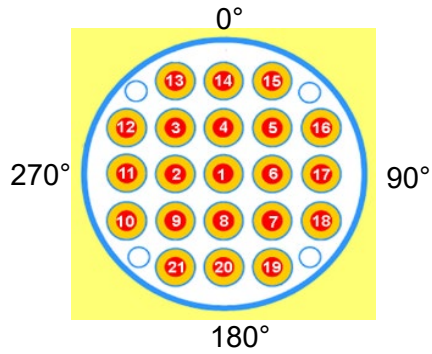
Eccentricity

- Circumferential homogeneity of hydrides appearance;
- Not very radial symmetry for the wall thinning:

angle	wall thickness, $\mu\text{m}$
0°	721
90°	724
180°	719
225°	716
270°	716

# Post-test clad #1 (DX-D4, 146 bar, 300 wppm H), elevation 520 mm: metallographic observation of hydrides and cladding thinning

Link to movie: <https://www.doi.org/10.5445/IR/1000189574>



Eccentricity

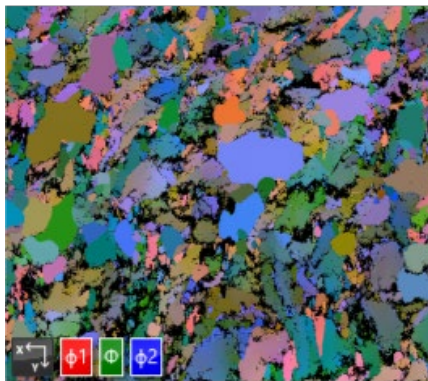
- Circumferential homogeneity of hydrides appearance;
- Not very radial symmetry for the wall thinning:

angle	wall thickness, µm
0°	716
90°	724
180°	720
225°	712
270°	713



# Grain growth during hydrogenation and following bundle test for Zry-4: fresh, hydrogenated, post-test samples

Euler Color 1



10µm

Euler Color 1

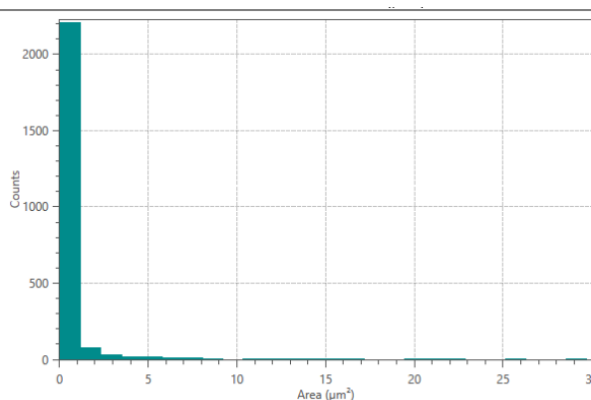


10µm

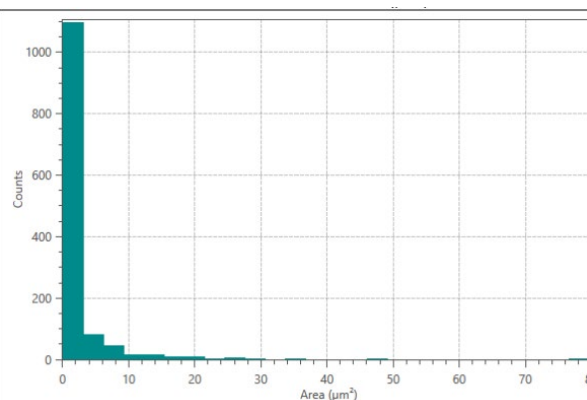
Euler Color 1



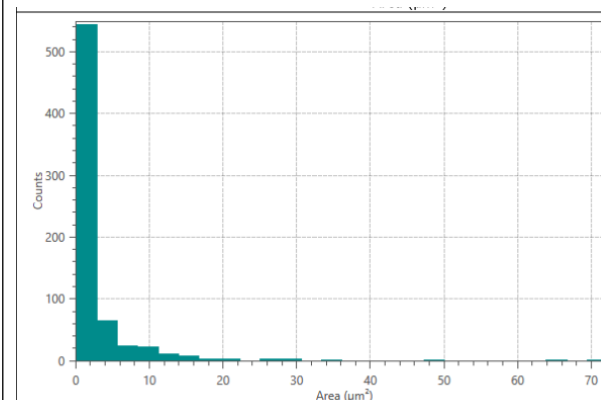
10µm



as-received: weight mean  $5.74 \pm 1.67 \mu\text{m}^2$ ,  
max  $28.58 \mu\text{m}^2$ , grains 2387

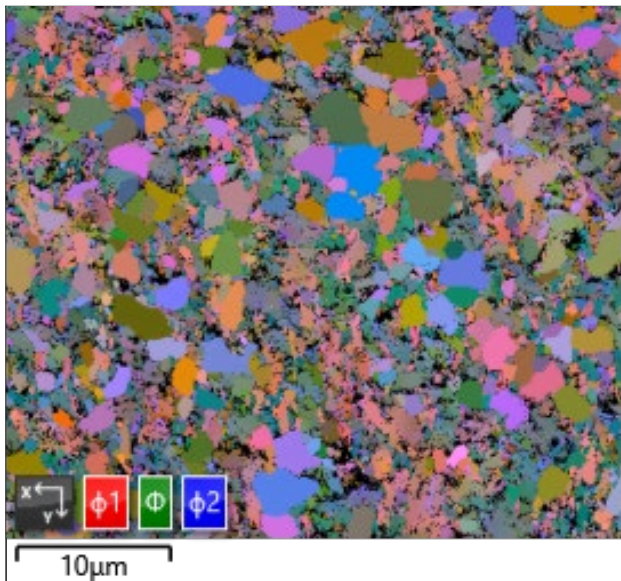


300 wppm H: weight mean  $12.79 \pm 4.54 \mu\text{m}^2$ ,  
max  $76.68 \mu\text{m}^2$ , grains 1282

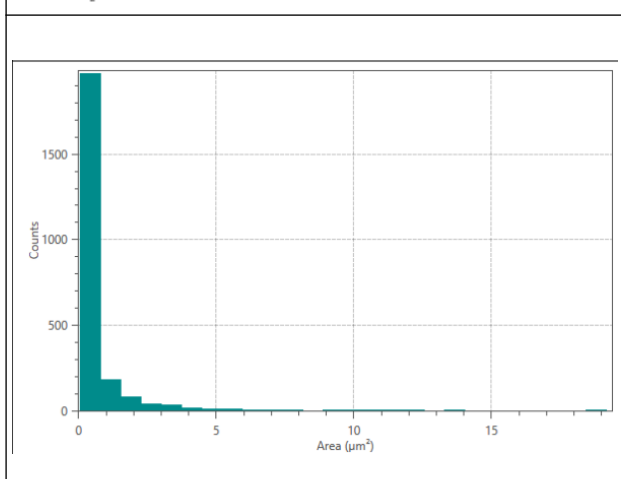
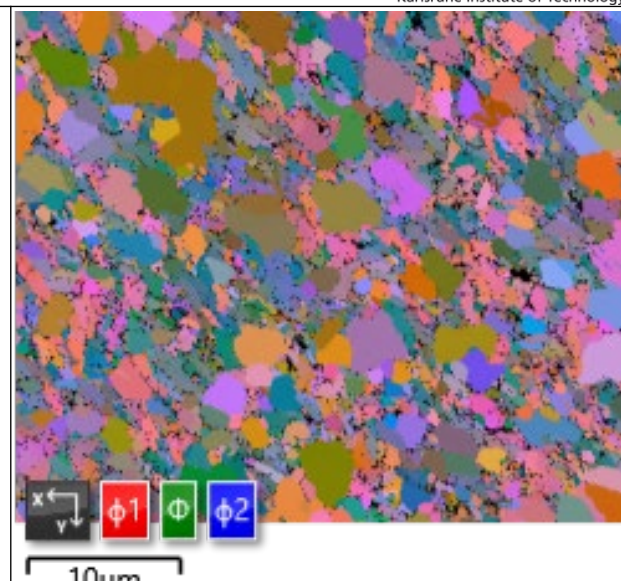


bundle, 300 wppm H: weight mean  $16.02 \pm 5.66 \mu\text{m}^2$ ,  
max  $69.46 \mu\text{m}^2$ , grains 685

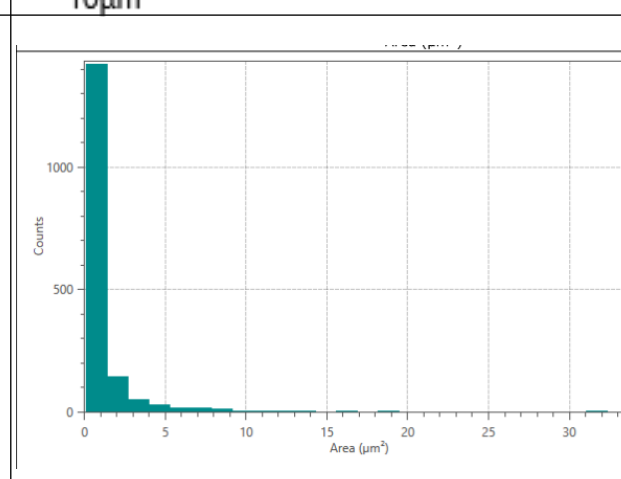
# Grain growth during hydrogenation and following bundle test for opt. ZIRLO: fresh, hydrogenated, post-test samples



not available



not available



as-received: weight mean  $2.92 \pm 1.16 \mu\text{m}^2$ ,  
max  $18.46 \mu\text{m}^2$ , grains 2363

300 wppm H

bundle, 300 wppm H: weight mean  $4.33 \pm 1.72 \mu\text{m}^2$ ,  
max  $32.37 \mu\text{m}^2$ , grains 1696

## Summary

- For the long-term SPIZWURZ bundle experiment, zirconium alloy tubes (opt. ZIRLO, Zry-4, DX-D4) were charged with hydrogen to 100 and 300 wppm in the special developed HOKI tube oven as homogeneously as possible along a length of 1.3 m.
- The hydrogenation was carried out at 450 °C by successively supplying fixed masses of hydrogen through the specially treated **inner** surface of claddings.
- After the hydrogen loading of the samples, the axial distribution of hydrogen was determined by laser scanning profilometry (calibrated by hot gas extraction).
- A long-term bundle test with 21 hydrogenated and pressurized cladding tubes began on 12.05.2023 and terminated on 17<sup>th</sup> January 2024. Two pressure set values were used: 106 and 146 bar. Due to small leaks in some of the rods, it was decided to maintain the pressure constant in all rods throughout the experiment (lasted 250 days) by periodically injecting the Ar+O<sub>2</sub> gas mixture refilled; oxygen was used for oxidation of the inner cladding surface to avoid hydrogen release from the cladding. The rod #18 was not pressurized and could be used as reference rod.
- The peak cladding temperature decreased in steps of  $\approx 15$  K from 400 to 165 °C (average cooling rate  $\approx 0.9$  K/day). The maximal cooling rate during each temperature step was 6 K/h, step duration was about 10 h.

## Summary (cont.)

- The post-test laser scanner measurements of the outer cladding diameter showed significant creep: radial deformation values are between 0.2 and 3.3% (diameter increase and the corresponding wall thinning).
- The largest creep of 3.3% was measured for opt. ZIRLO claddings hydrogenated to 300 wppm. The corresponding maximum creep value was 0.93% for Zry-4 and 1% for DX-D4.
- A clearly visible dependence of the degree of creep on the hydrogen concentration is observed for the opt. ZIRLO claddings: the creep of claddings hydrogenated to 300 ppm is 1.2-1.5 times higher than that of claddings hydrogenated to 100 ppm.
- A number of claddings show radially asymmetric wall thinning, which can be associated with the radial shift of the pellets from the central axis of the rod and the corresponding asymmetric heat supply along the circumference of the cladding.
- The metallographic investigations revealed a uniform distribution of hydrides throughout the entire cladding circumference for all three cladding types used. In the DX-D4 claddings, hydrogen primarily diffused toward the outer liner.
- The degree of hydride reorientation was significantly higher in the Zry-4 claddings compared to the opt. ZIRLO claddings.
- The difference in the behavior of the Zry-4 and opt. ZIRLO may be due, in part, to their different grain microstructures. Opt. ZIRLO claddings have a finer grain size than Zry-4. Moreover, although the temperatures during hydrogenation (450 °C) and the experiment itself (max. 400 °C) were relatively low, EBSD measurements showed grain growth from approx. 6 μm for the initial state to post-test 16 μm for Zry-4 (12 μm after hydrogenation), and from initial 3 μm to post-test 4.3 μm for opt. ZIRLO.

*Thank you for your attention*

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<http://quench.forschung.kit.edu/>



**Mikhail Kolesnik**

KIT

## **Hydride Morphology in Zirconium Tubes After SPIZWURZ Bundle Tests: Experimental Data and Preliminary Simulation Results**

Hydride embrittlement of zirconium cladding is a major safety concern when handling and long-term dry storage of spent nuclear fuel. The degree of embrittlement is strongly influenced by the morphology of hydrides, which includes their orientation, size, spacing, and connectivity. Under dry storage conditions, a thermomechanical cycle involving heating and subsequent slow cooling of fuel rods under internal excessive gas pressure can promote hydride reorientation in the cladding. This scenario can result in the formation of radially oriented hydrides, making the material more brittle than in its pre-storage state.

This study presents new detailed experimental data on hydride morphology in Zircaloy-4 tubes obtained from the SPIZWURZ bundle test conducted at the Karlsruhe Institute of Technology (KIT) at the LICAS facility. The test involved a 21-rod bundle that was subjected to a 250-day, stepwise cooling sequence under different internal gas pressures to simulate the thermo-mechanical conditions of dry storage. Measured parameters include the radial hydride fraction, hydride length and density, and continuity metrics such as the Hydride Continuity Coefficient (HCC) and Radial Hydride Continuity Path (RHCP).

The experimental results were compared with simulations obtained using two modeling approaches. The first approach is a kinetic ordinary differential equation (ODE)-based model capable of reproducing the average morphological parameters as functions of stress, temperature, and hydrogen content. The second approach is MORPHYD, a 3D numerical tool that simulates the nucleation and diffusion-controlled growth of disc-shaped hydrides on a virtual domain. This enables the evaluation of network connectivity and statistics of morphology parameters.

While not all samples have been fully analyzed, initial benchmarking results demonstrate consistent trends between experiments and the two modeling tools. These findings confirm the approaches' suitability for predicting hydride morphology evolution and provide a solid basis for validating them on the complete SPIZWURZ dataset.

# Hydride Morphology in Zirconium Tubes After SPIZWURZ Bundle Tests: Experimental Data and Preliminary Simulation Results

**M. Kolesnik, J. Stuckert, M. Grosse, S. Weick**

*30<sup>th</sup> International QUENCH –Workshop, Karlsruhe, Germany*

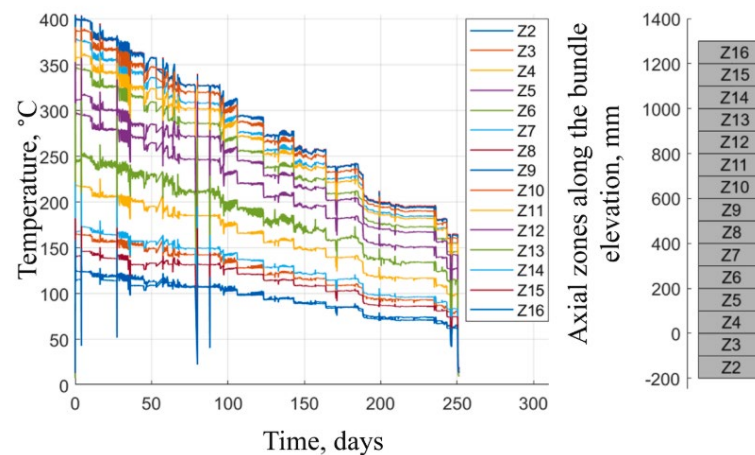
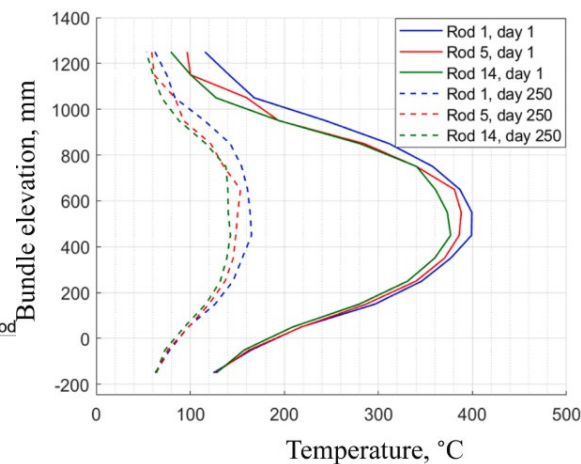
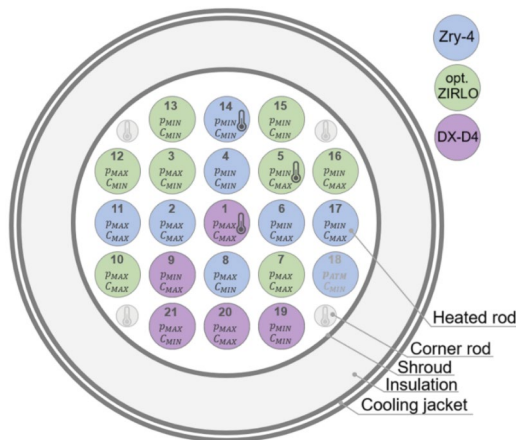
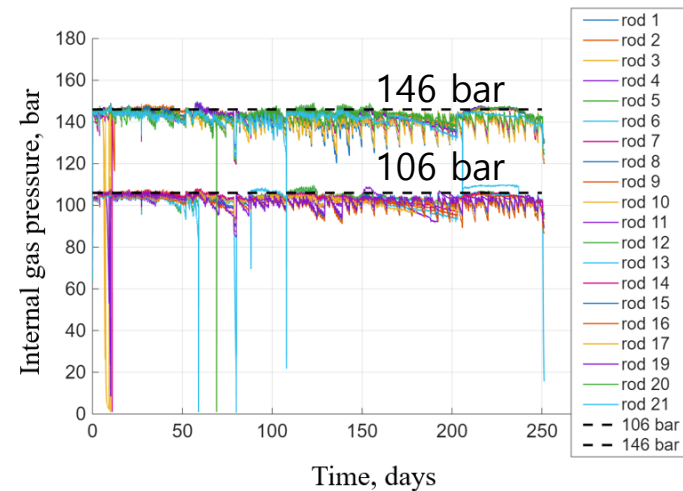
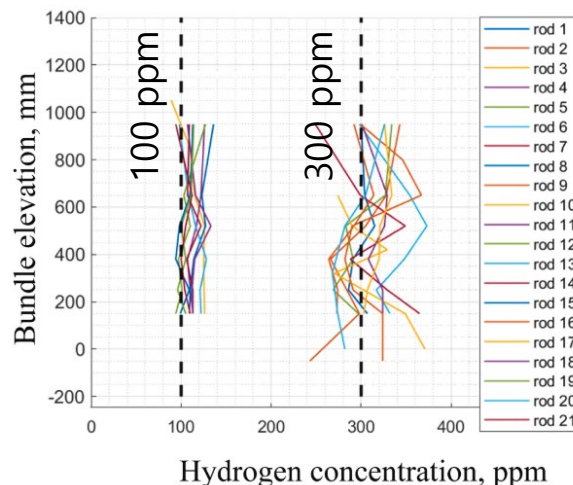
Institute for Applied Materials; Program NUSAFE



# SPIZWURZ bundle test experimental conditions

## SPIZWURZ bundle:

- 21 cladding tubes
- Zircaloy-4, opt. ZIRLO, duplex DX-D4
- internal gas loading
- stepwise cooling over 250 days

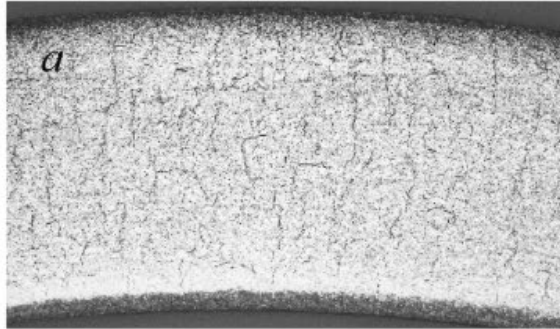




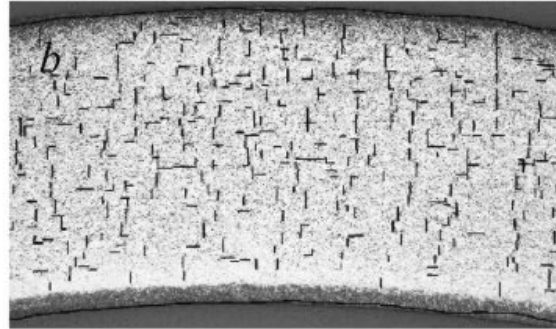
# SPIZWURZ bundle test

## hydride morphology measurement

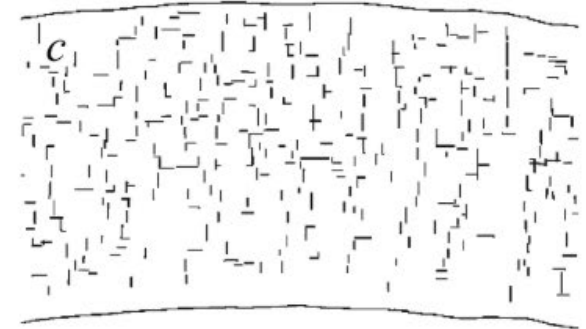
### Two-step micrograph processing



Initial micrograph



Manual phase



Numerical processing

### Measured parameters:

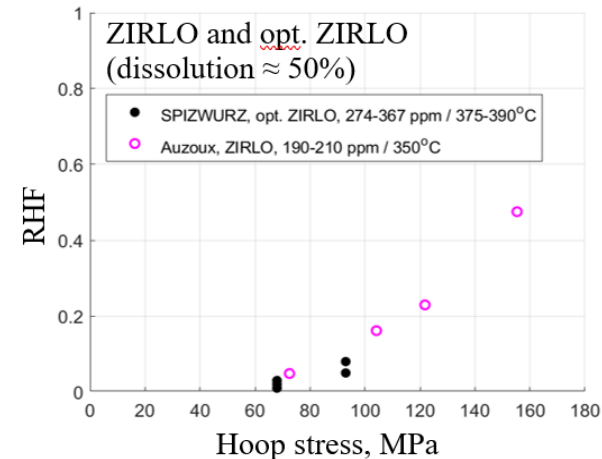
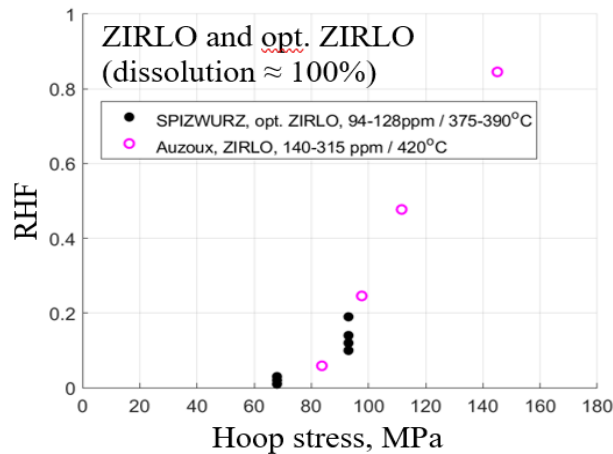
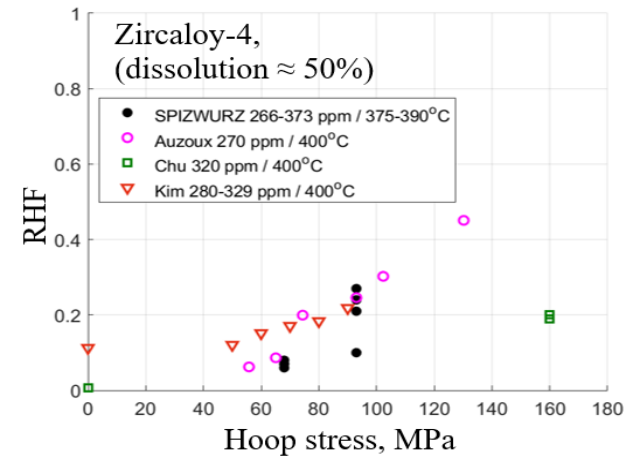
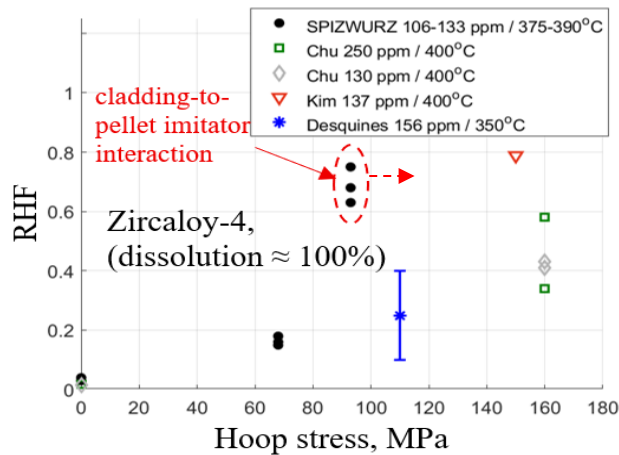
- Radial hydride fraction (RHF)
- Hydride Continuity Coefficient (HCC)\*
- Radial Hydride Continuity Path (RHCP)\*\*
- Length of hydrides (with statistical distribution)
- Surface density of hydrides
- Hydride length density

\*HCC – the total projection length of hydrides within 110  $\mu\text{m}$  in the radial direction, normalized by thickness

\*\*RHCP – fracture energy estimated from varying crack paths, normalized to the unhydrided sample

# SPIZWURZ bundle test results

## radial hydride fraction (RHF)

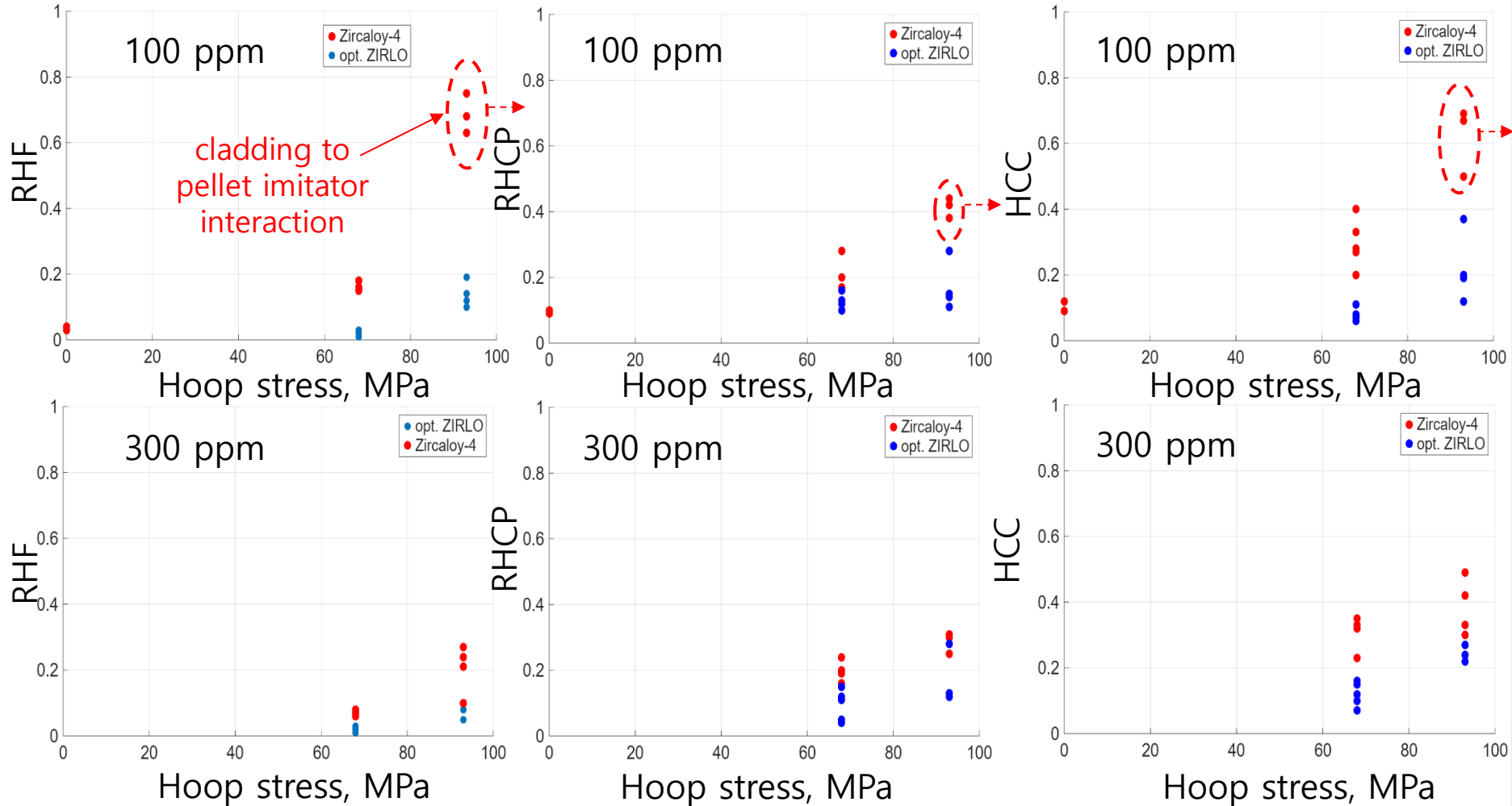


**RHF increases with hoop stress, in agreement with previously published data**

- [1] Q. Auzoux et al., J. Nucl. Mat. 494 (2022) 153893, DOI: 10.1016/j.jnucmat.2022.153893
- [2] J. Desquines et al., WRFPM (2023), 80-86, DOI: 10.1007/978-981-99-7157-2\_8
- [3] H.C. Chu, S.K. Wu and R.C. Kuo, J. Nucl. Mat. 373 (2008) 319-327, DOI: 10.1016/j.jnucmat.2007.06.012
- [4] Y.J. Kim et al. J. Nucl. Sci. Technol. 52 (2014) 717-727, DOI: 10.1080/00223131.2014.978829

# SPIZWURZ bundle test results

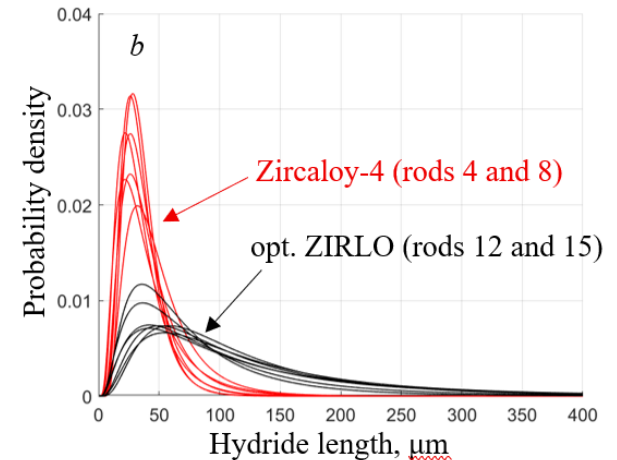
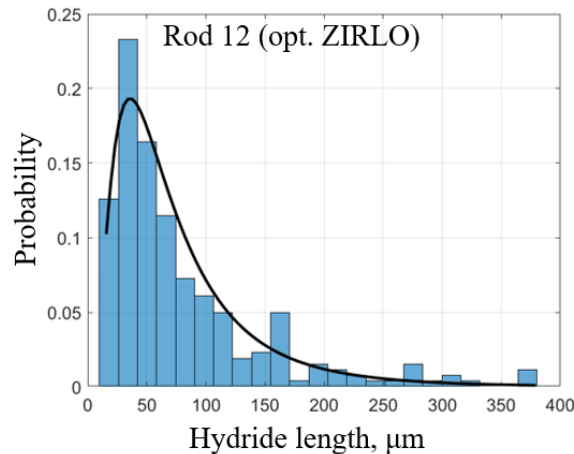
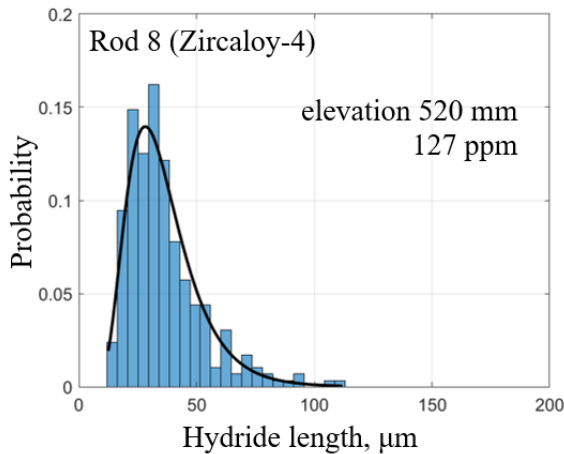
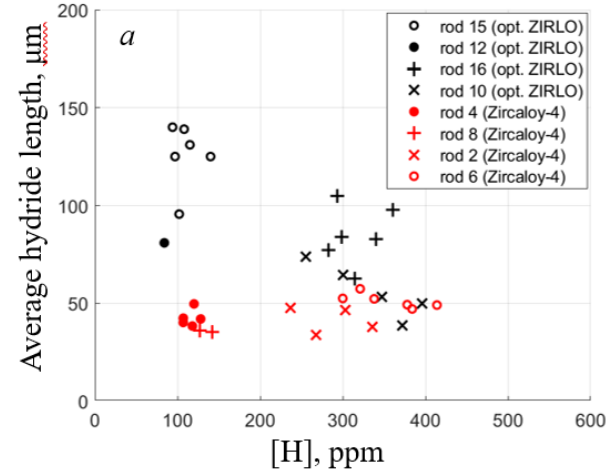
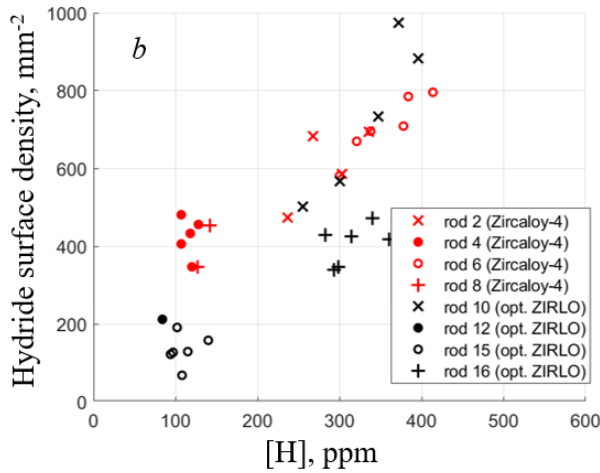
## *hydride reorientation: Zircaloy-4 vs. opt. ZIRLO*



**Hydride reorientation is more pronounced in Zircaloy-4 than in the opt. ZIRLO**

# SPIZWURZ bundle test results

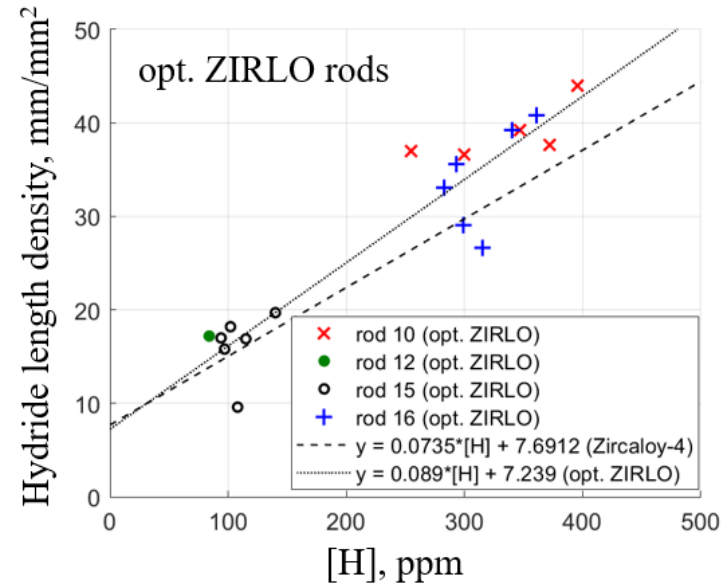
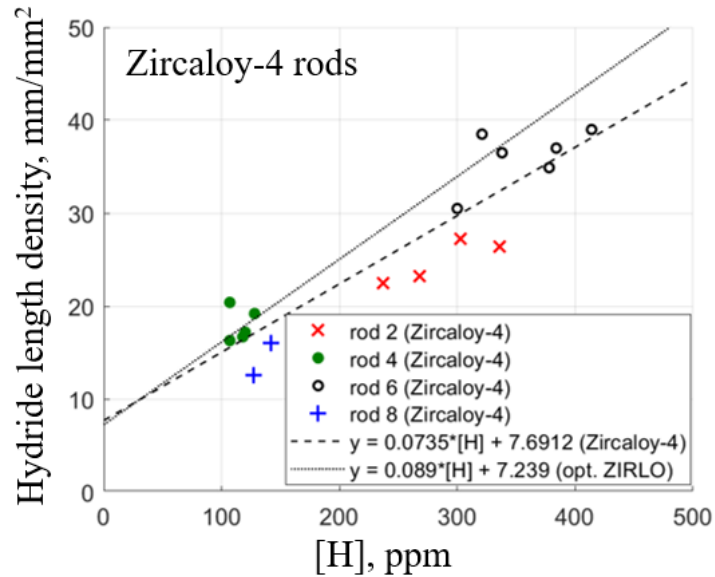
## length of hydrides



**The average and maximum hydride lengths in the opt. ZIRLO are two to three times longer than those in Zircaloy-4**

# SPIZWURZ bundle test results

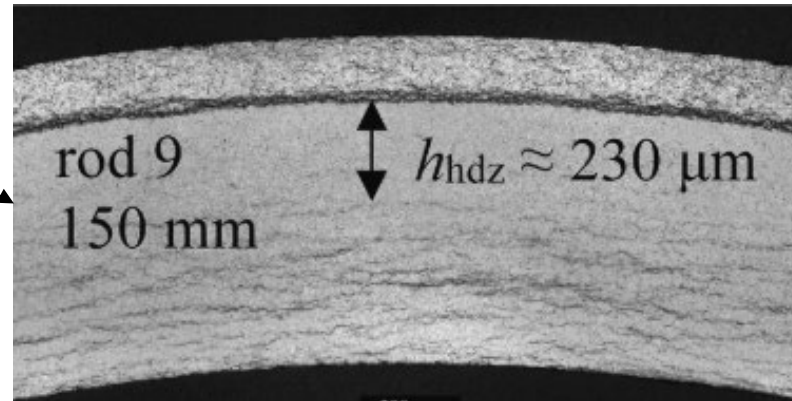
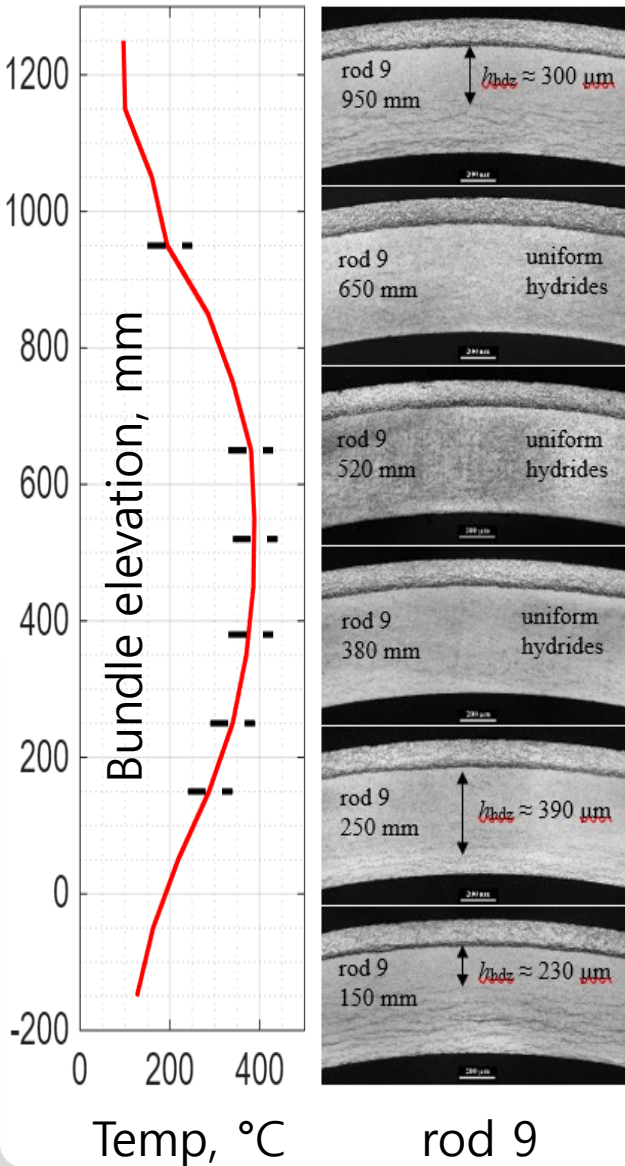
## hydride length density



**The hydride length density is almost proportional to the hydrogen content and is independent of the alloy type**

# SPIZWURZ bundle test results

## hydride morphology in duplex alloy DX-D4



**Dominant trend: redistribution of hydrogen between the substrate and the liner**

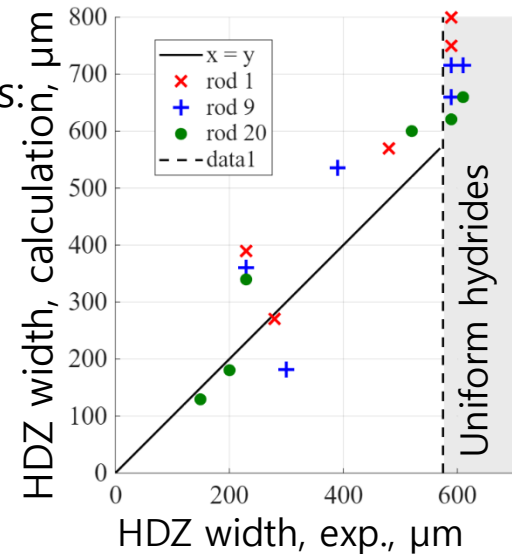
The width of the HDZ at the end of the thermocycle can be estimated as:

$$h_{hdz} = 2\lambda \cdot \sqrt{\int_0^t D_H(T(\tau)) \cdot d\tau}$$

$$\lambda e^{\lambda^2} \cdot \operatorname{erfc}(\lambda) = \frac{C_{ss} - C_{interface}}{C_{sub,tot} - C_{interface}} \cdot \frac{1}{\sqrt{\pi}}$$

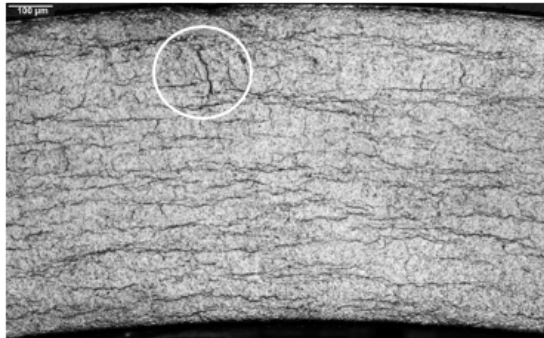
↓

$$\lambda \approx 0.01 \quad (\text{for } 300 \text{ ppm})$$

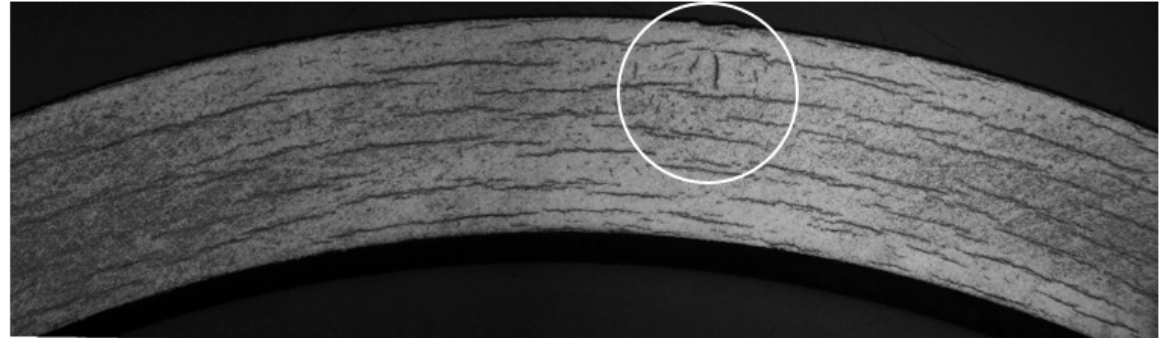


# SPIZWURZ bundle test results

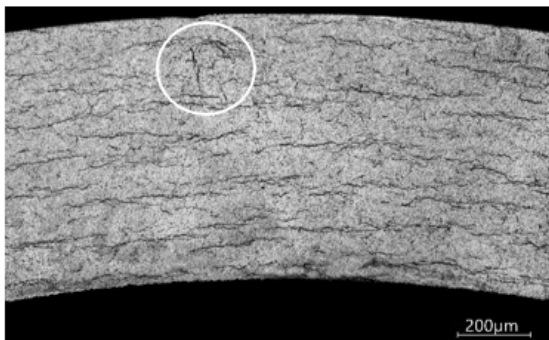
## hydride morphology "anomalies"



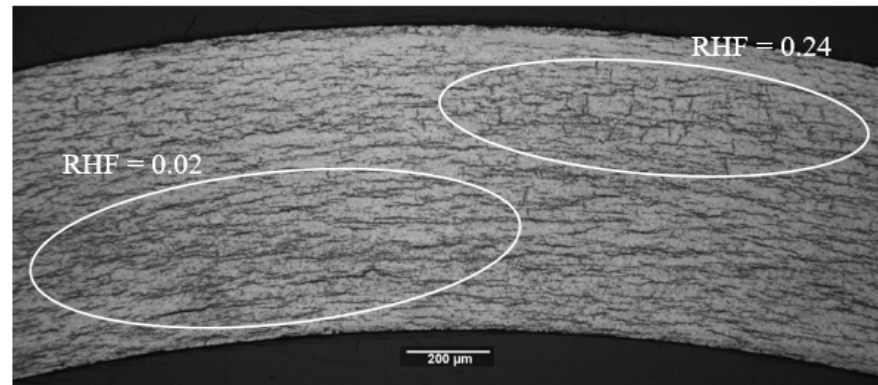
rod 2 (150 mm), RHF = 0.19 (mean)



rod 13 (950 mm), RHF = 0.03 (mean)



rod 4 (950 mm), RHF = 0.15 (mean)



rod 7 (150 mm), RHF = 0.07 (mean)

**The total number of tube cross-sections analyzed is of the order of 100**

# SPIZWURZ bundle simulation

## Model 1 description (ODE-based)

### Ordinary differential equation (ODE) system for precipitation:

Cumulative radial hydride fraction

Nucleation of hydrides is according to the classical heterogeneous nucleation approximation

Instantaneous radial hydride fraction

Gibbs energy change

$$\left\{ \begin{array}{l} \frac{dC_s}{dt} = \frac{C_s - C_e}{\tau_0}, \quad \tau_0 = \frac{\Delta^2}{\alpha^2 D_H} \\ \frac{d\theta}{dt} = \frac{F_r - \theta}{C_h} \cdot \frac{dC_h}{dt}, \quad C_h = C_{tot} - C_s \\ \frac{dn_r}{dt} = \int_{E_{d,min}}^{E_{d,max}} n \cdot g(E_d) \cdot Z(E_d) \cdot j_n \cdot F_r \cdot \exp(-\Delta G(E_d)/kT) \cdot dE_d \\ \frac{dn_t}{dt} = \int_{E_{d,min}}^{E_{d,max}} n \cdot g(E_d) \cdot Z(E_d) \cdot j_n \cdot (1 - F_r) \cdot \exp(-\Delta G(E_d)/kT) \cdot dE_d \\ F_r = \frac{1 - f_{tex}}{1 + f_0 \cdot \exp(-\sigma \cdot \Omega_0/kT)} + f_{tex} \\ \Delta G(E_d) = \Omega_n (g_m - \Delta\mu/v_H) + S_n \gamma - E_d \end{array} \right.$$

### Ordinary differential equation (ODE) system for dissolution:

$$\left\{ \begin{array}{l} \frac{dC_s}{dt} = \frac{C_s - C_e}{\tau_0} \\ \frac{d\theta}{dt} = 0 \\ \frac{dn_{r,t}}{dt} = 0 \end{array} \right.$$

[1] M. Kolesnik *et al.*, *Comp. Mater. Sci.* 189 (2021) 110260, DOI: 10.1016/j.commatsci.2020.110260

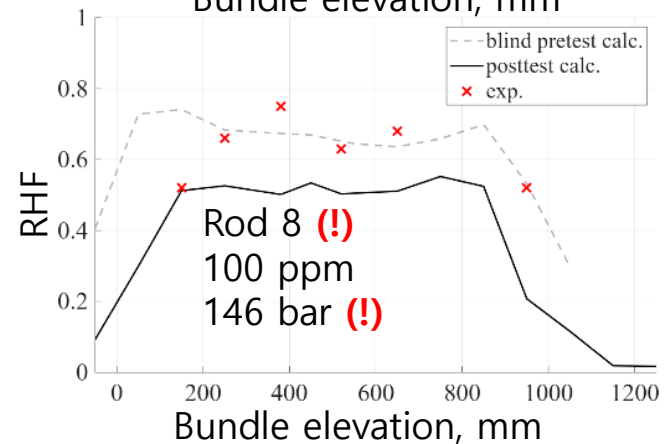
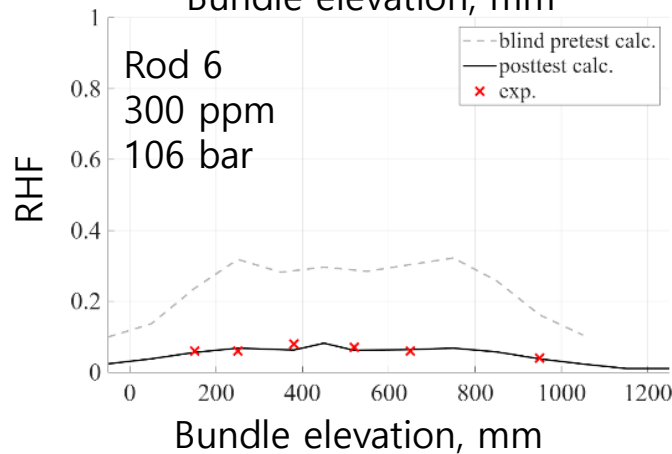
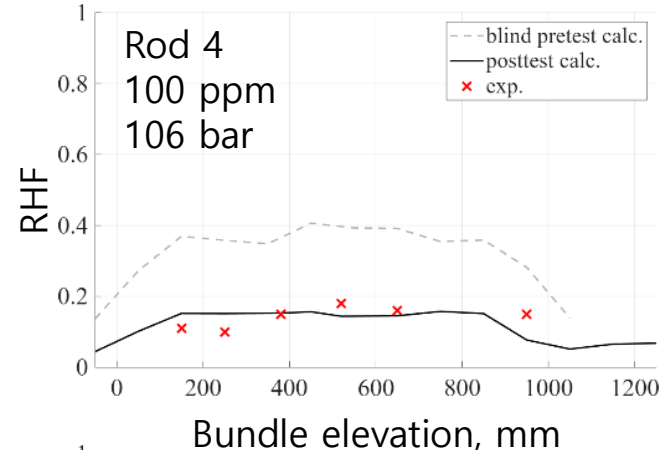
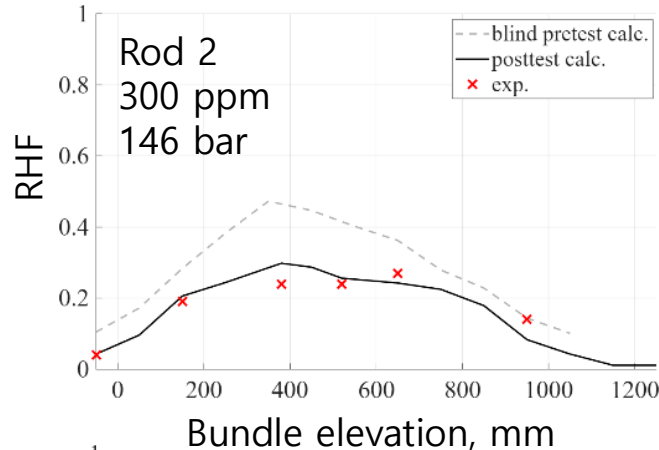


# SPIZWURZ bundle simulation

## Model 1, simulation results

### Rods 2, 4, 6 and 8 (Zircaloy-4):

located symmetrically within the bundle and have all possible combinations of hydrogen content (100 and 300 ppm) and internal pressure (106 and 146 bar)

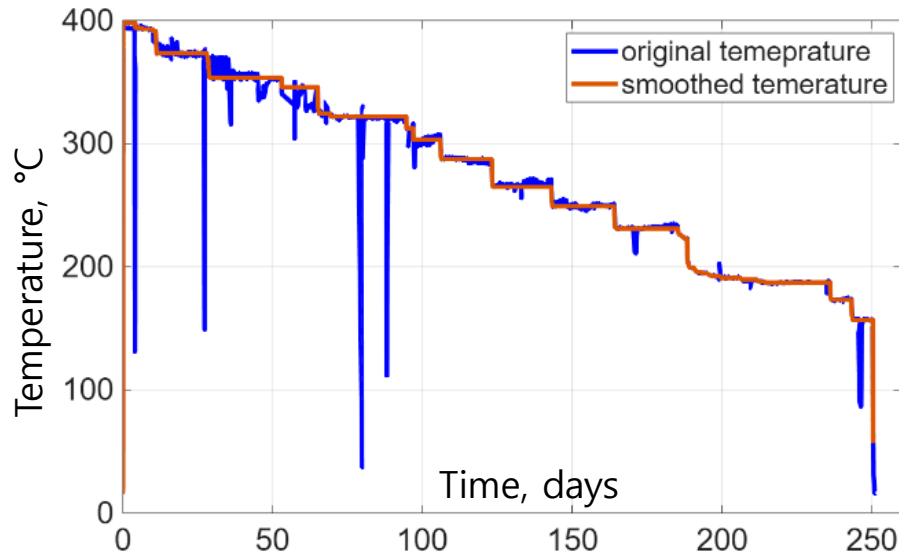
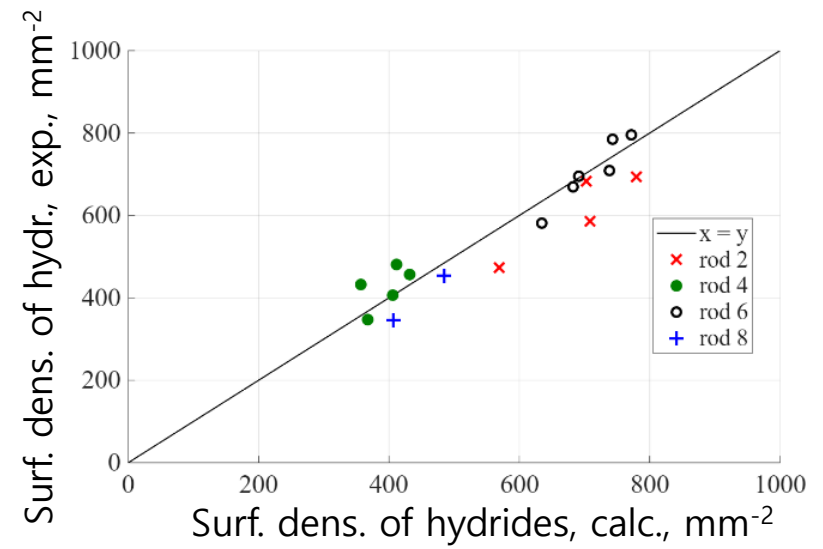
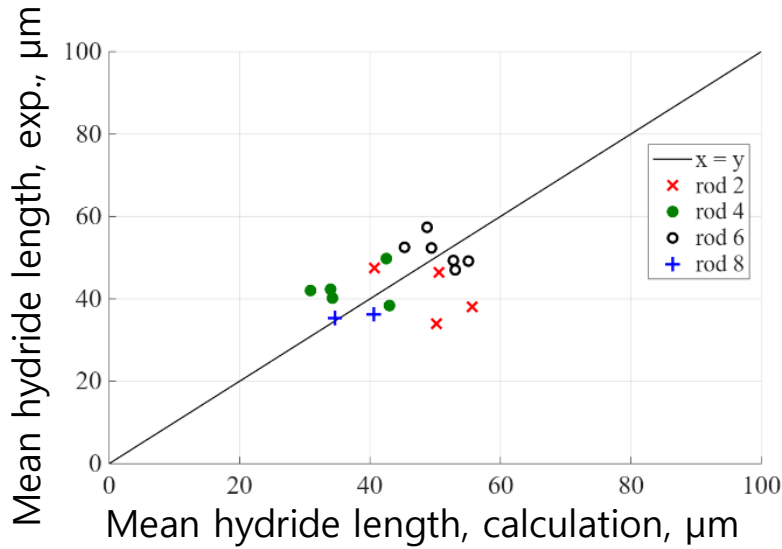


The difference in pre- and post-simulations originates from:

- (i) the actual hydrogen concentration and (ii) the datasets used to fit the model parameters.

# SPIZWURZ bundle simulation

## Model 1, simulation results

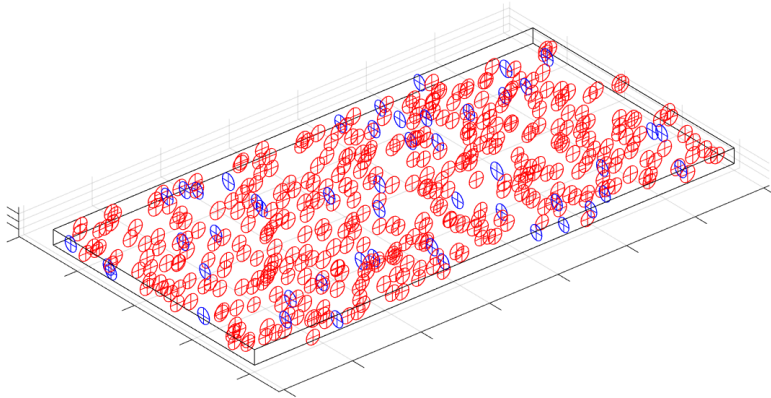


# SPIZWURZ bundle simulation

## Model 2 description (MORPHYD module)

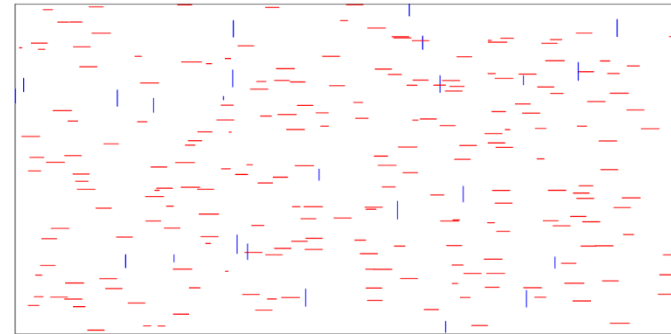
### Nucleation and growth of hydrides

- disk-shaped hydrides
- pre-defined nucleation sites
- classical nucleation theory
- diffusional growth
- competition of neighboring hydrides for the hydrogen in solid solution



### Cross-section analysis

- morphology analysis as with experimental cross-sections
- any hydride morphology metric
- statistical analysis of metrics



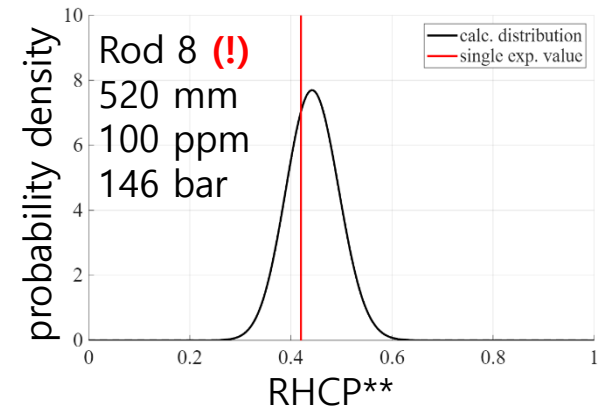
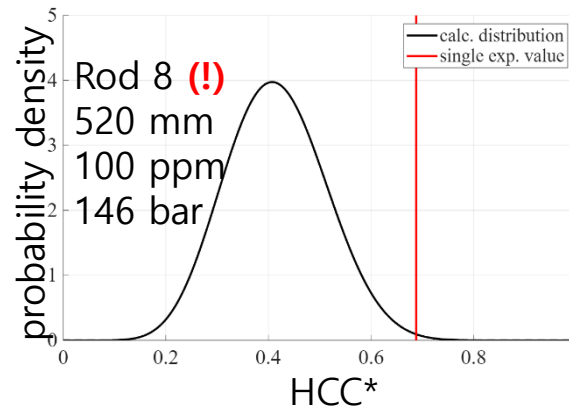
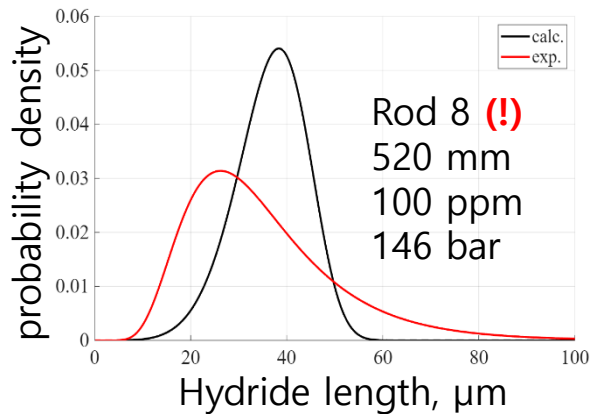
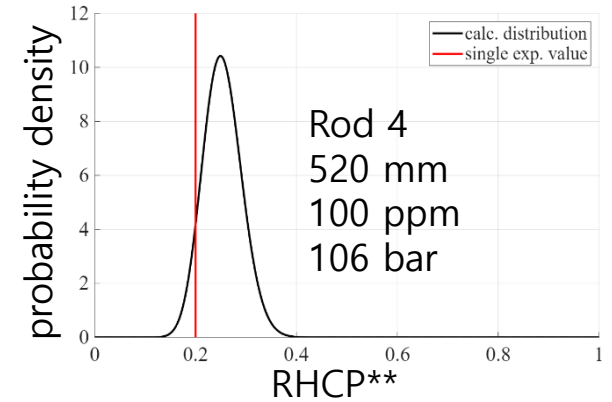
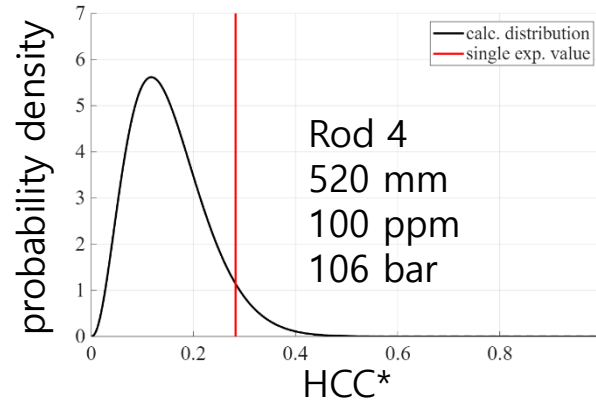
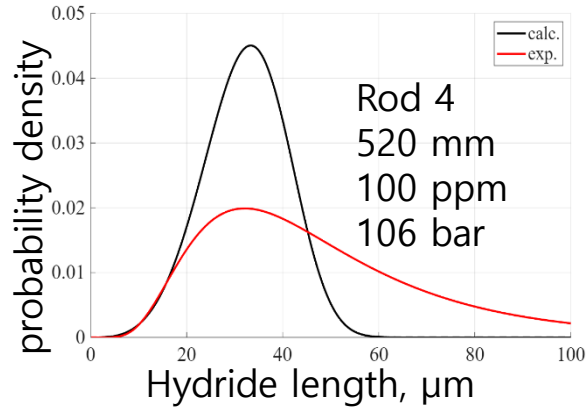
### Current limitations of the MORPHYD module:

(i) precipitation only (no dissolution), (ii) valid for small hydrides

- [1] M. Kolesnik and T. Aliev, *Phys. of Met. and Metal.* 104 (2023) 1414-1425, DOI: 10.1134/S0031918X22602074  
[2] T. Aliev and M. Kolesnik, *Let. on Mater.* 13 (2023) 143-148, DOI: 10.22226/2410-3535-2023-2-143-148

# SPIZWURZ bundle simulation

## Model 2 (MORPHYD), simulation results



\*HCC – the total projection length of hydrides within 110  $\mu\text{m}$  in the radial direction, normalized by thickness  
 \*\*RHCP – fracture energy estimated from varying crack paths, normalized to the unhydrided sample

- The measured RHF for Zircaloy-4 and opt. ZIRLO is consistent with the published data. Zircaloy-4 samples have a higher stress-induced reorientation than opt. ZIRLO under SPIZWURZ conditions;
- Both the mean and maximum hydride lengths in the opt. ZIRLO are two to three times longer than those in Zircaloy-4. Accordingly, the hydride density in opt. ZIRLO is lower than that in Zircaloy-4;
- The hydride length density is proportional to the total hydrogen concentration and is almost independent on the alloy type;
- In the duplex alloy DX-D4, after heating and slow cooling, hydrogen moves from the substrate to the liner;
- Several samples exhibited local anomalies in hydride morphology. These anomalies could significantly increase the degree of local hydride embrittlement;
- Simulations of various morphological parameters (RHF, HCC, RHCP and hydride length) showed acceptable agreement with the experiment.

# Thank you for your attention

<https://www.iam.kit.edu/awp/english/163.php>

<http://quench.forschung.kit.edu/>



**Aleksandra Rezchikova**

GRS

## **SPIZWURZ Blind Benchmark**

Ensuring the integrity of fuel rods during extended interim storage is critical for the safe management of spent nuclear fuel. Due to the challenges associated with conducting experiments under real conditions, associated with the use of irradiated materials and the involved long time-scales, assessing the state of spent fuel relies heavily on simulations. As a result, the development of reliable numerical tools becomes of paramount importance for predicting the behavior of spent fuel during the entire storage period.

Creep and embrittlement due to hydrogen hydride formation are significant degradation mechanisms for the cladding tubes during extended interim storage of spent nuclear fuel. To better understand these phenomena, the joint project SPIZWURZ between KIT and GRS was initiated to investigate the behavior of cladding tubes under storage conditions. The core of this research was the SPIZWURZ bundle experiment, carried out at the LICAS facility by KIT, and specifically designed to examine how slow cooling influences the properties of fuel cladding. The experiment involved a bundle of 21 fuel rod simulators, which were cooled over a period of 250 days with the maximum averaged cooling rate being 0.94°C per day. The maximum temperature reached within the bundle was 405°C at the start of the cooling transient. While the cladding tubes used were non-irradiated, they were pre-loaded with hydrogen to the levels of 100 ppm and 300 ppm to simulate hydrogen concentrations both below and above the solubility limit. Additionally, the experimental setup included three different cladding materials (Zircaloy-4, opt.ZIRLO, Duplex DX D4) and two pressurization levels of 103 and 142 bar, making the experimental matrix highly complex.

This SPIZWURZ bundle experiment also served as the foundation for an international blind benchmark coordinated by GRS, with contributions from 11 participants representing 10 different organizations. Using the temperature and pressure histories from the experiment, along with the estimated initial hydrogen content, participants were asked to calculate the creep strains and the hydrogen behavior. These calculated results were compared against experimentally measured creep and the radial hydride fractions derived from metallographic image analysis.

This blind benchmark provided a valuable opportunity to evaluate the accuracy of different models and computational approaches in predicting the state of the cladding tubes after a slow cooling transient, conditions that are highly relevant to interim storage. The presentation will summarize the results obtained from this evaluation.



SPIZWURZ

Blind Benchmark Results

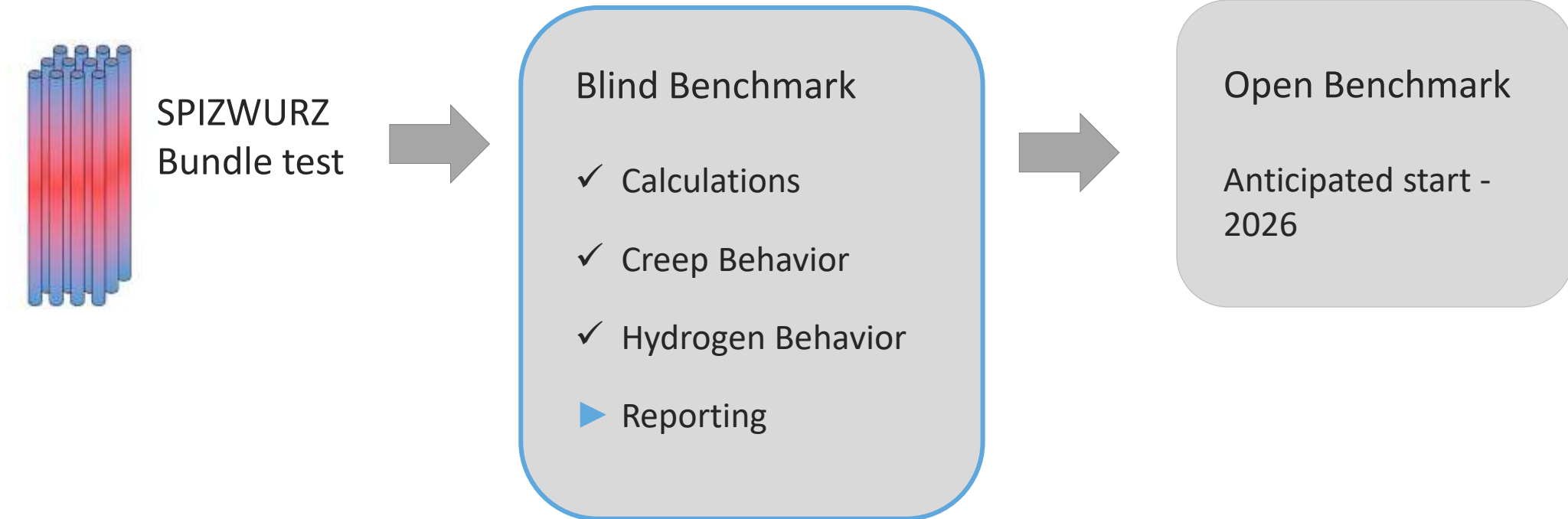
30<sup>th</sup> International QUENCH Workshop

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Aleksandra Rezchikova, 16th December 2025



# SPIZWURZ Blind Benchmark



# SPIZWURZ Blind Benchmark: Participation

## 11 Participants from 10 Organisations

Comisión Nacional de  
Energía Atómica (CNEA)

Gesellschaft für Anlagen- und  
Reaktorsicherheit (GRS)

Karlsruhe Institute of Technology  
(KIT)

Axpo Switzerland

Framatome Germany

Paul Scherrer Institute (PSI)

Centro de Investigaciones  
Energéticas, Medioambientales y  
Tecnológicas (CIEMAT)

EDF France

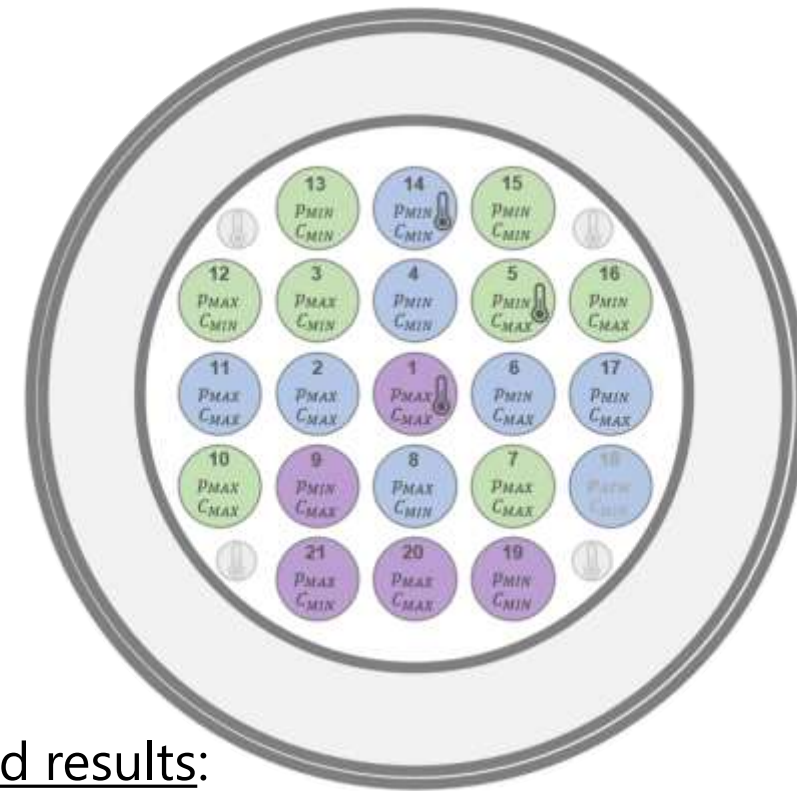
ÚJV Řež

Seoul National University  
(SNU)

# SPIZWURZ Blind Benchmark

Key factors to consider when comparing rods:

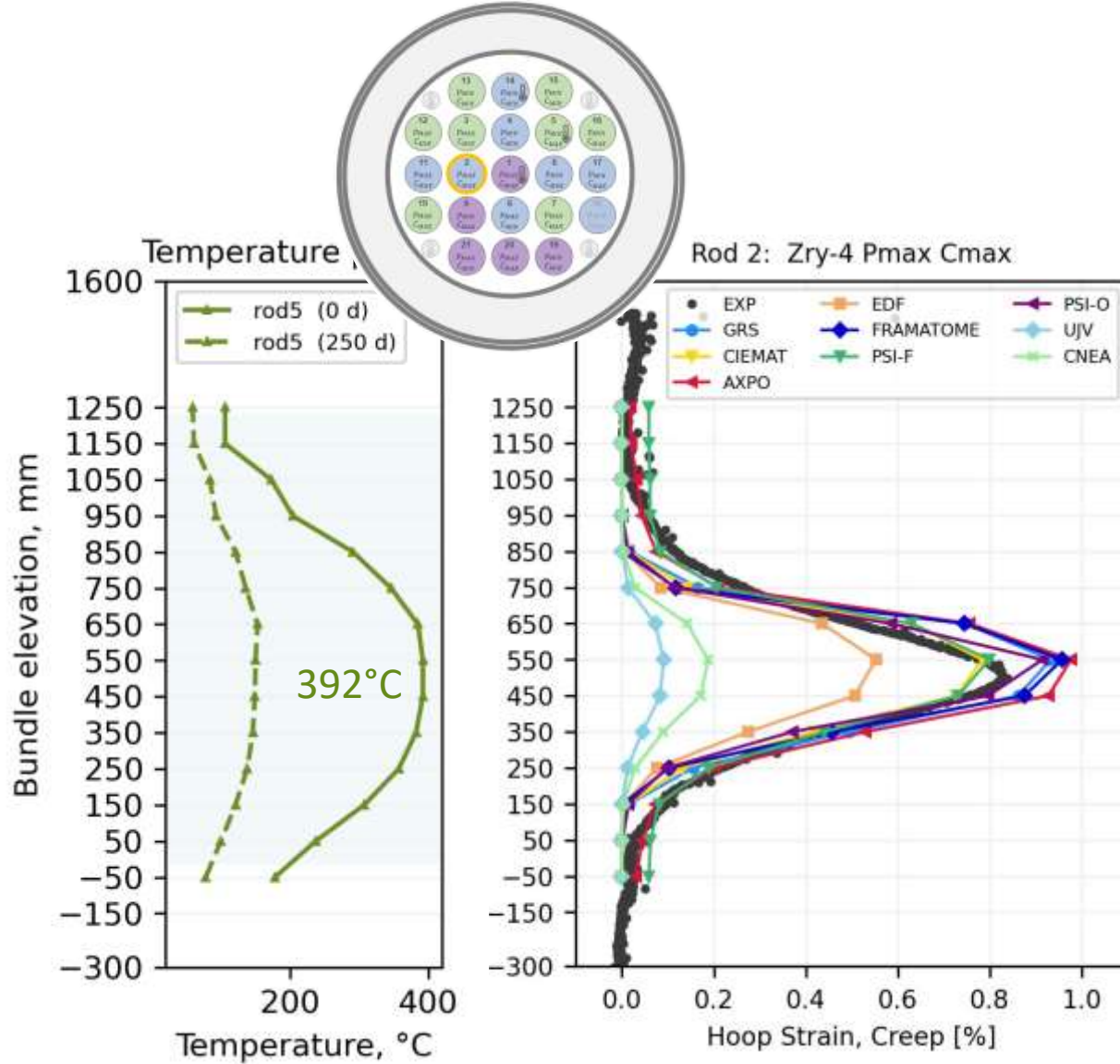
- Rod position inside the bundle
- Variations in hydrogen content
- Pressure evolution throughout the test



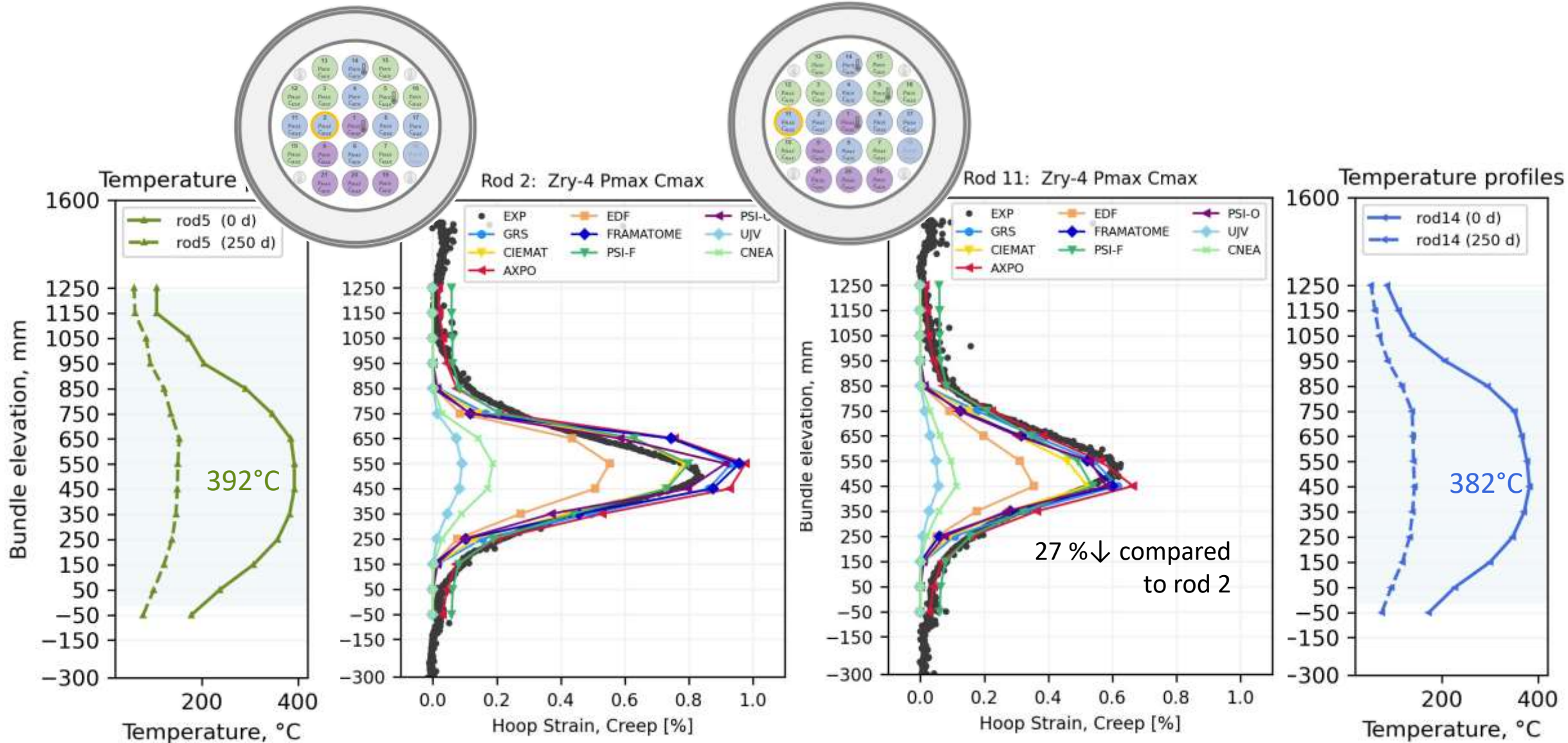
Key considerations when comparing experimental and simulated results:

- Differences in initial hydrogen content
- Influence of pellet-cladding interaction (PCI) — notable in Rods 6, 8, and 12

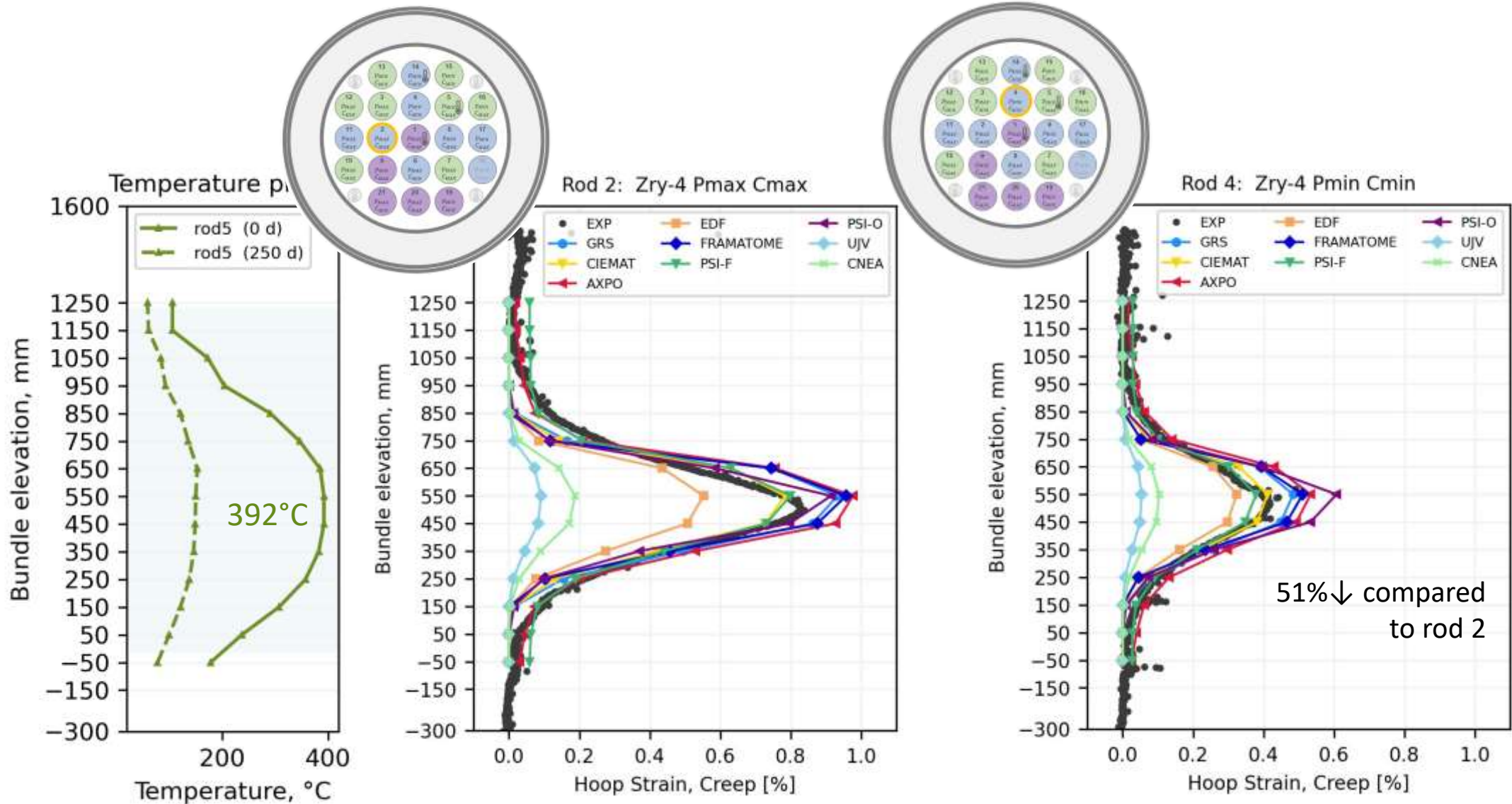
# Zircaloy-4 Creep



# Zircaloy-4 Creep: Effect of Rod Position

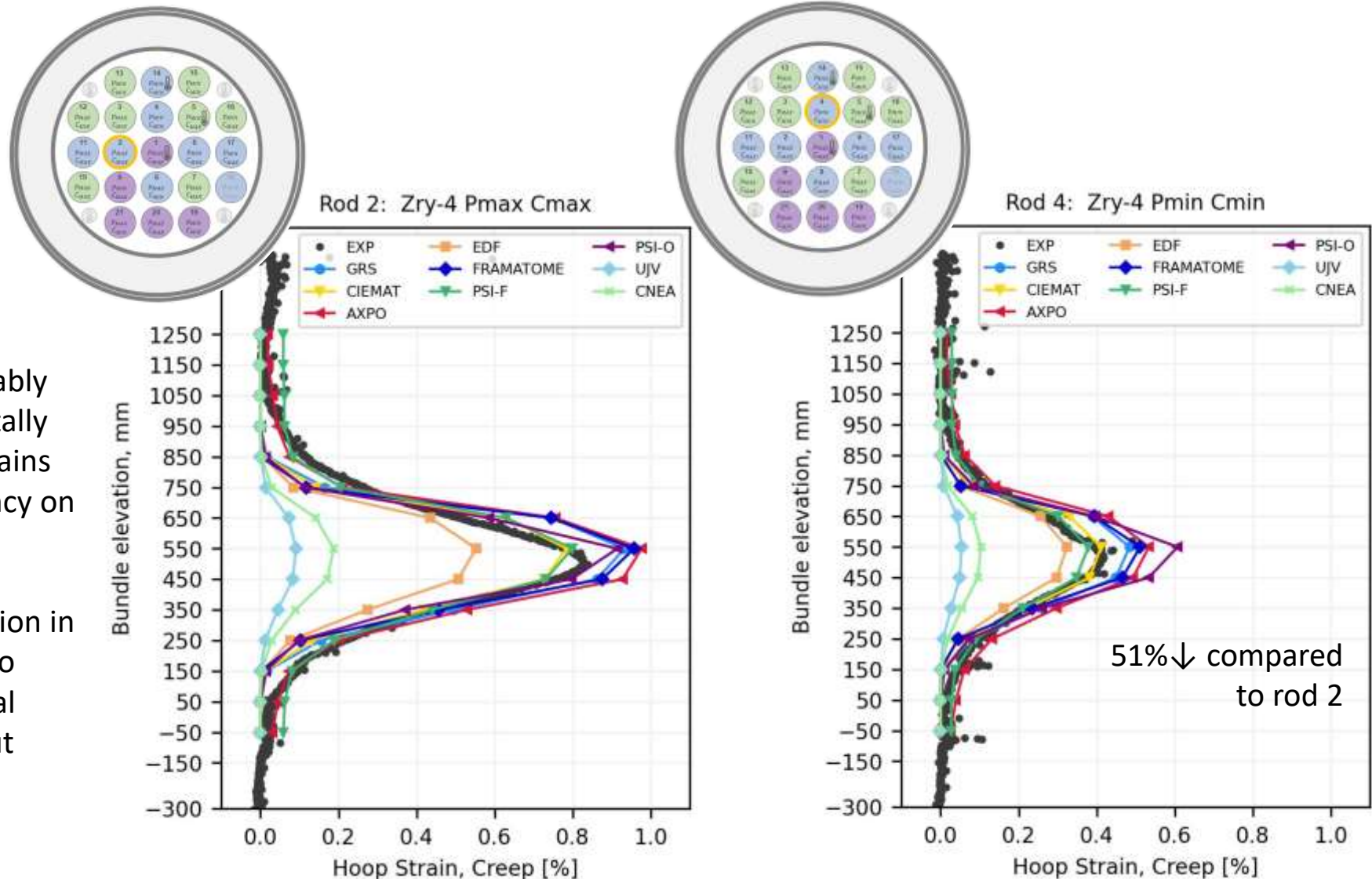


# Zircaloy-4 Creep: Pressure Effect



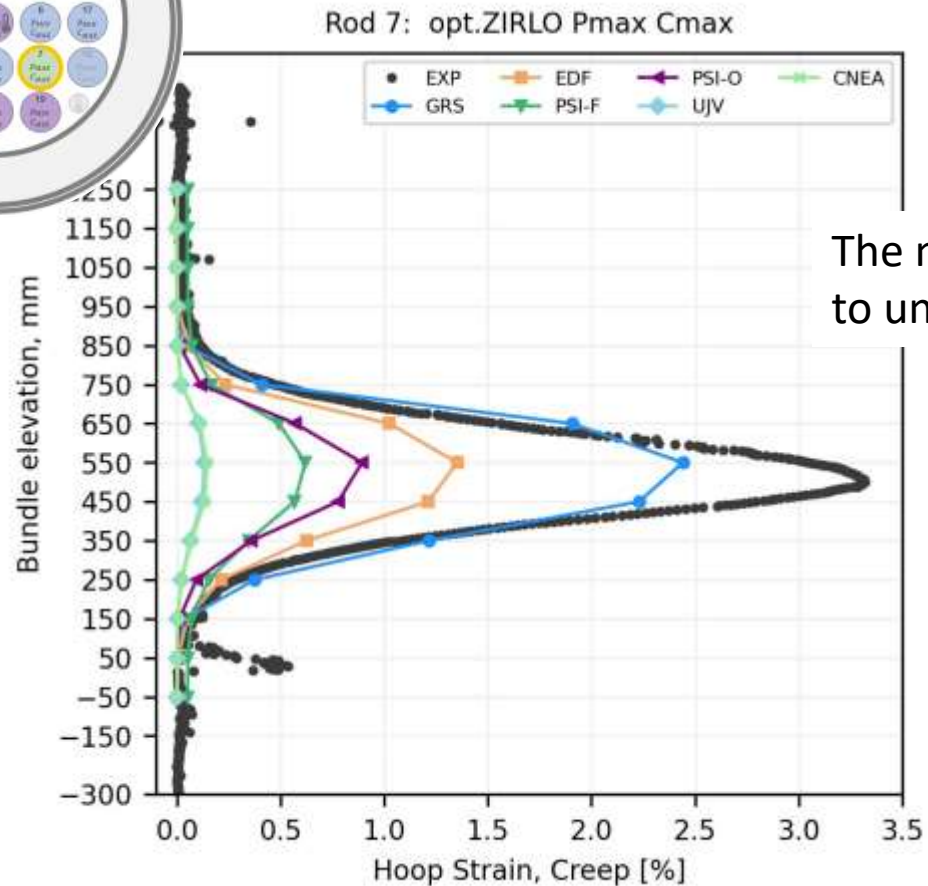
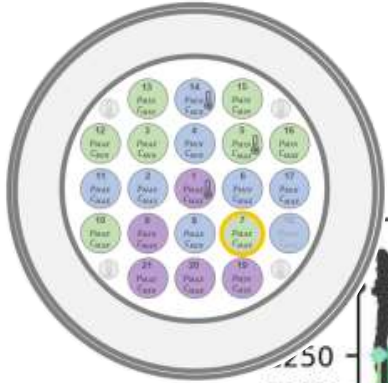
# Zircaloy-4 Creep: Pressure Effect

- Most modeling approaches reasonably capture experimentally measured creep strains and their dependency on temperature and pressure
- Creep underprediction in 'colder' zones due to limited experimental data for model input



# Opt.ZIRLO Creep: Effect of Rod Position

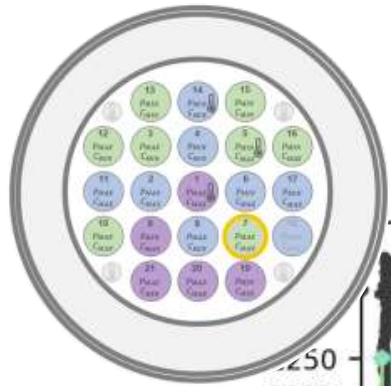
4.15x  $\uparrow$  compared  
to Zry-4 rod 2



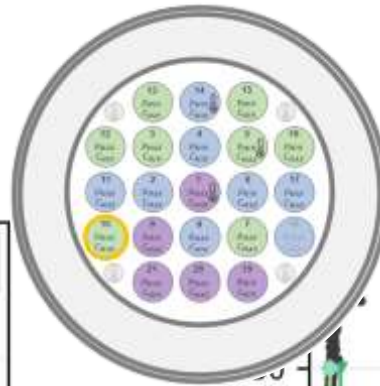
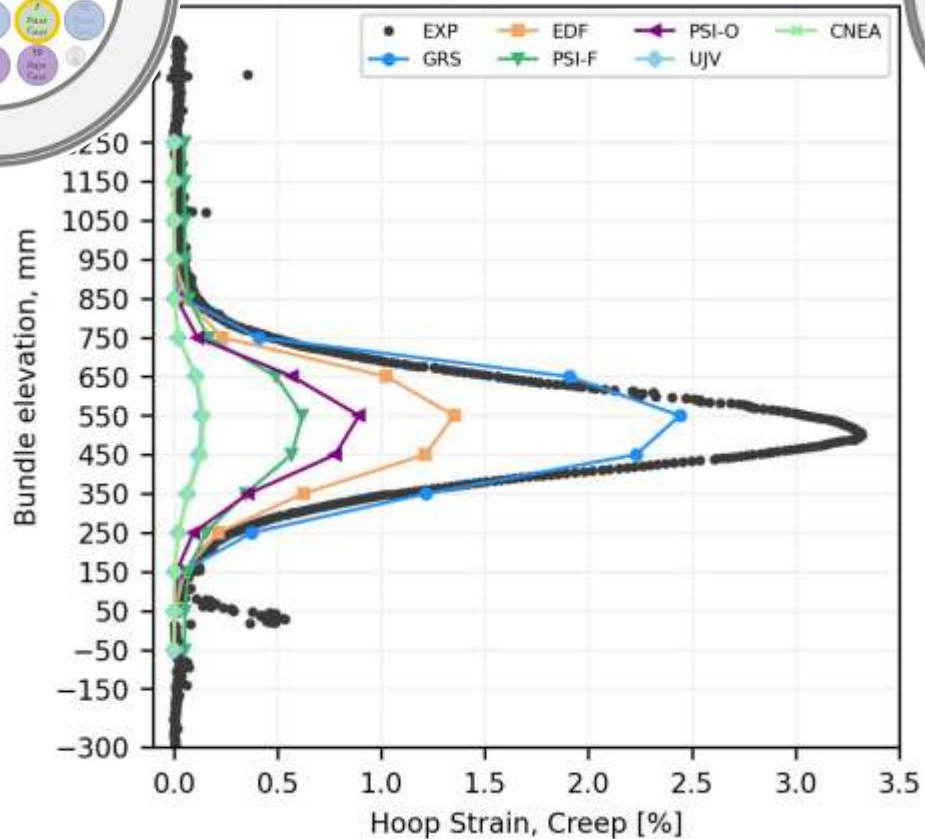
The models based on Zry-4 data tend to underpredict the creep of Zirlo rods



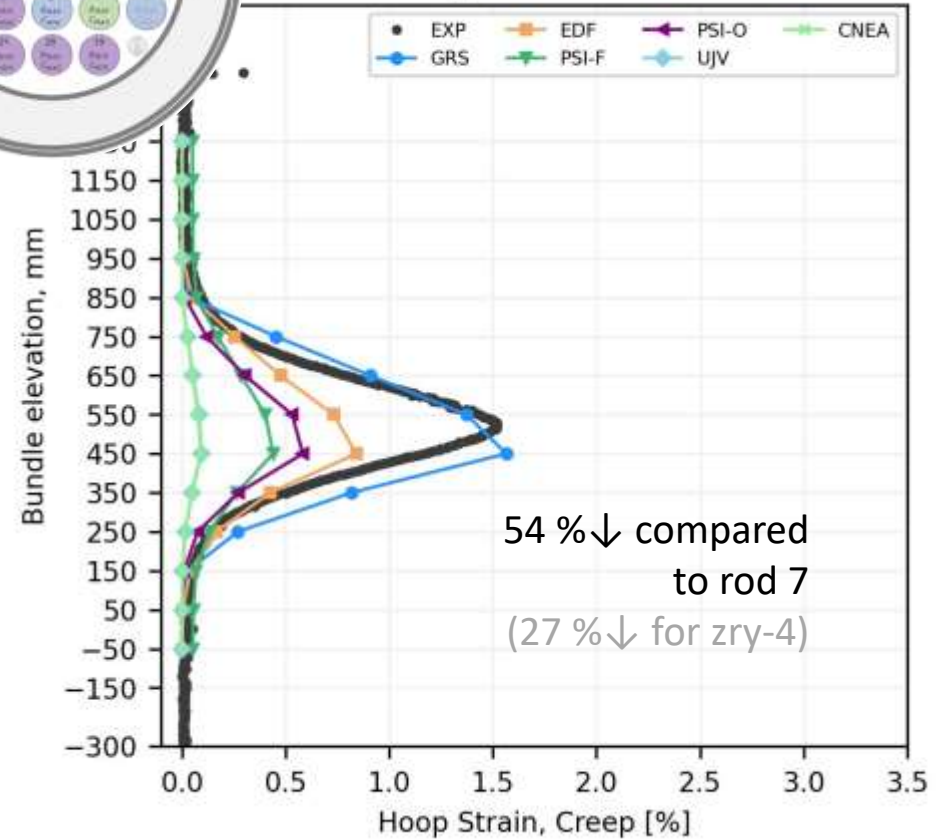
# Opt.ZIRLO Creep: Effect of Rod Position



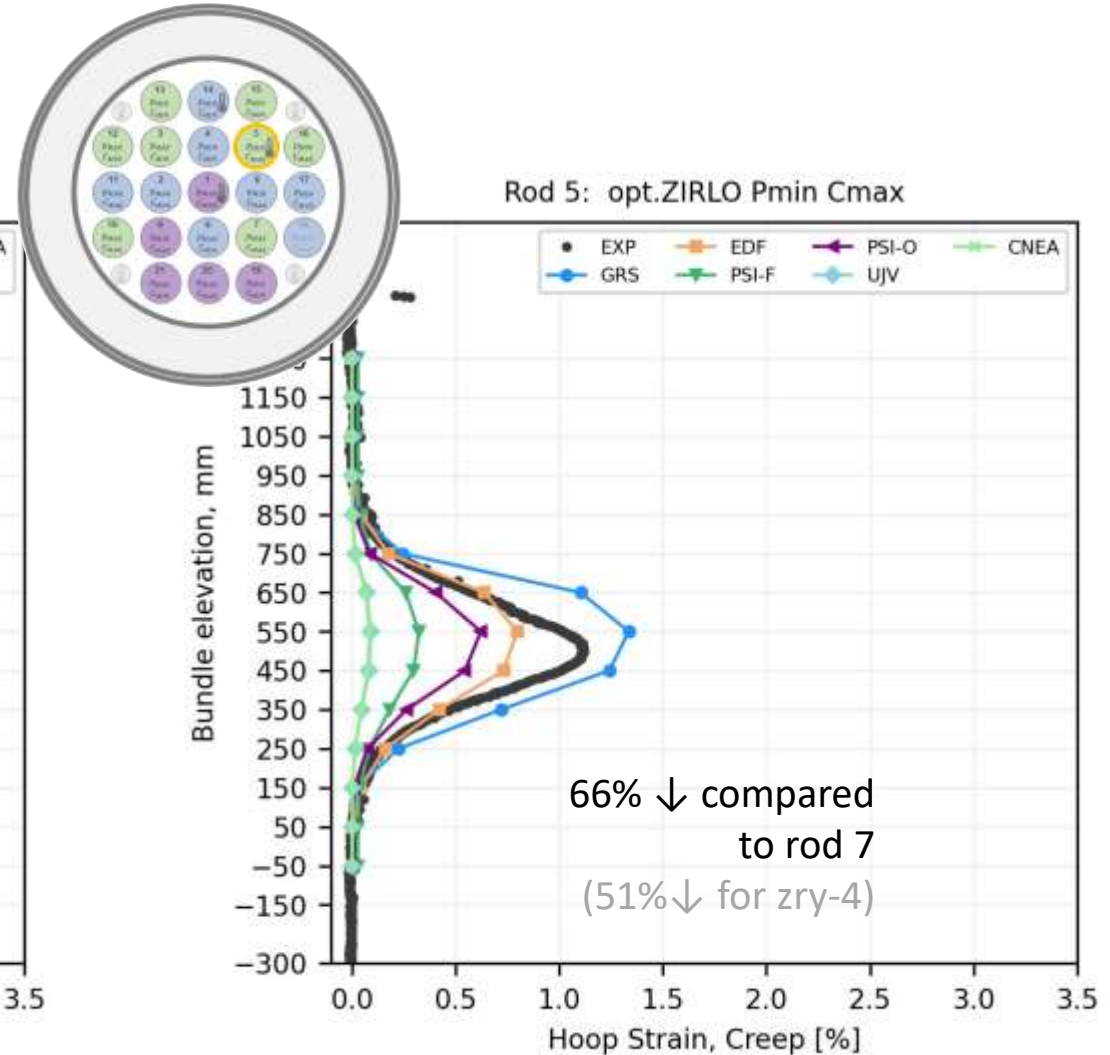
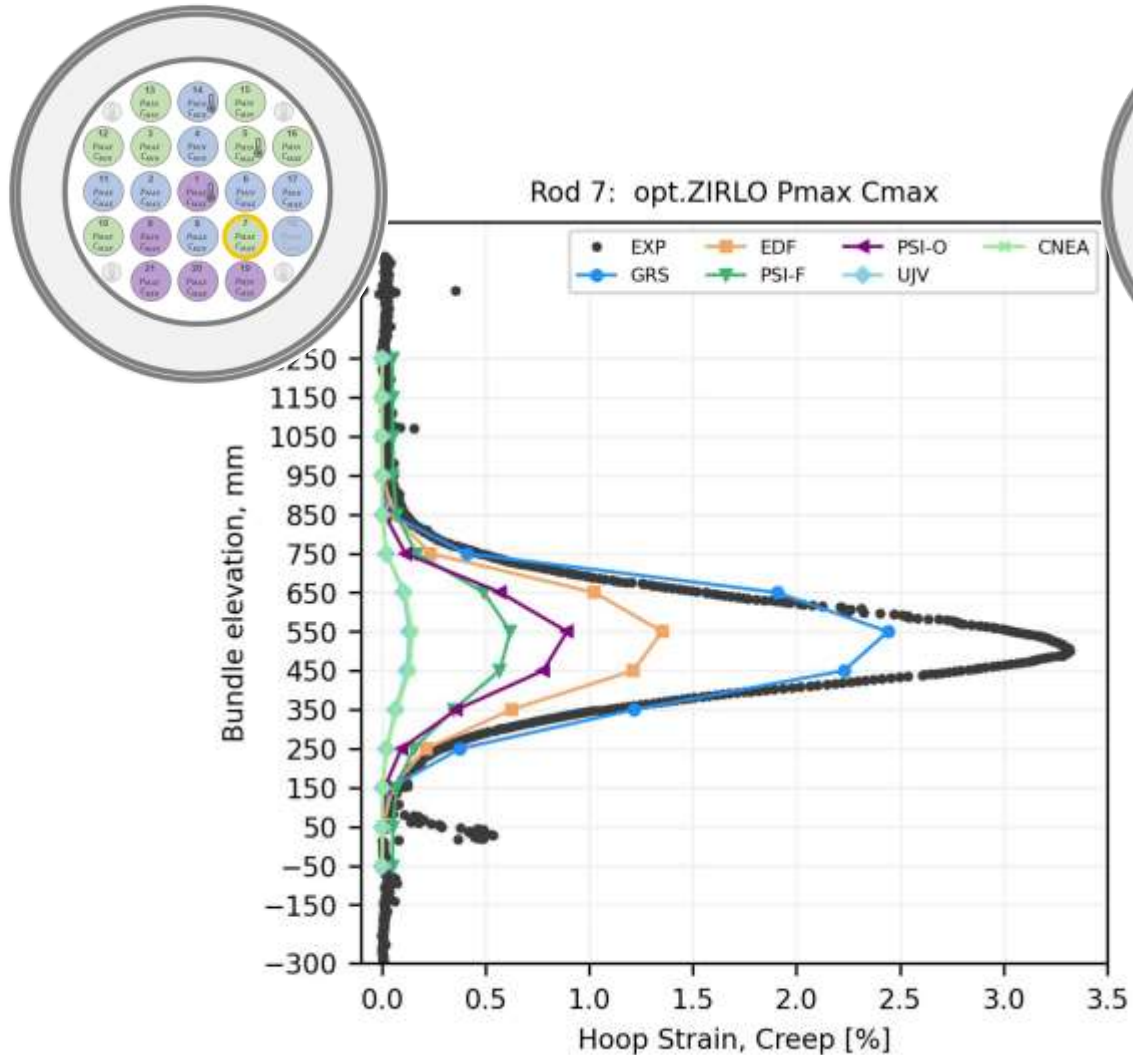
Rod 7: opt.ZIRLO Pmax Cmax



Rod 10: opt.ZIRLO Pmax Cmax



# Opt.ZIRLO Creep: Pressure Effect

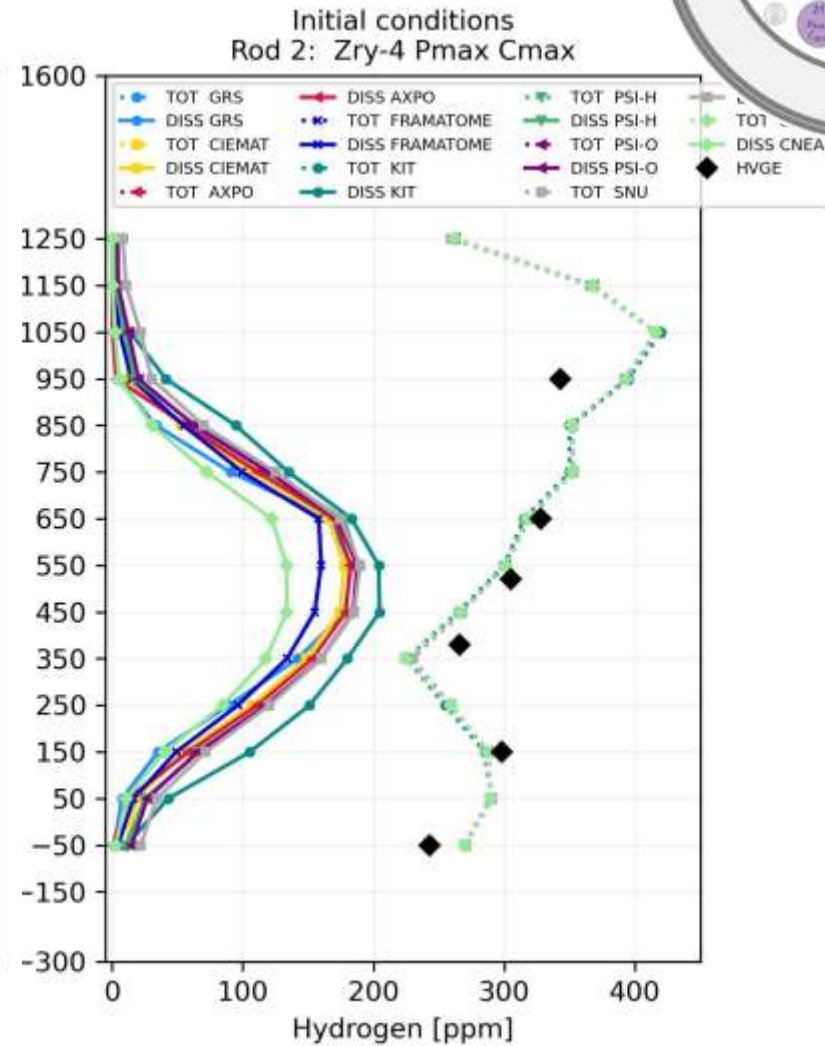
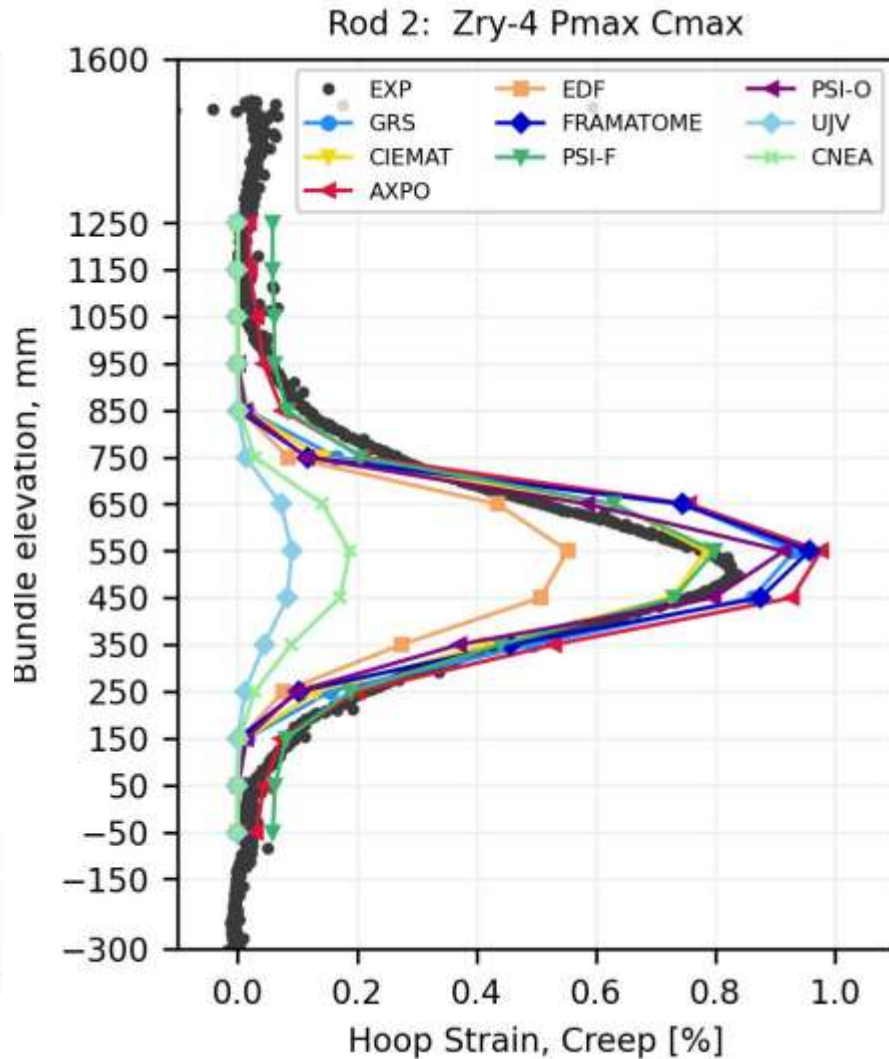
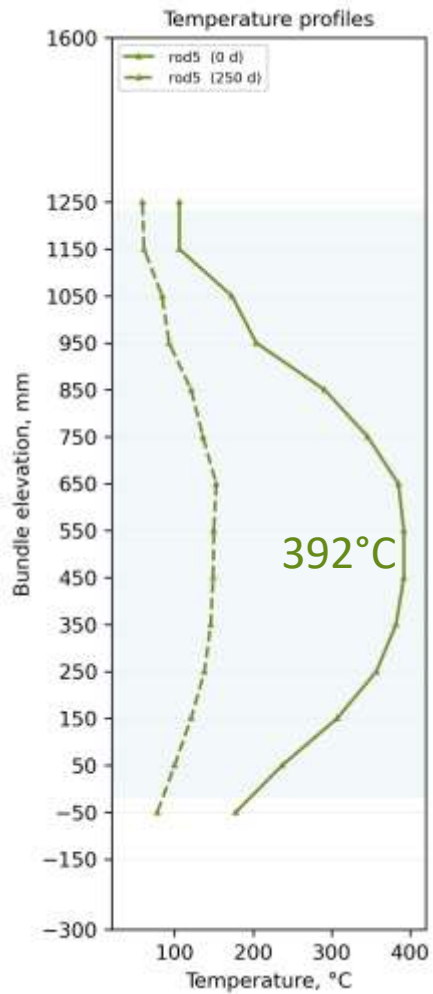
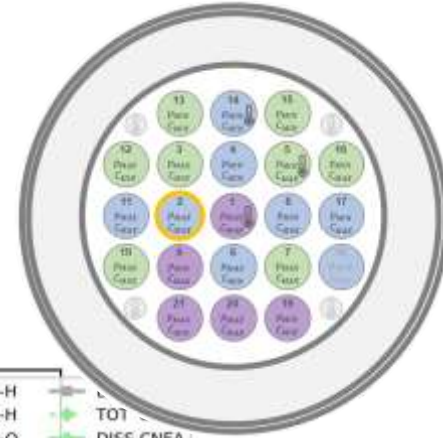


## SPIZWURZ Blind Benchmark: Creep

- Existing numerical models capture well Zry-4 and DX D4 creep strains at the considered conditions, but generally underpredict creep strains for optimized ZIRLO.
- Different creep models are required for different cladding materials:
  - Duplex and Zry-4 rods show similar creep behavior, allowing them to be modeled with comparable formulations.
  - Optimized ZIRLO exhibits significantly different creep behavior, with a much stronger sensitivity to pressure and temperature changes.
  - Negligible impact of hydrogen on creep of Zry-4 and DX D4 content. Hydrogen likely promotes creep of opt.ZIRLO at high pressure, but this effect is uncertain due to experimental variability.

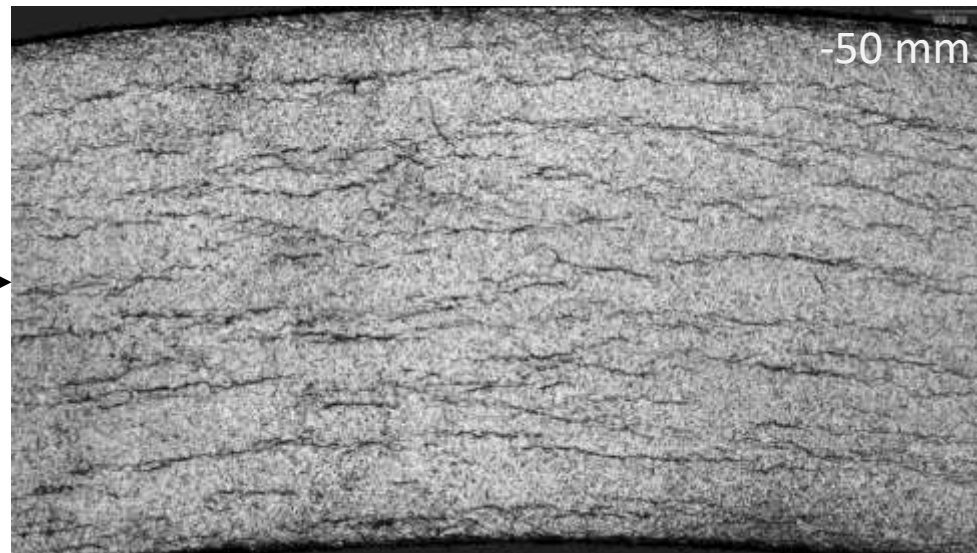
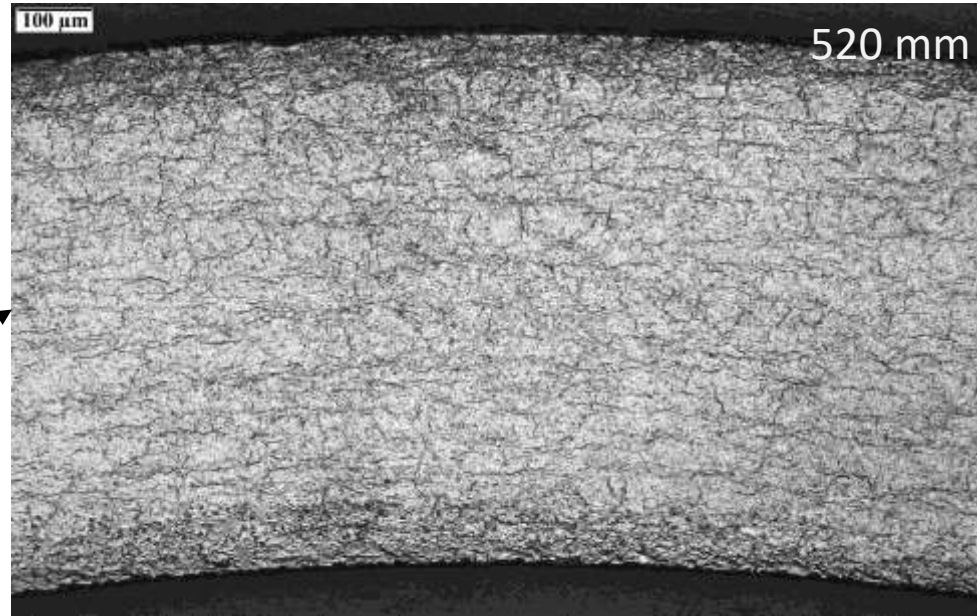
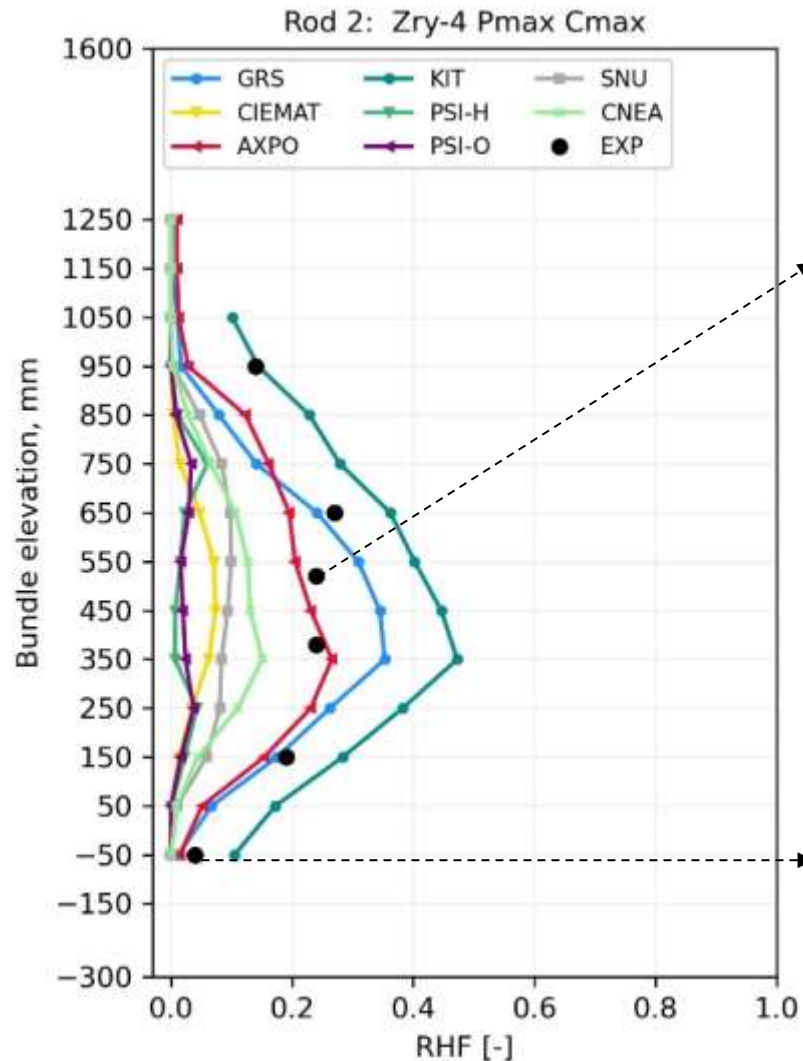
# Zircaloy-4: Rod 2

## 91MPa 300wppm Inner



# Zircaloy-4: Rod 2

## 91MPa 300wppm Inner



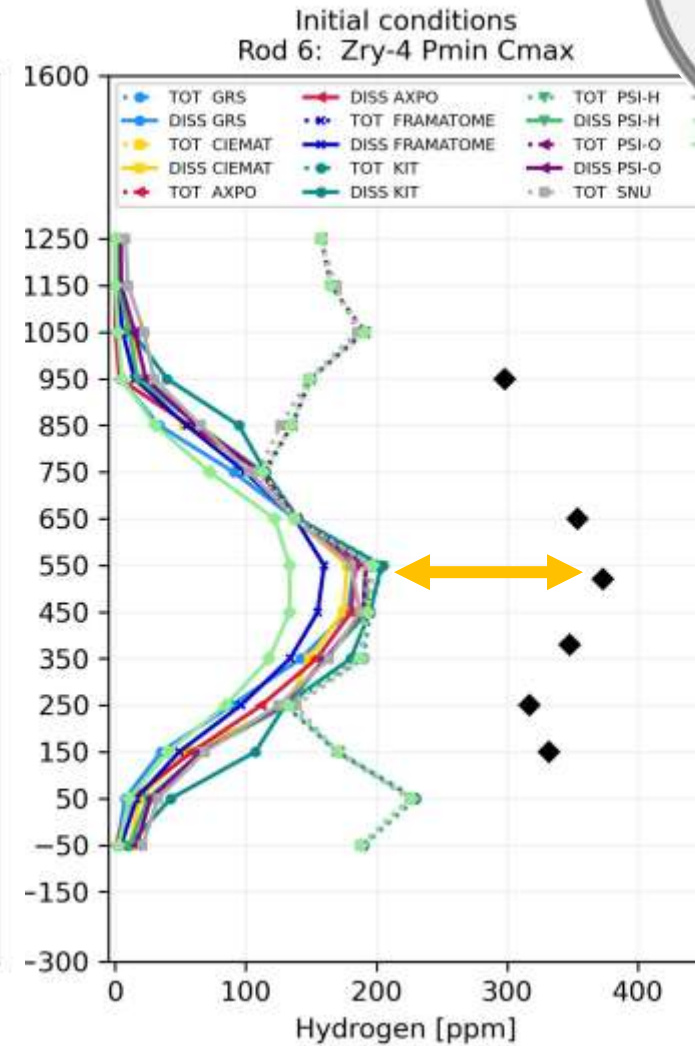
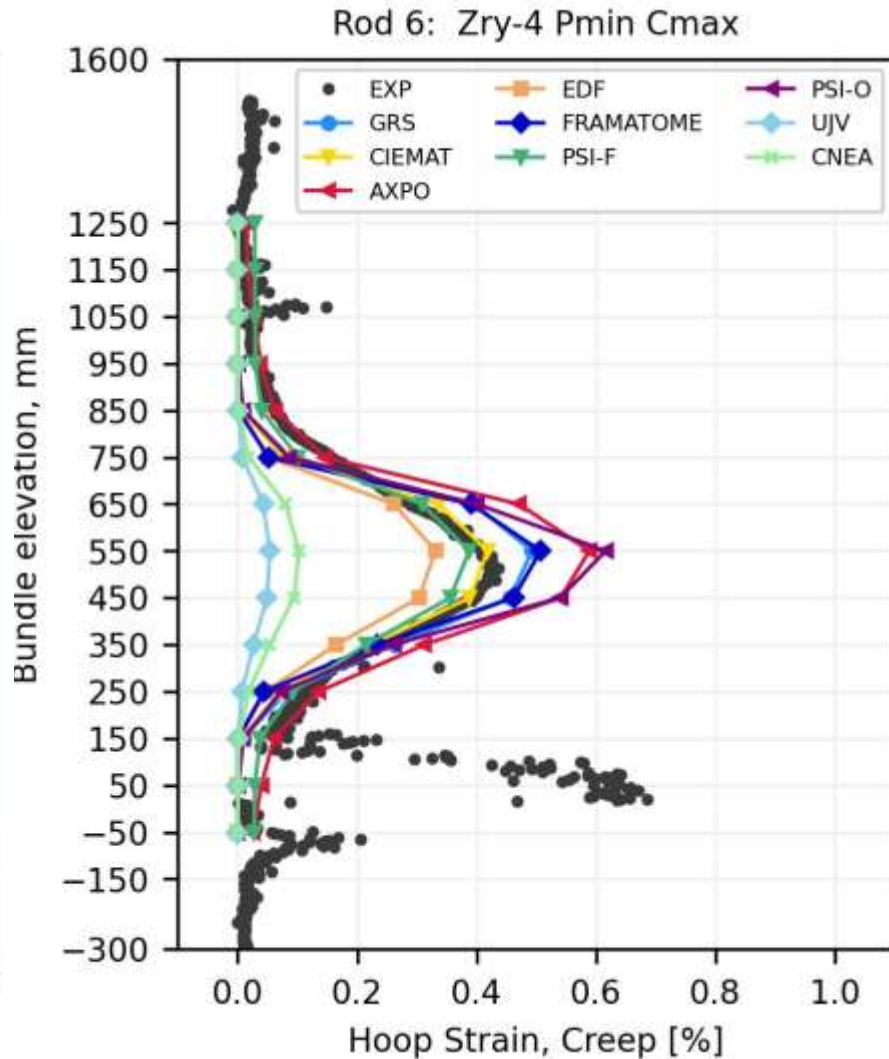
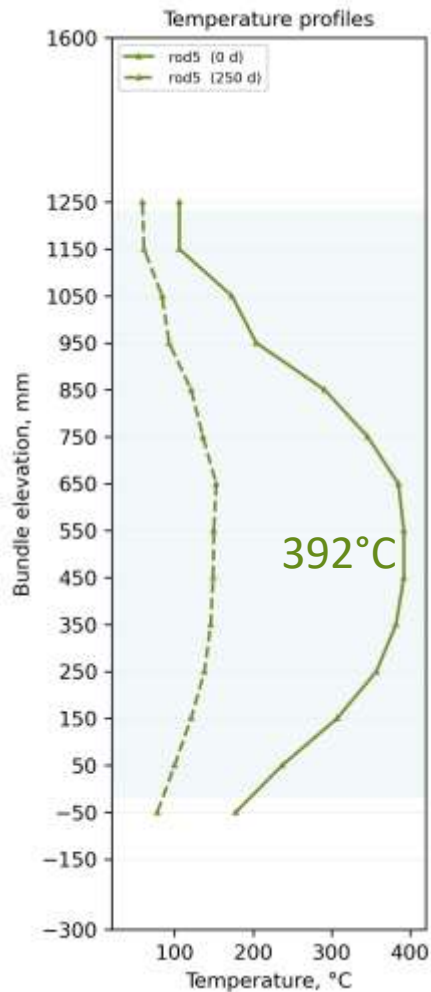
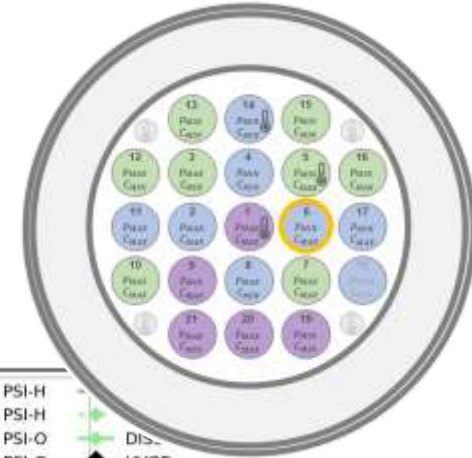
Extracted RHF shows a maximum of 27% at 650 mm

RHF predictions vary broadly from 0 to 50%

350 mm peak linked to lower initial H content

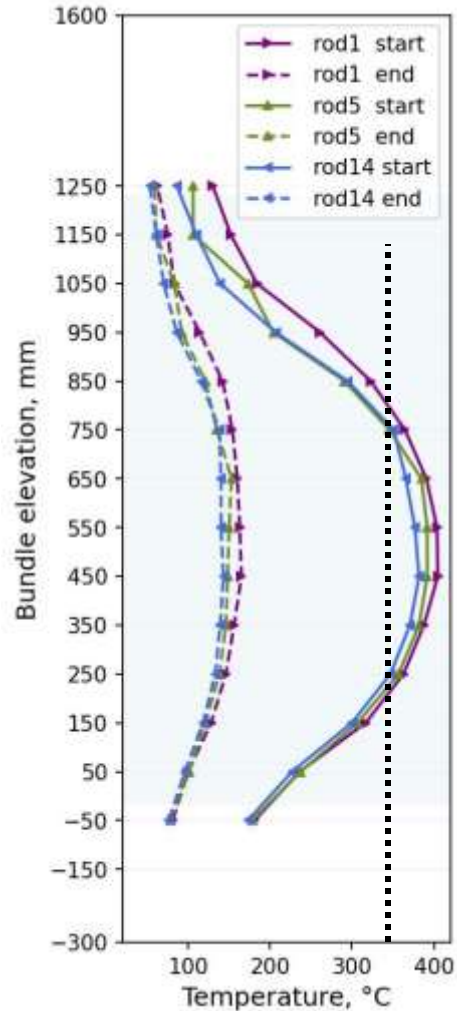
# Zircaloy-4: Rod 6

## 66MPa 300wppm Inner

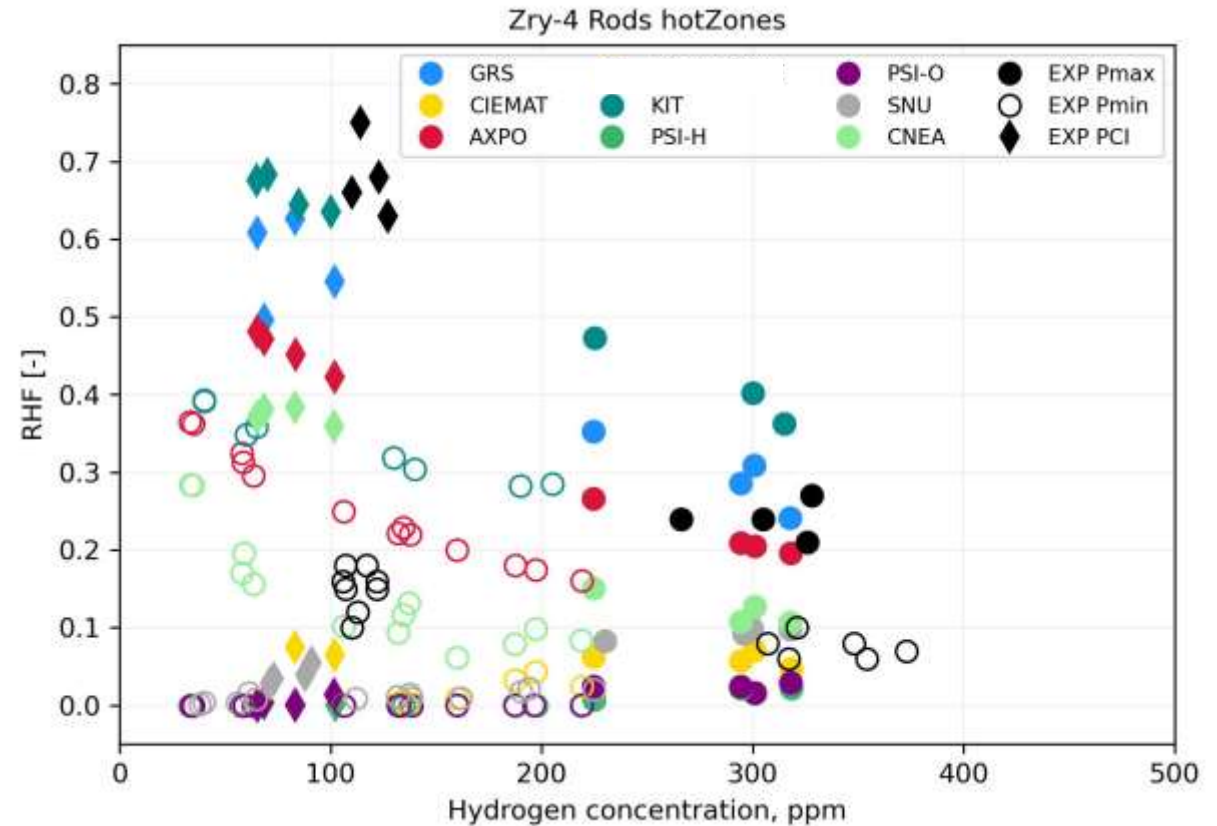


large discrepancy between HVGE and estimated hydrogen concentrations

# Zry-4: Initial Hydrogen Concentration VS RHF

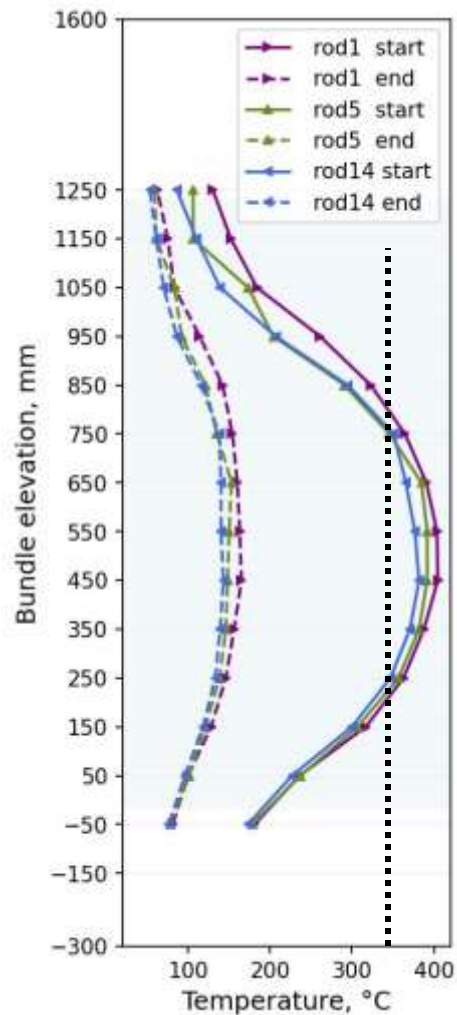


Zones 4-9  
Temperatures  
above 350°C



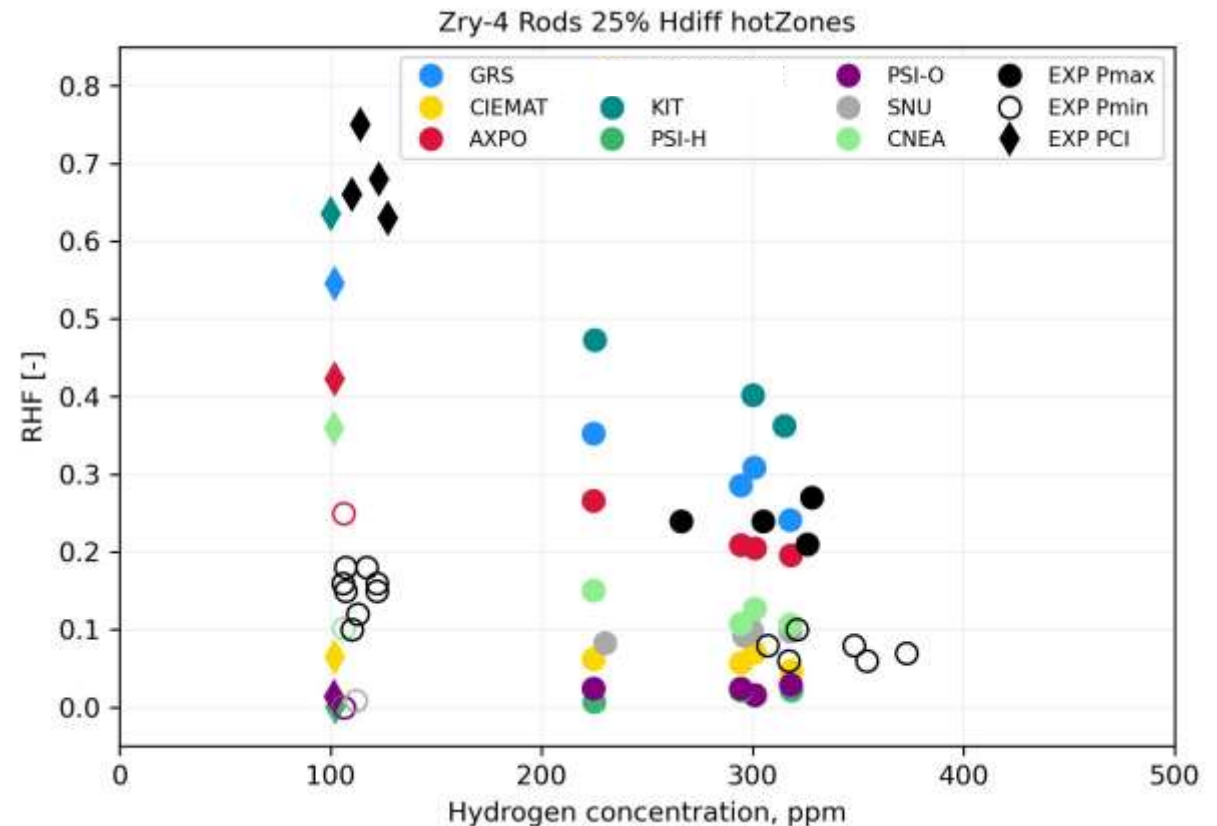
Simulations show a negative correlation between RHF and increasing initial hydrogen concentration, which is supported by experimental results

# Zry-4: Initial Hydrogen Concentration VS RHF



Zones 4-9  
Temperatures  
above 350°C

$$|C_{H,HVGE} - C_{H,ini}| < 25\% \text{ of } C_{H,target}$$

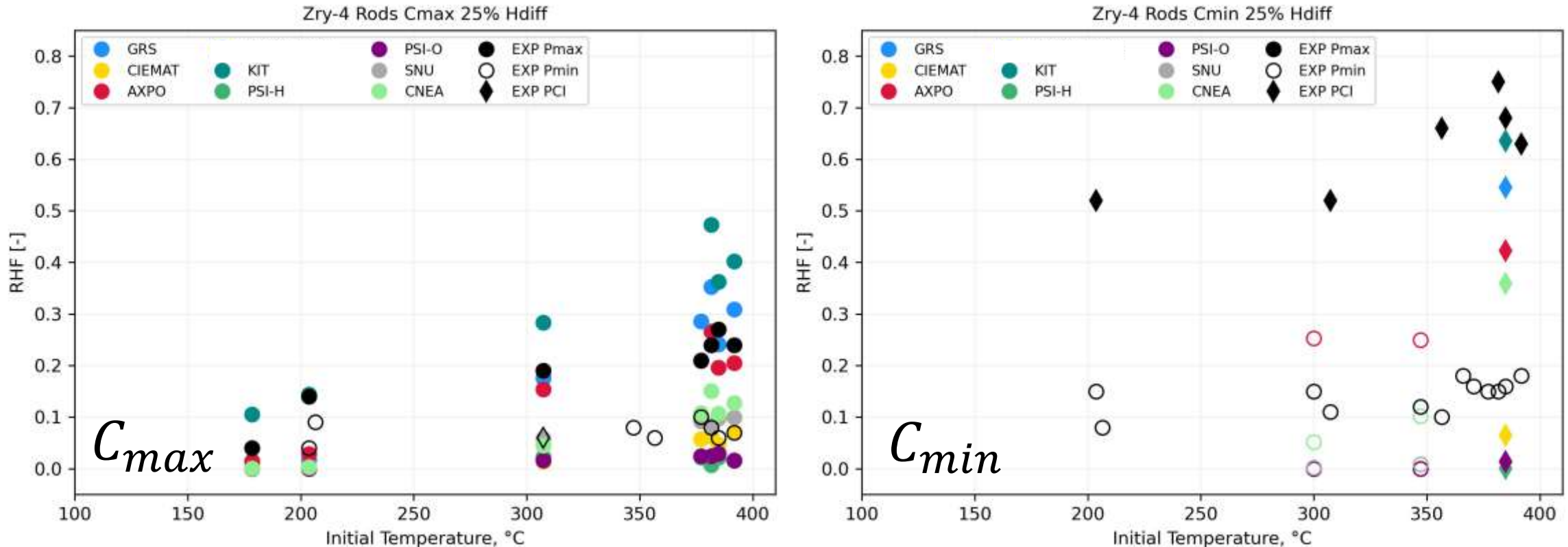


Simulations show a negative correlation between RHF and increasing initial hydrogen concentration, which is supported by experimental results



# Zry-4: Starting Temperature VS RHF

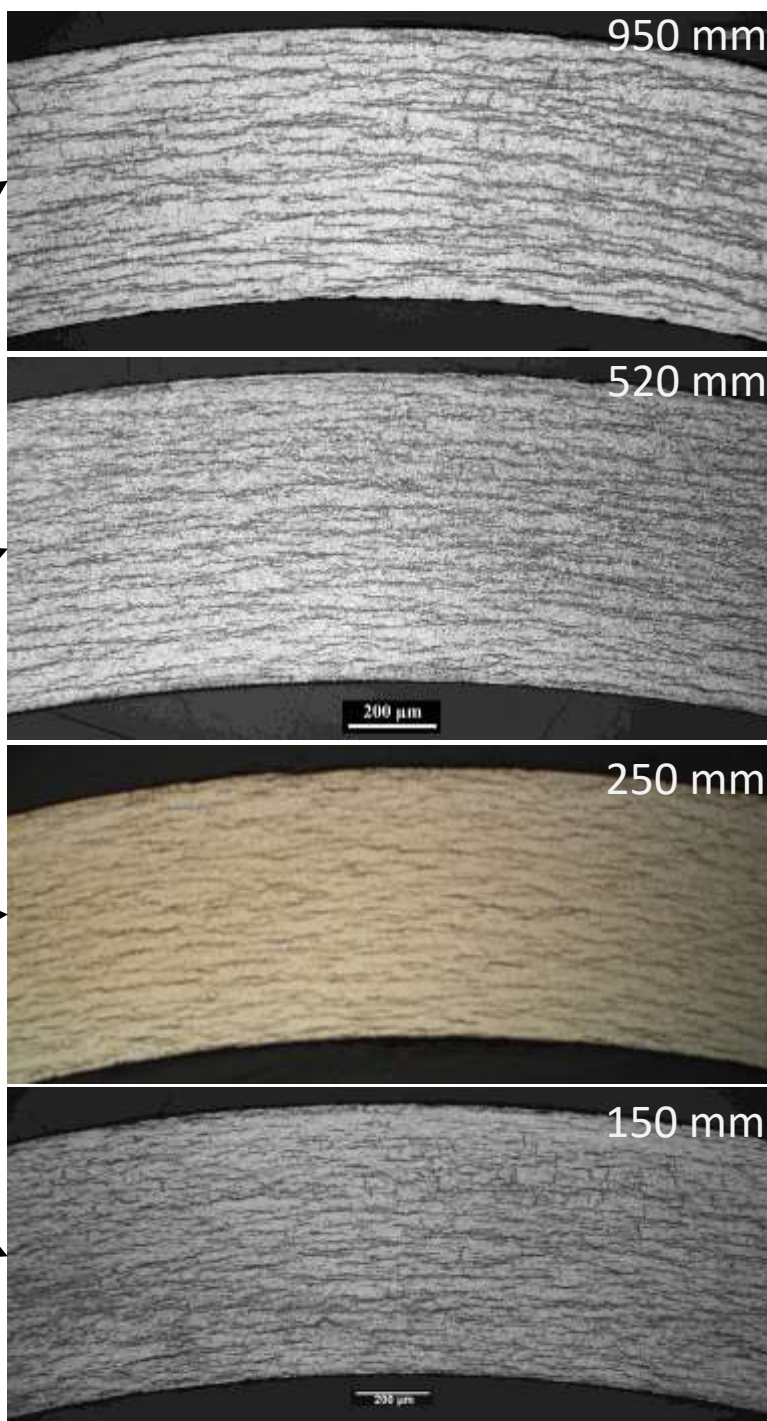
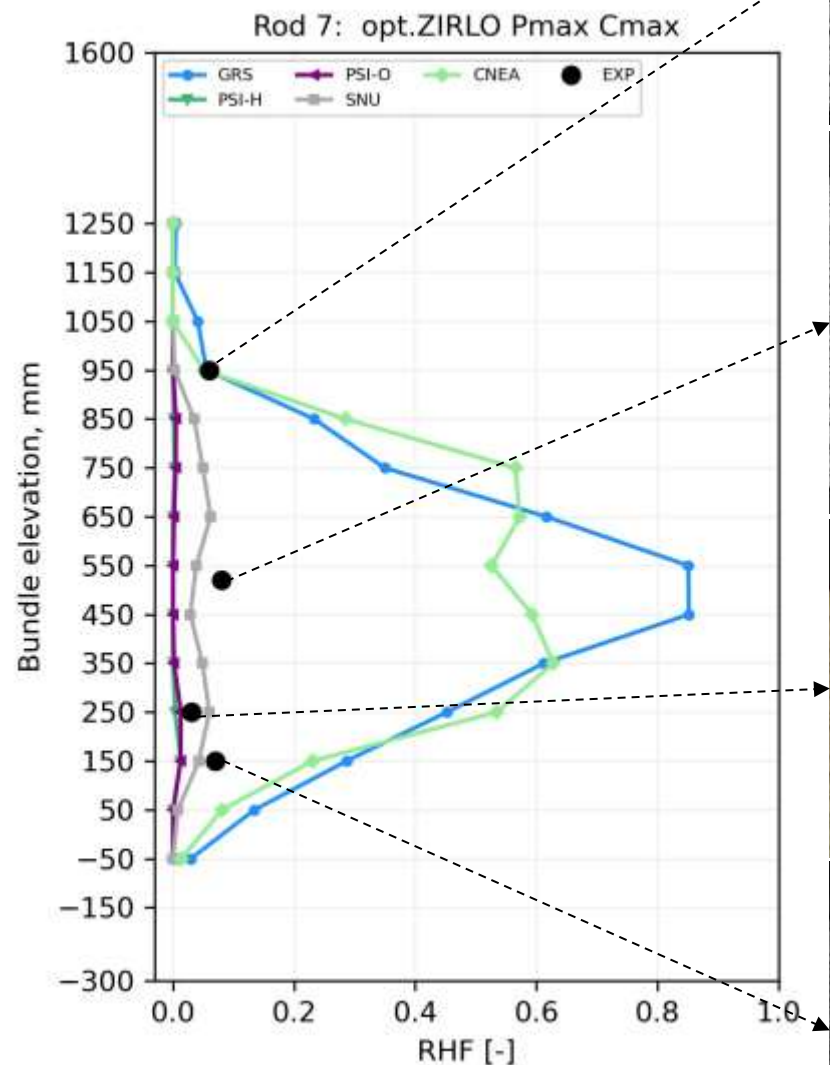
$$|C_{H,HVGE} - C_{H,ini}| < 25\% \text{ of } C_{H,target}$$



- Experiments demonstrate higher RHF at lower hydrogen concentrations, a trend partially captured by some calculations.
- Some calculations correctly capture the increase in RHF with rising initial temperatures in the zones
- Limited comparison for Cmin due to large discrepancy between initial and measured hydrogen concentrations

# Opt.ZIRLO: Rod 7

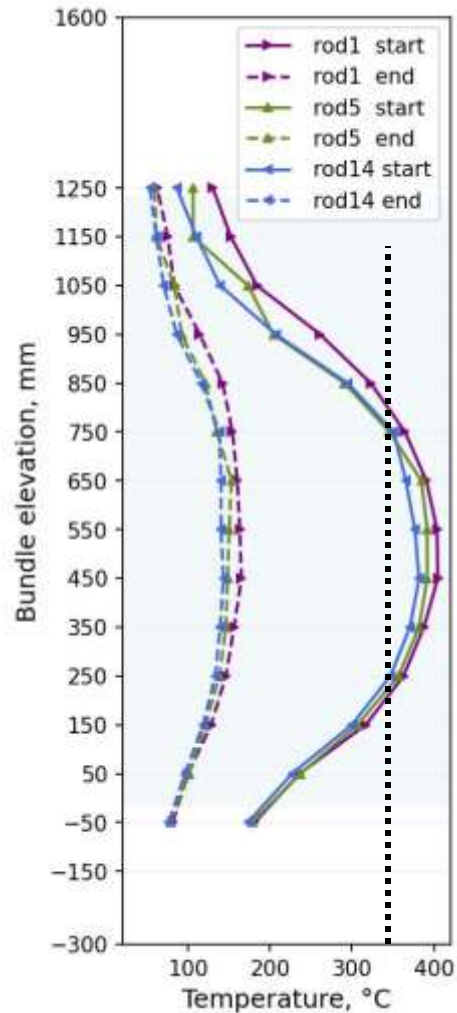
## 91MPa 300wppm Inner



Fewer radial hydrides than in Zry-4 observed under similar conditions in opt.ZIRLO.

A threefold difference between the initial hydrogen concentrations used and the measured hydrogen limits the comparison.

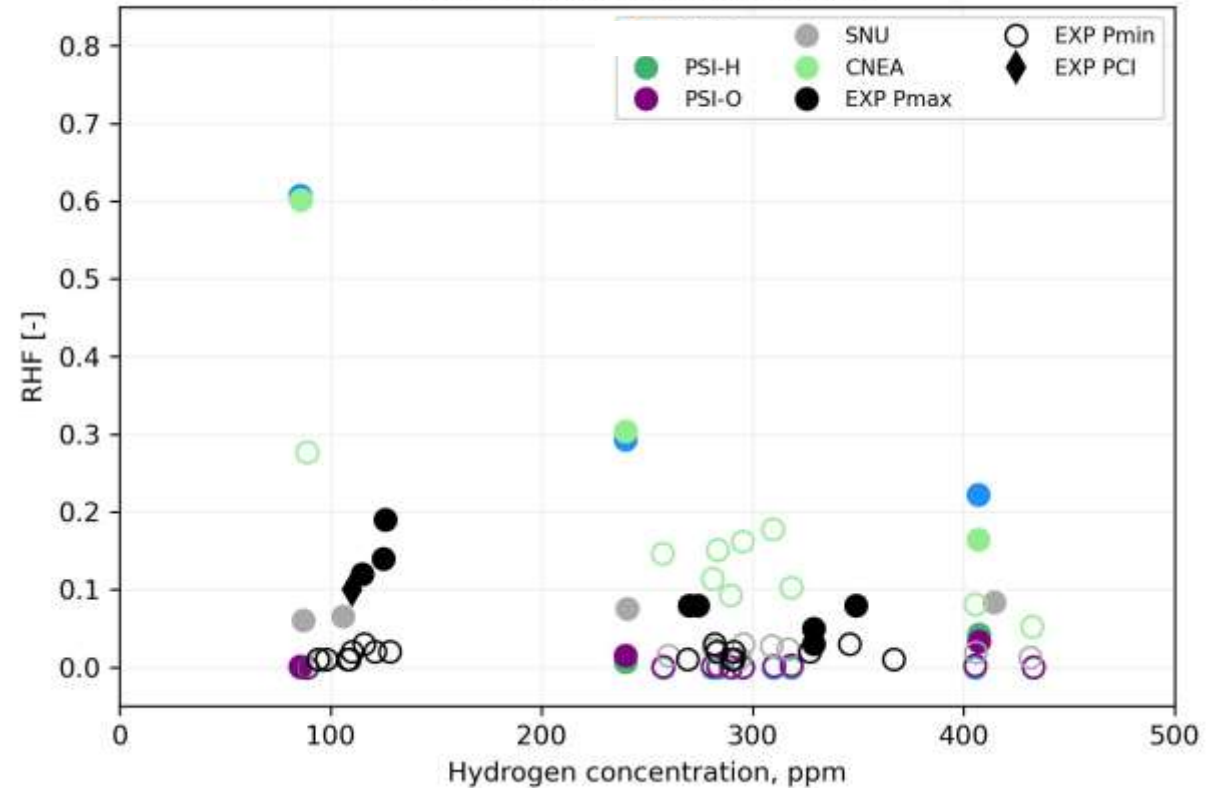
# Opt.ZIRLO: Initial Hydrogen Concentration VS RHF



Zones 4-9  
Temperatures  
above 350°C

$$|C_{H,HVGE} - C_{H,ini}| < 30\% \text{ of } C_{H,target}$$

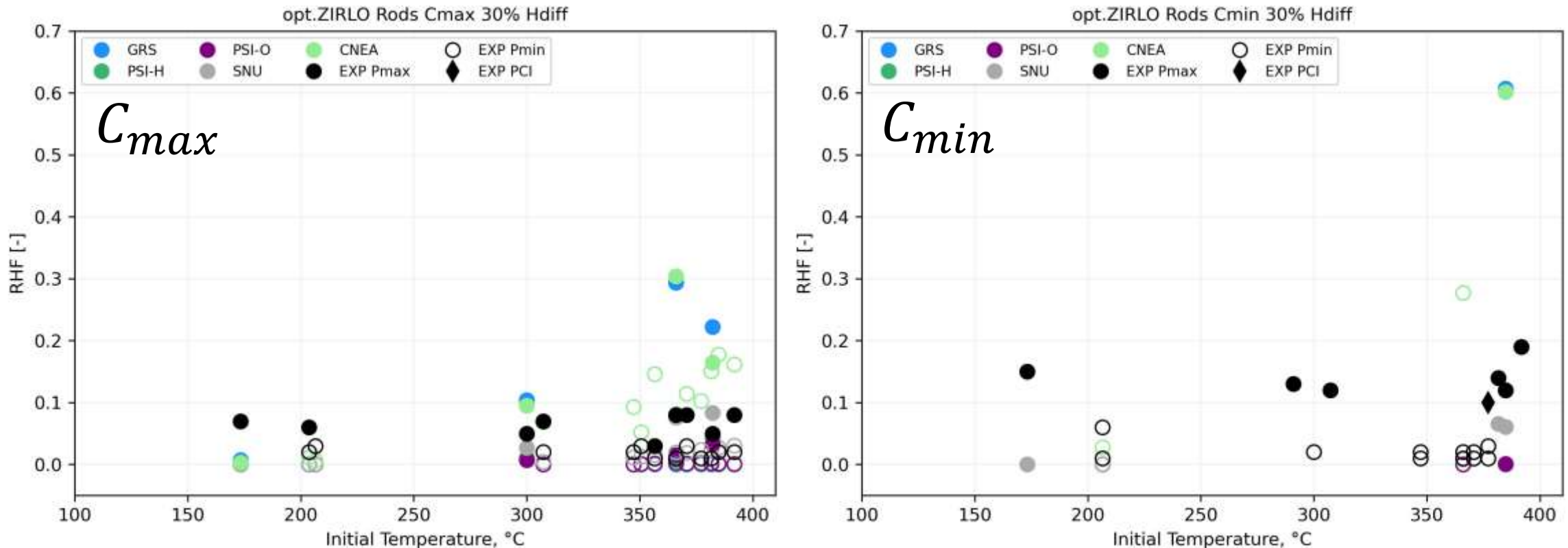
opt.ZIRLO Rods 30% Hdiff hotZones



Modeling approaches that underestimated RHF for Zry-4 align better with experiments for opt. ZIRLO.

# Opt.ZIRLO: Starting Temperature VS RHF

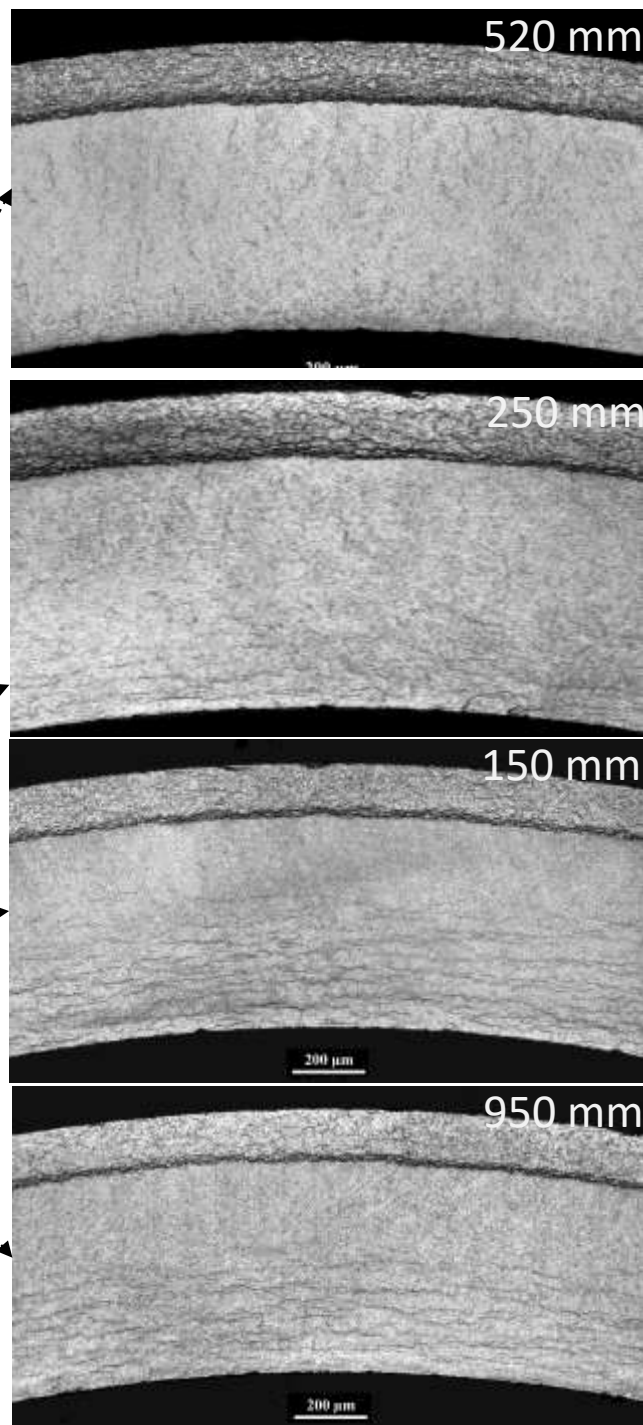
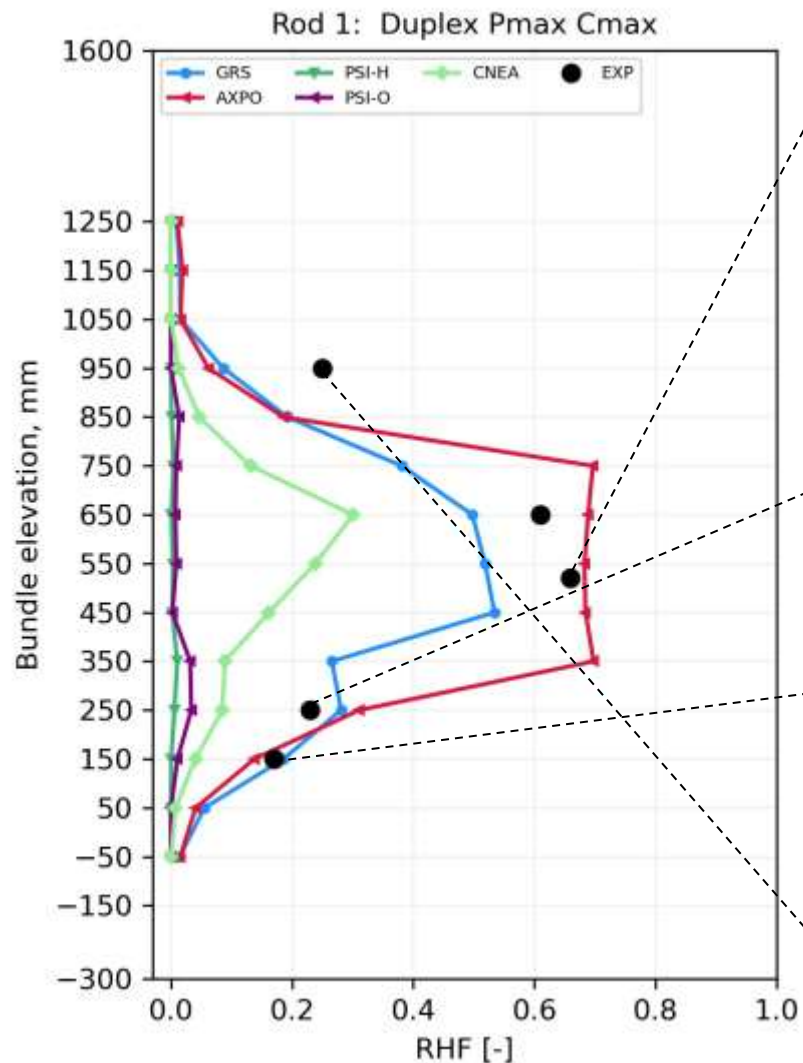
$$|C_{H,HVGE} - C_{H,ini}| < 30\% \text{ of } C_{H,target}$$



- Limited comparison due to large discrepancy between initial and measured hydrogen concentrations
- Experiments show slightly higher RHF at lower hydrogen concentrations, a trend not well captured by the simulations.
- Experiments show similar RHF for different starting temperatures, whereas simulations indicate an increasing RHF with higher temperatures.

# DX D4: Rod 1

## 91MPa 300wppm Central



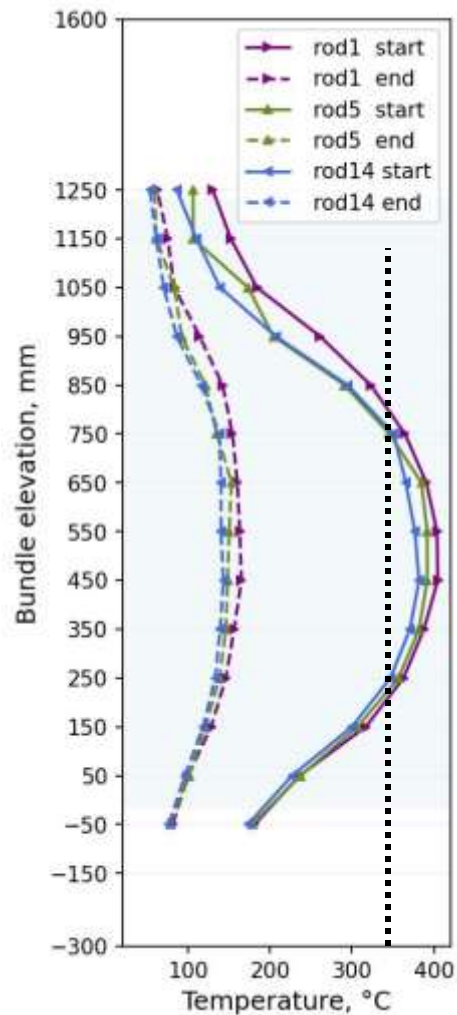
Hydride reorientation is stronger compared to Zry-4.

The extent of the depleted zone is temperature-dependent

Radial hydride orientation increases toward the liner

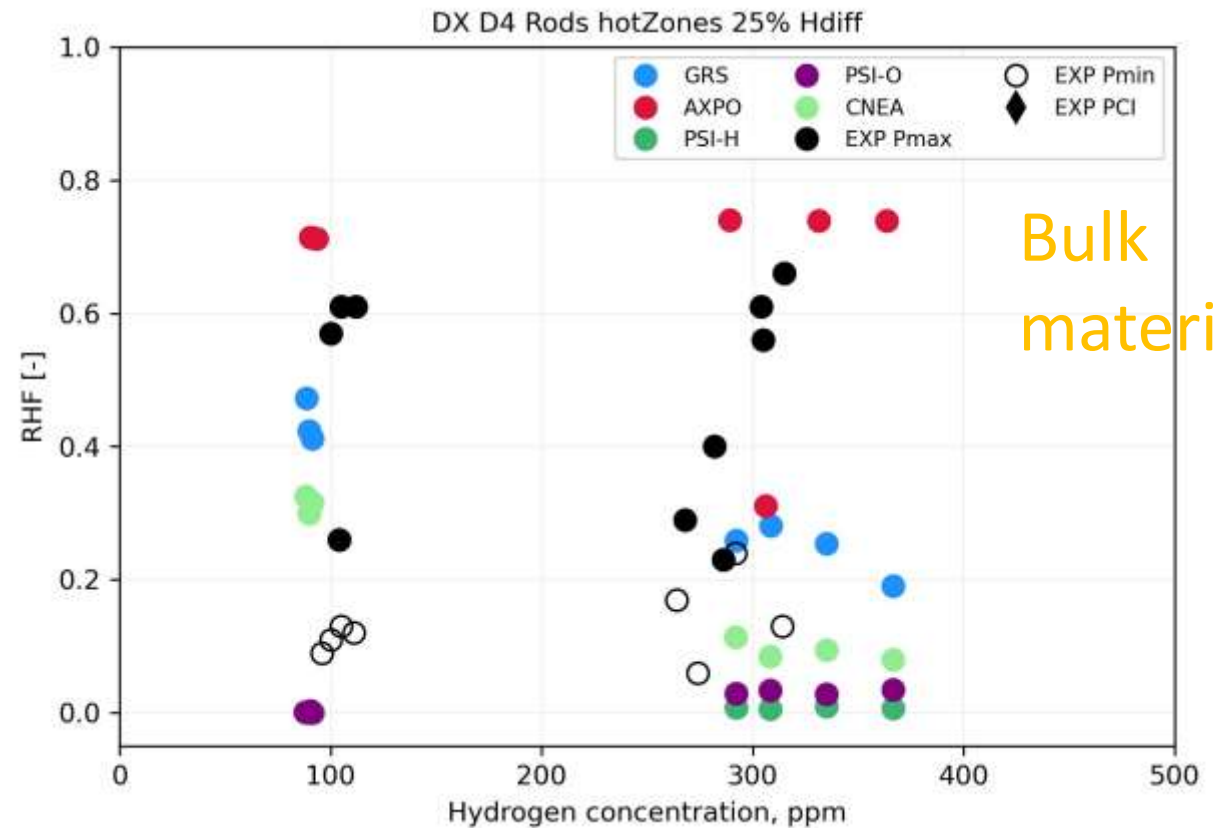
Most participants modeled only the bulk region of the duplex rods

# DX D4: Initial Hydrogen Concentration VS RHF



Zones 4-9  
Temperatures  
above 350°C

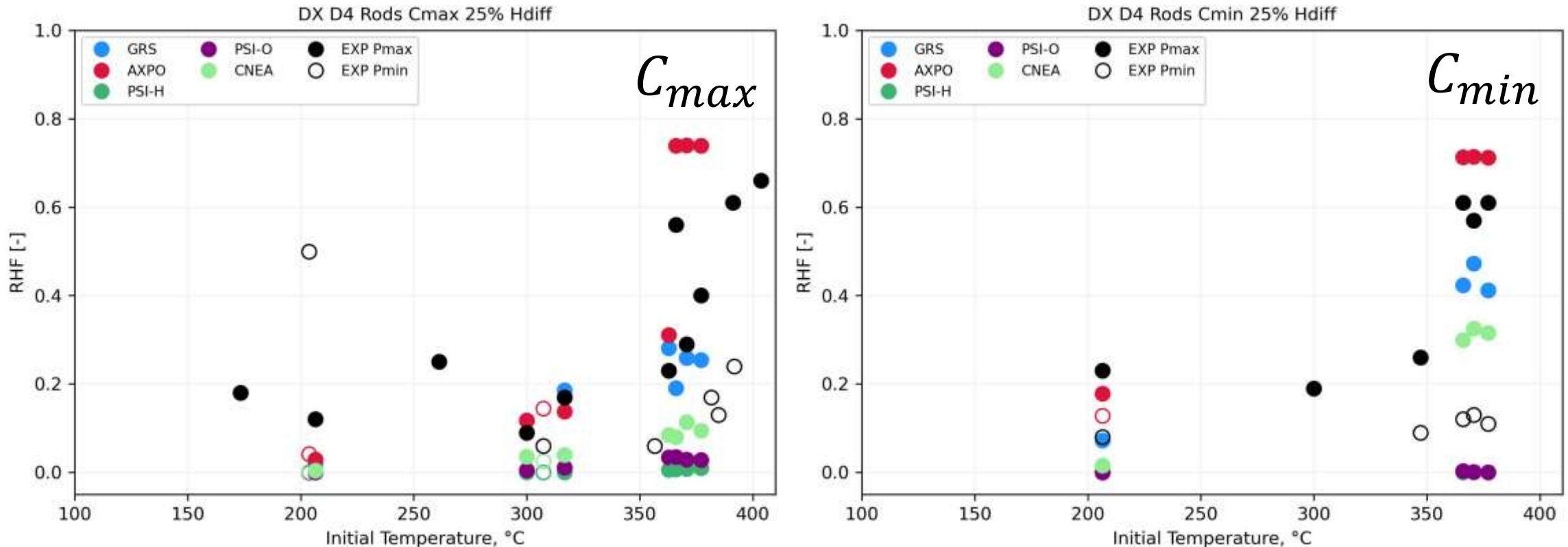
$$|C_{H,HVGE} - C_{H,ini}| < 25\% \text{ of } C_{H,target}$$



The modeling approach, which considers both liner and bulk, better captures the higher than in Zry-4 RHF.

## DX D4: Starting Temperature VS RHF

$$|C_{H,HVGE} - C_{H,ini}| < 25\% \text{ of } C_{H,target}$$



- Experiments show little difference in RHF between low and high hydrogen concentrations, while most simulations show an increasing trend for Cmin.
- Especially at high pressure, RHF increases significantly with rising starting temperature, captured partially.
- Limited comparison due to differing boundary conditions

## Next steps

The preparation of the final report is underway.

Further Benchmark Activities:

- Use HVGE values to define initial hydrogen content.

- Focus on rods suitable for comparison that are unaffected by PCI.

- Model duplex rods with emphasis on radial behavior.



Gesellschaft für Anlagen- und  
Reaktorsicherheit (GRS) gGmbH  
Schwertnergasse 1  
50667 Köln



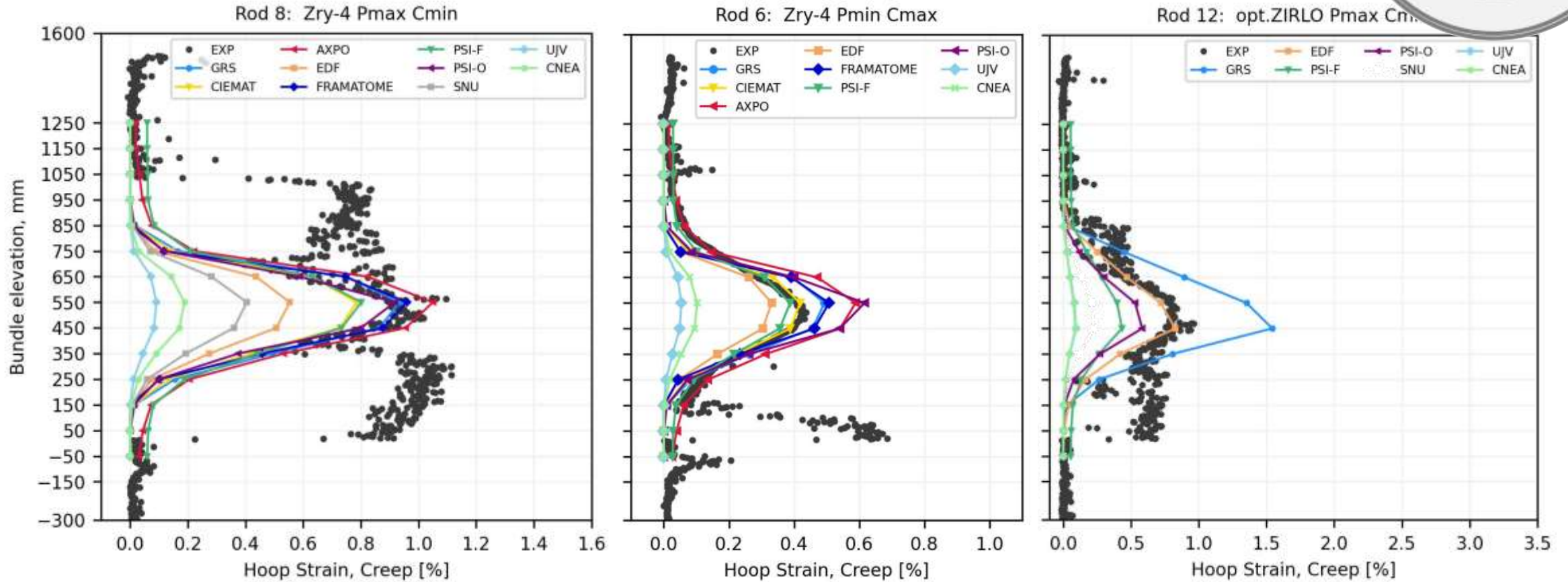
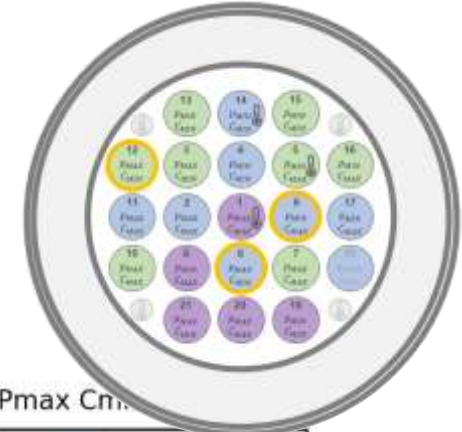
→ [www.grs.de](http://www.grs.de)

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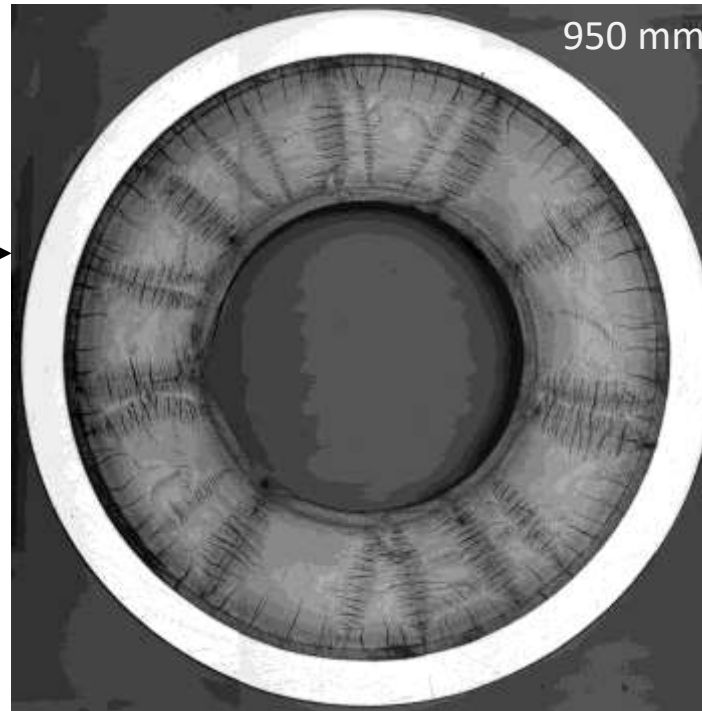
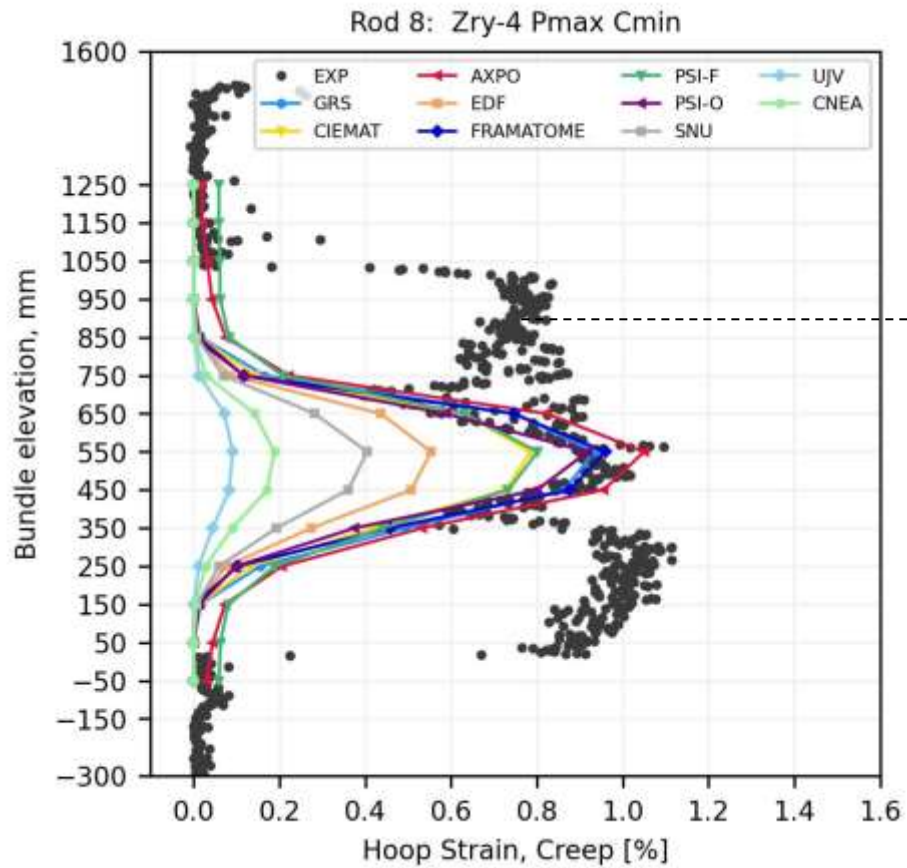
**FOLLOW US**



# Pellet-Cladding Interaction

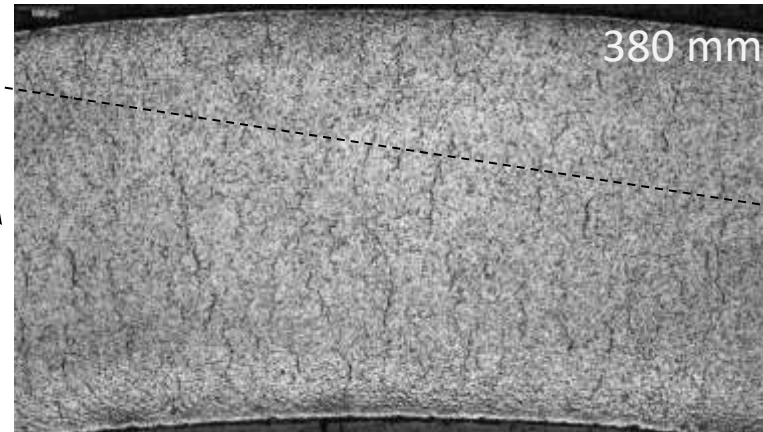
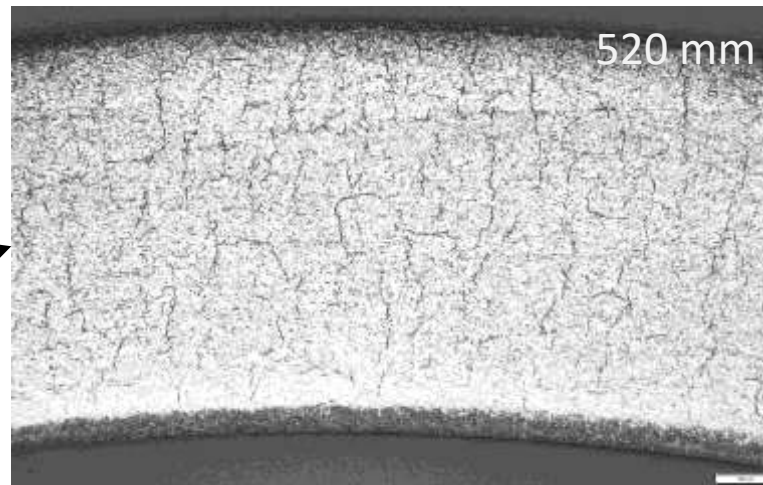
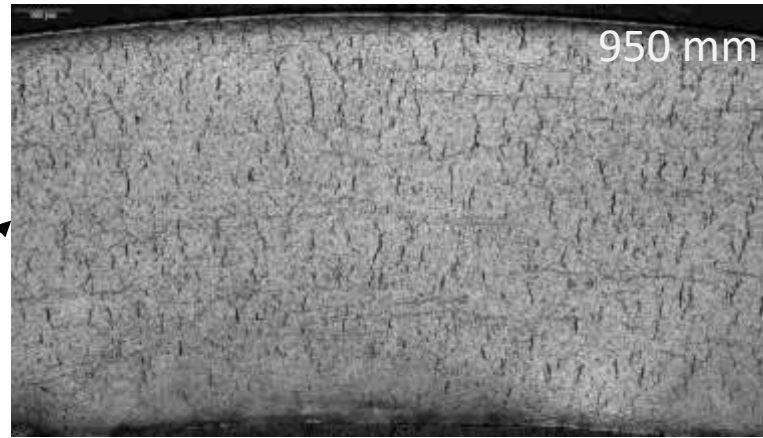
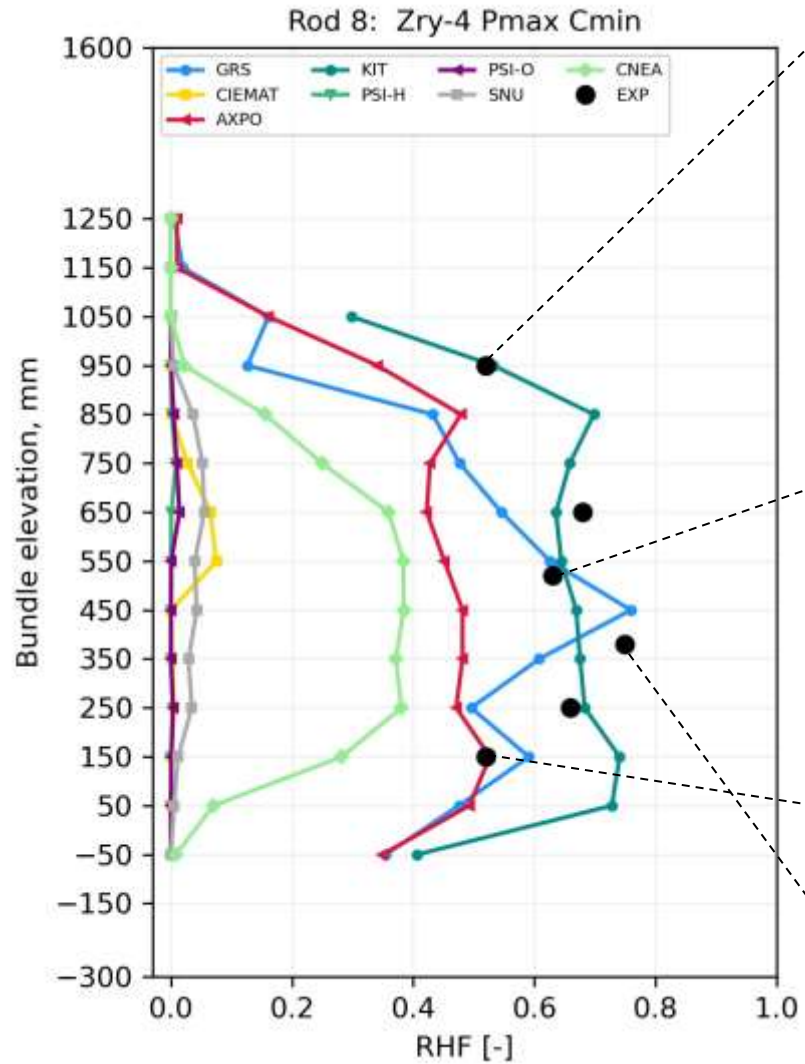


# Pellet-Cladding Interaction



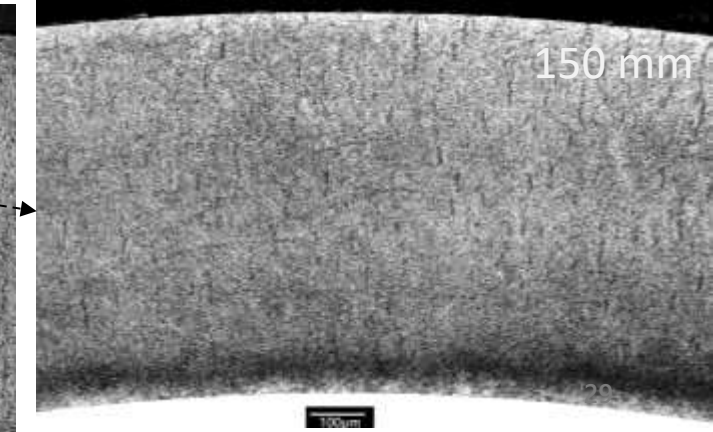
# Zircaloy-4: Rod 8

## 91MPa 100wppm Inner

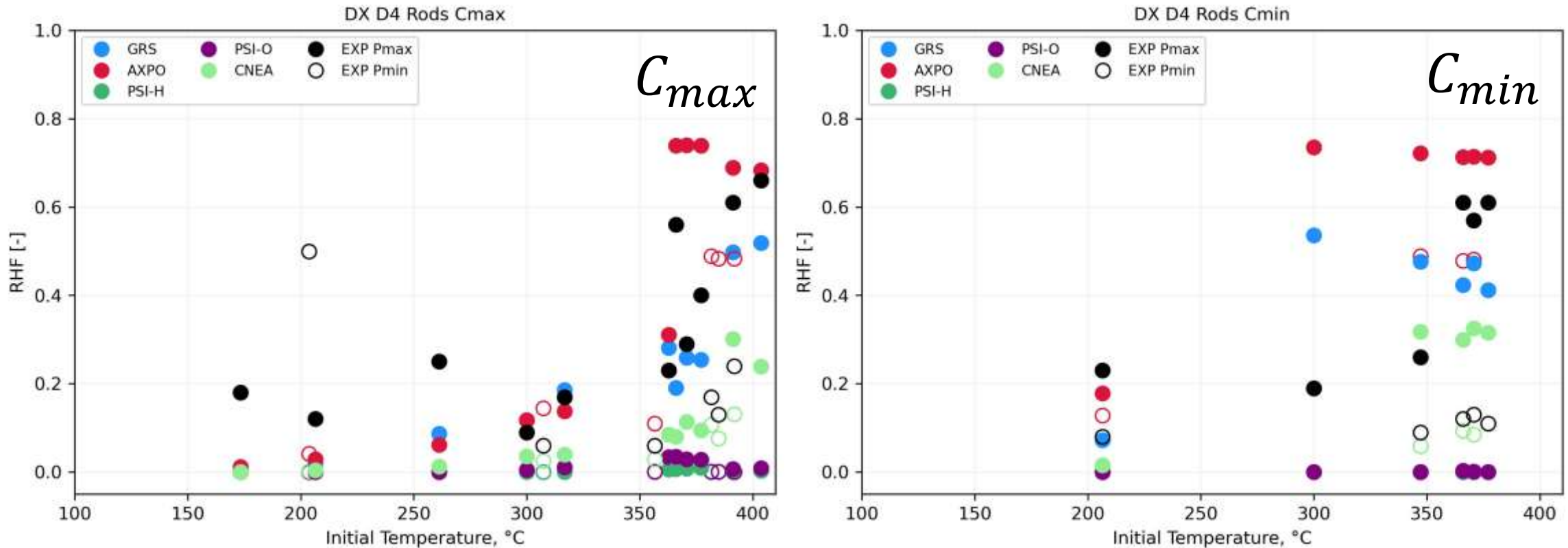


Radial hydrides present across all examined axial planes, including cold zones  
Pressure-induced higher hydrogen dissolution?

H.E. Weekes, D. Dye, J.E. Proctor, D. Smith, C. Simionescu, T.J. Prior, M.R. Wenman, The effect of pressure on hydrogen solubility in Zircaloy-4, Journal of Nuclear Materials, Volume 524, 2019, Pages 256-262, ISSN 0022-3115, <https://doi.org/10.1016/j.jnucmat.2019.07.012>.



# DX D4: Starting Temperature VS RHF



- Experiments show little difference in RHF between low and high hydrogen concentrations, while most simulations show an increasing trend for  $C_{min}$ .
- Especially at high pressure, RHF increases significantly with rising starting temperature, captured partially.



**Johannes Bertsch**

PSI

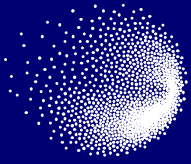
## **Hydrogen in Claddings – Investigations on Hydrogen Axial Mobility, Role of Liner and Creep**

Under reactor operation, corrosion takes place at the hot surface of nuclear fuel rods in the cooling water. The H<sub>2</sub>O is split up; while the oxygen leads to the formation of an oxide layer on the fuel cladding surface, a part of the hydrogen diffuses into the cladding. In water cooled reactors, the cladding typically consists of a zirconium alloy. At higher temperatures hydrogen remains in solid solution, but precipitates into a zirconium-hydrogen compound, hydrides, with decreasing temperature. These hydrides are brittle and can affect the mechanical properties of the cladding. However, the cladding being the first barrier against the release of highly radioactive fission products must keep its integrity during and after reactor service.

After reactor service and under intermediate dry storage conditions, the fuel rods remain at a certain temperature because of decay heat and keep internal pressure because of fission gas. This leads to creep of the cladding. Hydrogen in solid solution accelerates creep, hydrides slow it down. In addition, several factors make hydrogen diffuse, i.e., gradients in hydrogen concentration, in temperature, in chemical composition or in mechanical stress. Existing hydrides attract further hydrogen and grow. These effects can lead to hydrogen/hydrides accumulations and thus to weak spots in the material.

Claddings can have a compound design, namely a thin liner on the cladding substrate. The liner – for the use in pressurized water reactors at the outer cladding surface to improve corrosion resistance, and for boiling water reactors at the inner side to mitigate pellet-cladding interaction – is a purer zirconium alloy. Due to its different terminal solid solubility for hydrogen compared to the substrate, the liner accumulates hydrides during cooling down. Therefore, a liner influences the creep behavior and hydrogen mobility in the cladding. While the diffusion of hydrogen towards a liner has been well examined, the overlaying of cladding tube axial hydrogen diffusion and attraction by a liner is unknown.

To explore the role of a liner for creep and axial hydrogen diffusion, two PhD projects have been launched at PSI. Both projects use claddings with and without a liner. In the case of axial diffusion, a hydrogen concentration gradient is created by electrochemical hydrogenation; the creep test samples are homogeneously hydrogenated in a gaseous environment. Besides microstructural characterizations, the samples are investigated with high resolution neutron imaging to explore the hydrogen/hydrides distribution before and after diffusion and creep testing. The work is accompanied by model calculations, in case of creep focusing on the stress distribution using FEM, in case of axial diffusion on the mobility and precipitation of hydrides. First results and the development of the projects are described.



**PSI** Center for Nuclear Engineering  
and Sciences

# Hydrogen in Claddings – Investigations on Hydrogen Axial Mobility, Role of Liner and Creep

Current PhD projects

Johannes Bertsch, Benedetta Buzzatti, Liliana Duarte,  
Sebastian Niedermeyer, Robert Zubler

30<sup>th</sup> International QUENCH Workshop, 2025, Dec 16-18, KIT

- Intro
- Axiality
- Creep
- Outlook



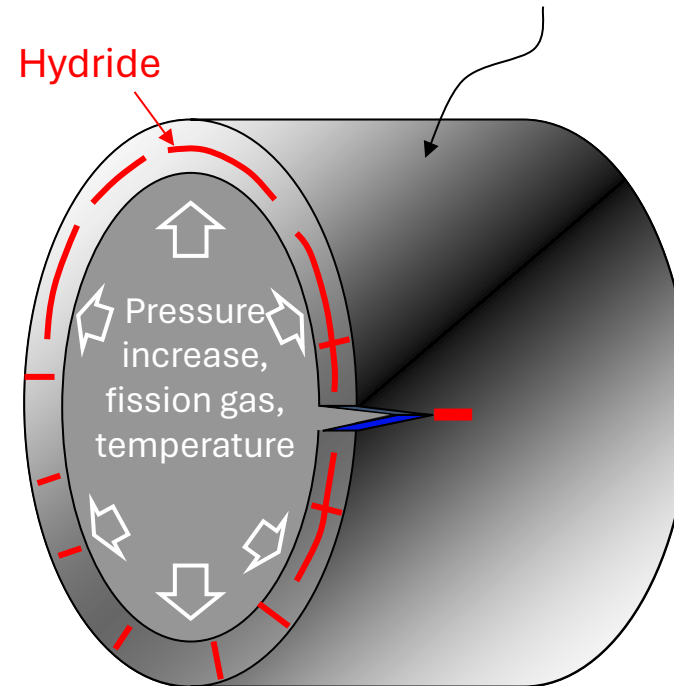
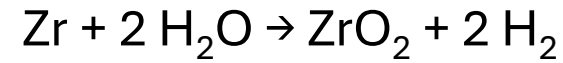
# Introduction

## Hydrogen Uptake, Diffusion and Precipitation

During fuel service in the reactor hydrogen is created and diffuses into the cladding

- Embrittlement (**fracture toughness**)
- Precipitation of hydrides (**solubility!**)
- Change of **creep properties**
- **Reorientation** of hydrides
- **DHC** – Delayed Hydride Cracking

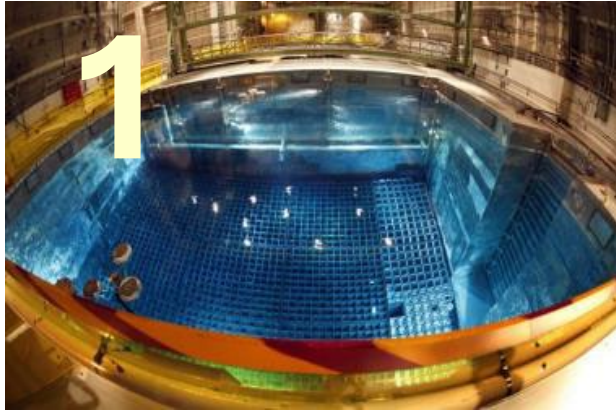
Those effects are aggravated with burn-up and deteriorate the mechanical stability of the fuel cladding.



Reduction of safety (cladding integrity) is not acceptable!

# Introduction

## Cladding Thermomechanics – Transportation, Handling and Dry Storage



After operation: cladding embrittlement due to hydrogen redistribution and precipitation

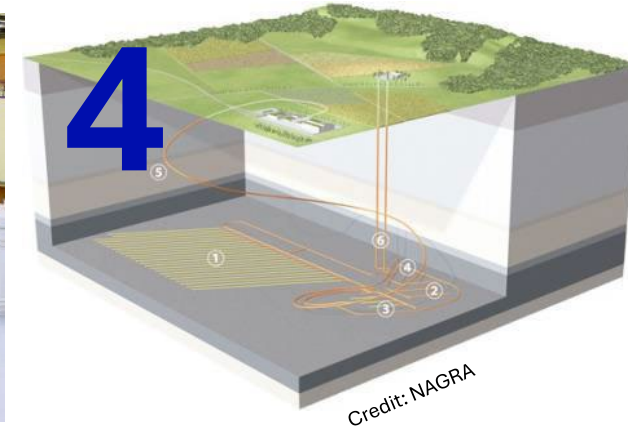
2

- Unloading from pool
- Vacuum drying
- Packaging into transport/storage cask

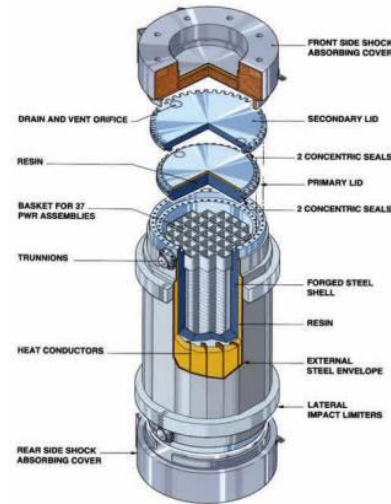
- Temperature ↑ (decay)
- Pressure ↑ (fission gas)
- Hydrogen in solution



- Dry storage
- Temperature going down ↓
- Hydrides precipitation, embrittlement
- Liner cladding



- Final handling
- Repacking



TN24 cask produced by Orano TN

$$J_{\text{Diffusion}} = J_{\text{Fick}} + J_{\text{Soret}} + J_{\text{Stress}} + J_{\text{Material Gradient}}$$

HNGD\* model

- 1 Fickian Diffusion: net flux to regions of **lower hydrogen concentration**
- 2 Soret Effect: hydrogen migrates towards **cooler regions**
- 3 Stress-induced diffusion: towards zones of **hydrostatic tensile stress**
- 4 Material-driven diffusion: flux influenced by **microstructural features, irradiation damage, or liner presence**



**Spent fuel is cooling off, but hydrogen is still on the move!**

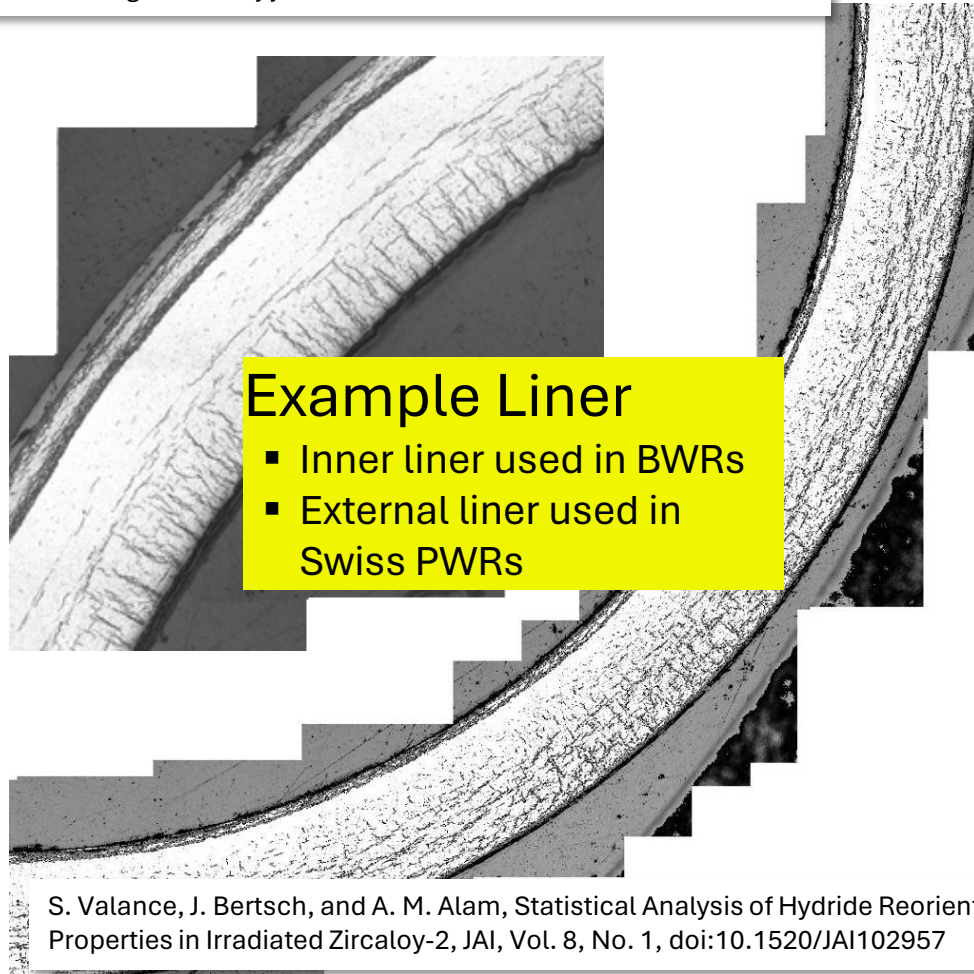
Sebastian Niedermeyer, Investigation of Hydrogen and Hydrides Distribution in Axial Cladding Direction at PSI, BGZ Workshop, 2025, Nov 25-26, Berlin

\* **H**ydrides **N**ucleation, **G**rowth and **D**issolution model

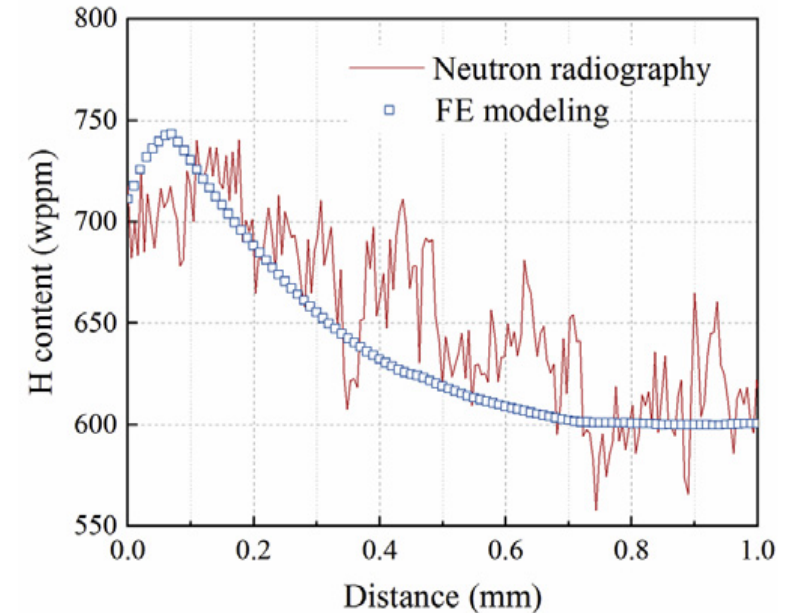
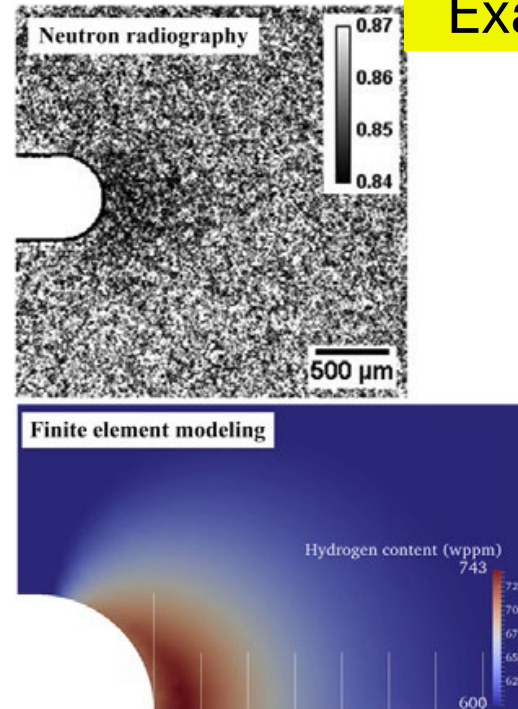
# Introduction

## Hydrogen Diffusion and Precipitation, Influence of Liner and Stress

S. Valance, J. Bertsch, Hydrides reorientation investigation of high burn-up PWR fuel cladding, Journal of Nuclear Materials 464 (2015) 371–381, <http://dx.doi.org/10.1016/j.jnucmat.2015.05.003>



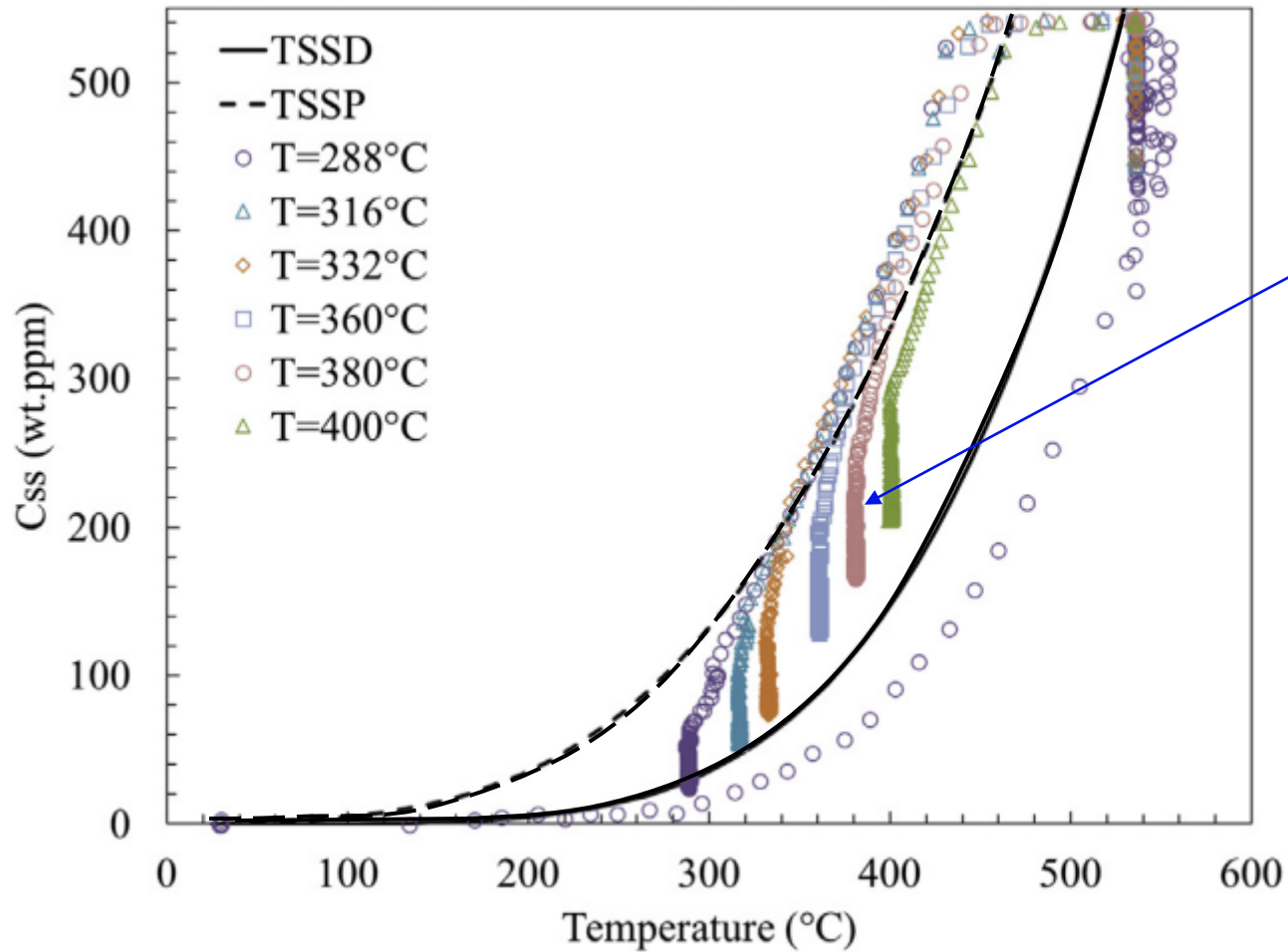
### Example Stress



W. Gong, P. Trtik, S. Valance, J. Bertsch, Hydrogen diffusion under stress in Zircaloy: High-resolution neutron radiography and finite element modeling, Journal of Nuclear Materials 508 (2018) 459e464, <https://doi.org/10.1016/j.jnucmat.2018.05.079>

# Introduction

## Hydrogen Diffusion and Precipitation

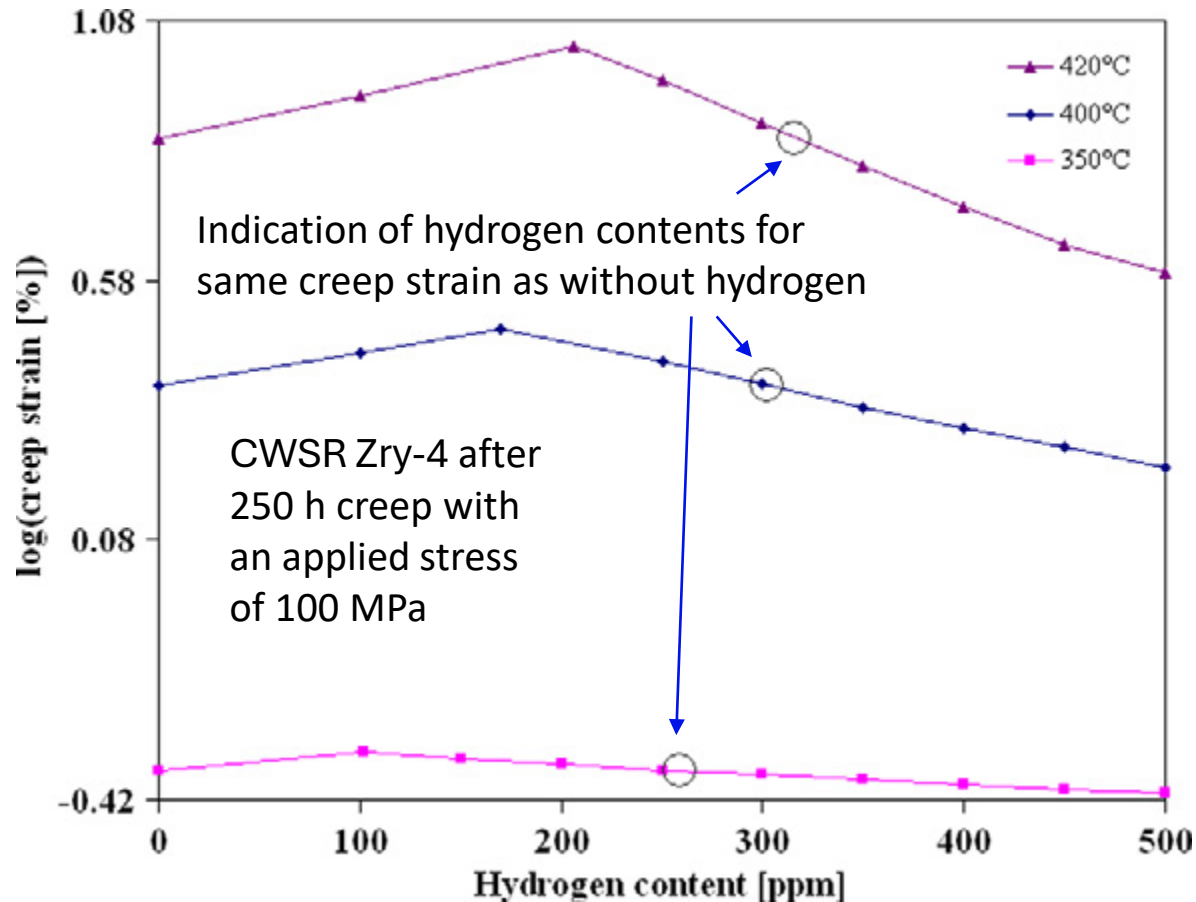


- Hysteresis ( $TSSP \neq TSSD$ )
- Different curves for liner and substrate
- Growing hydrides attract hydrogen
- More hydrides in liner

E. Lacroix, A.T. Motta, J.D. Almer, Experimental determination of zirconium hydride precipitation and dissolution in zirconium alloy, *Journal of Nuclear Materials* 509 (2018) 162e167, <https://doi.org/10.1016/j.jnucmat.2018.06.038>

# Introduction

## Hydrogen, Hydrides and Creep



### Primary factors:

- Temperature
- Stress
- Hydrogen concentration

### Secondary factors:

- Hydrogen in solid solution
  - Hydrides orientation
- } Stress dependent

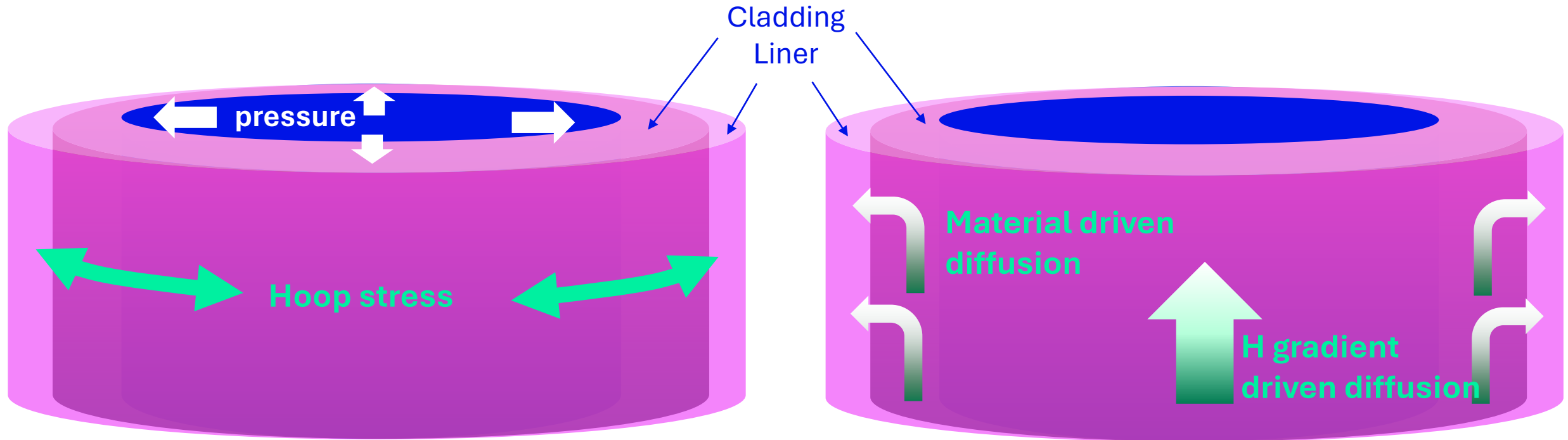
### Additional factors:

- Liner
  - different hydrogen terminal solubility
  - different mechanical properties

V. Mallipudi, S. Valance, J. Bertsch, Meso-scale analysis of the creep behavior of hydrogenated Zircaloy-4, Mechanics of Materials 51 (2012) 15–28, <http://dx.doi.org/10.1016/j.mechmat.2012.03.003>

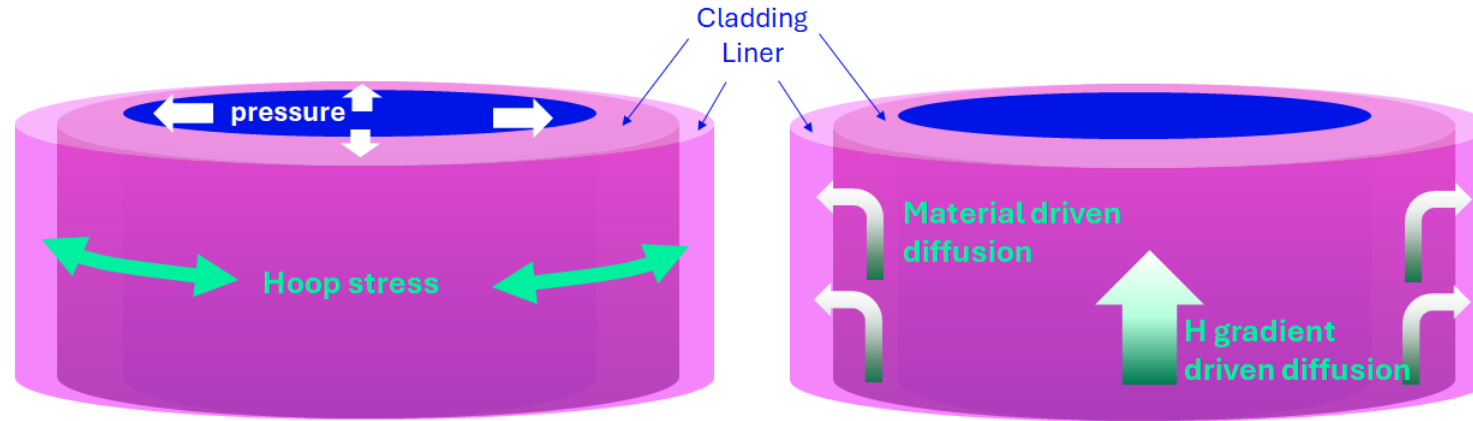
# Introduction

## Hydrogen, Temperature, Stress – 2 Cases for **Liner Cladding**



# Introduction

Hydrogen, Temperature, Stress, Liner – 2 cases



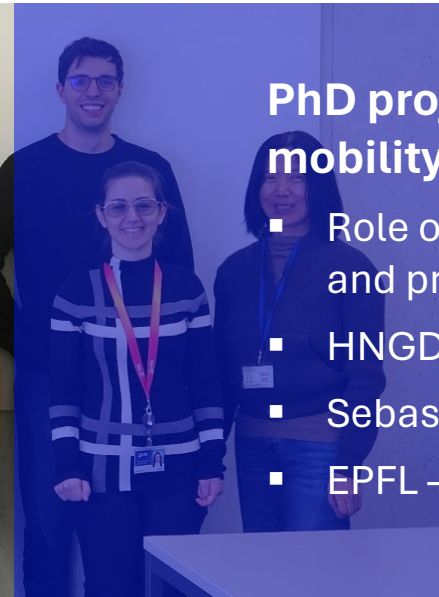
## PhD project on creep

- Role of stress and liner, stress driven hydrogen diffusion and resulting creep properties
- Benedetta Buzzatti
- ETH – Zürich



## PhD project on axial hydrogen mobility

- Role of liner on axial diffusion and precipitation
- HNGD model
- Sebastian Niedermeyer
- EPFL – Lausanne

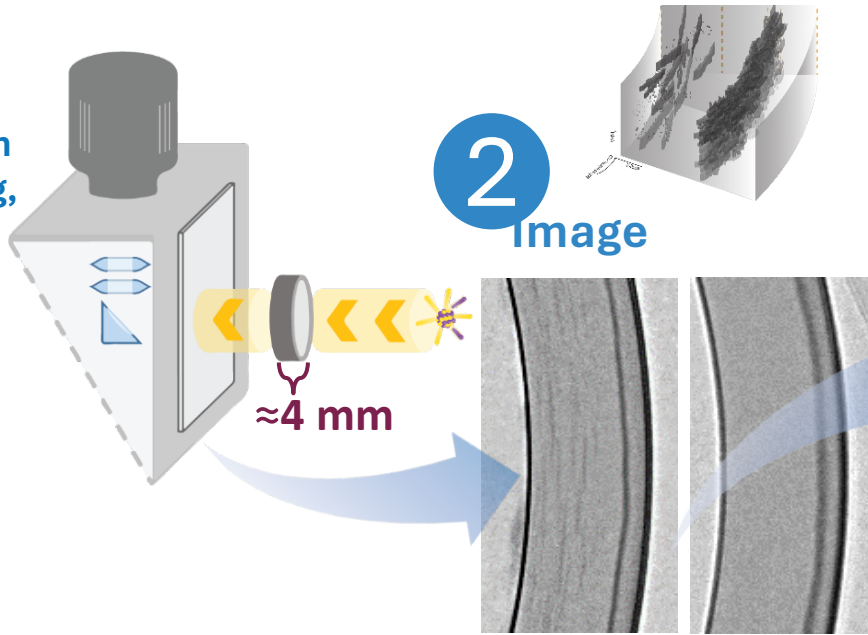




# Both PhD projects – High Resolution Neutron Imaging (HR-NI)

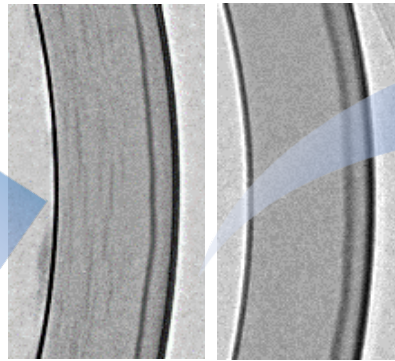
1

Neutron Imaging, ICON SING



2

Image



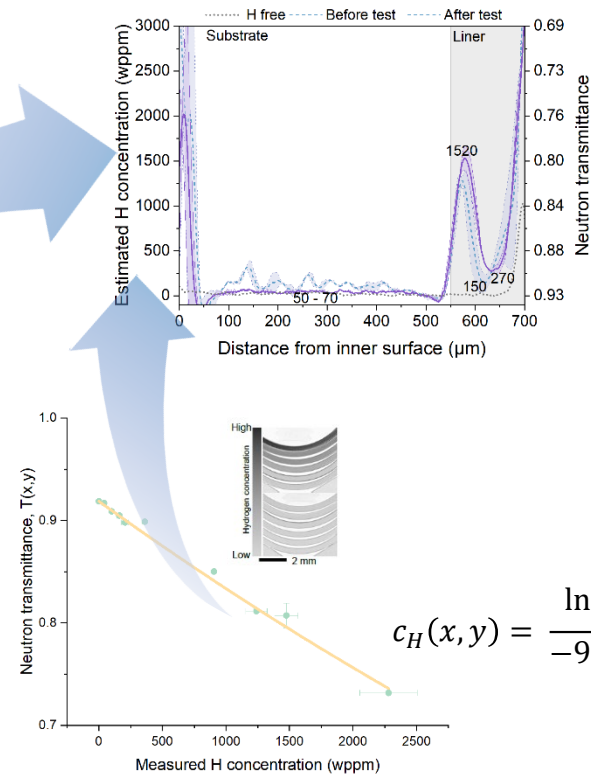
500  $\mu\text{m}$  transmittance >0.98 <0.7

Attenuation coefficient for neutrons

H	Zr
3.44	0.29

3

Quantification



$$c_H(x, y) = \frac{\ln\left(\frac{T(x, y)}{0.9227}\right)}{-9.73E - 05}$$

- Spatial resolution < 10  $\mu\text{m}$
- Hydrogen from ~10 to several 1000 wppm, concentration resolution a few tens of wppm

O. Yetik et al, 29th International QUENCH Workshop, 2024, Nov 21, KIT

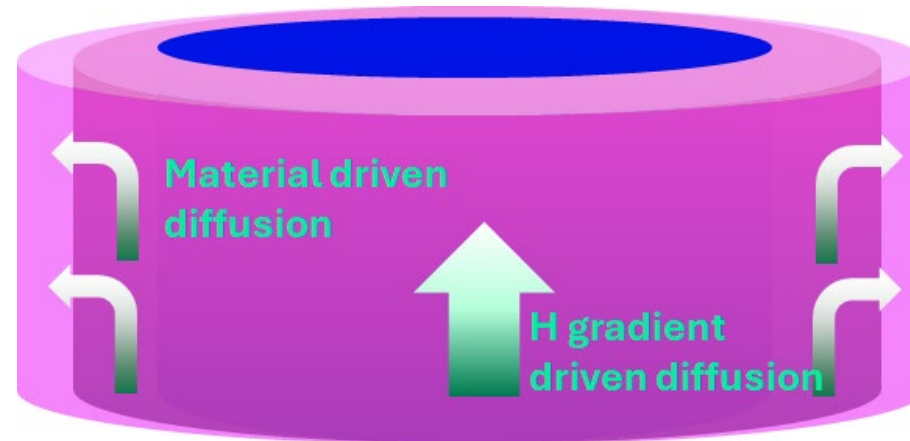
# Both PhD projects – HR-NI at SINQ



- Intro
- Axiality
- Creep
- Outlook

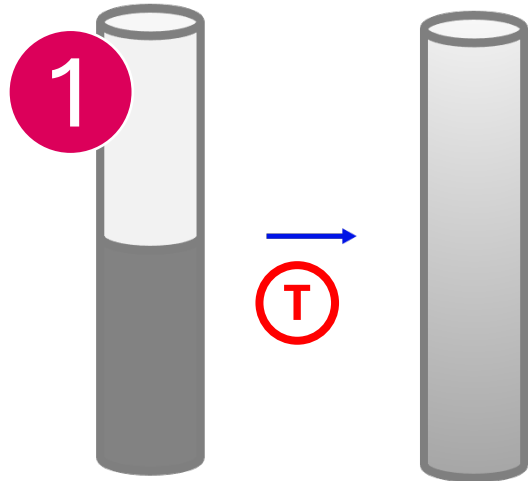
Comprehensive understanding of axial hydrogen diffusion is essential for **predictive modeling** and **safety assessment** of nuclear fuel rods.

- Texture
- Liner

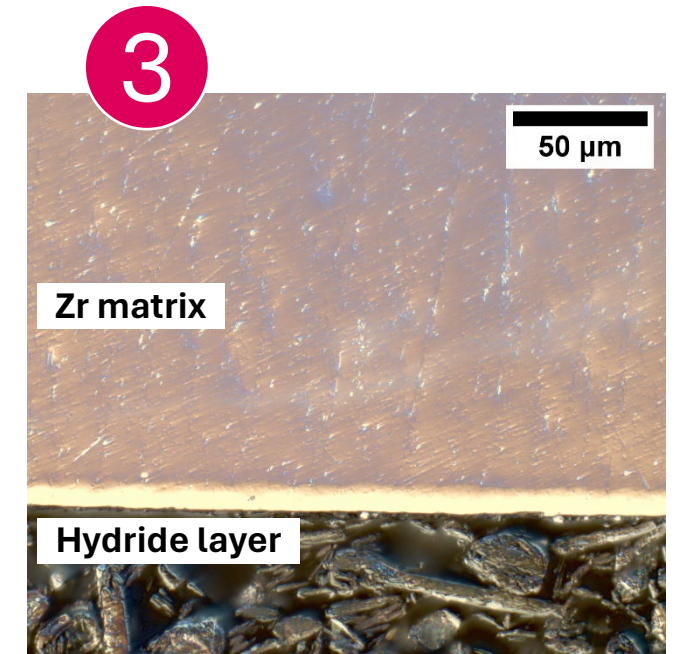
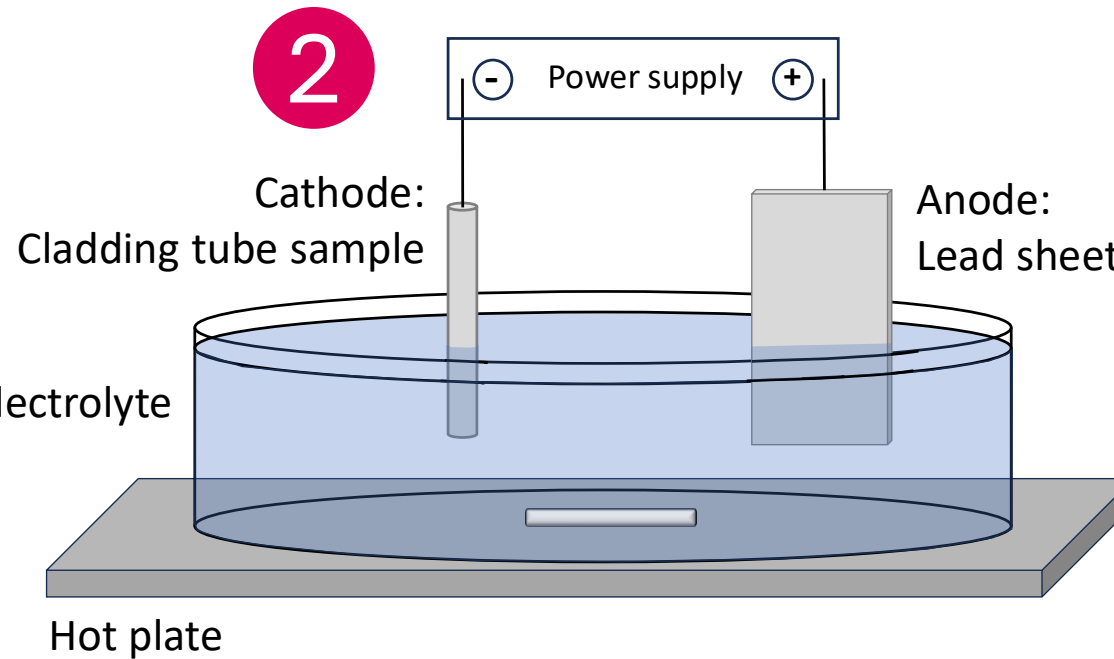


# Experimental Approach – Electrochemical Hydrogenation

Approach  
Concentration Gradient

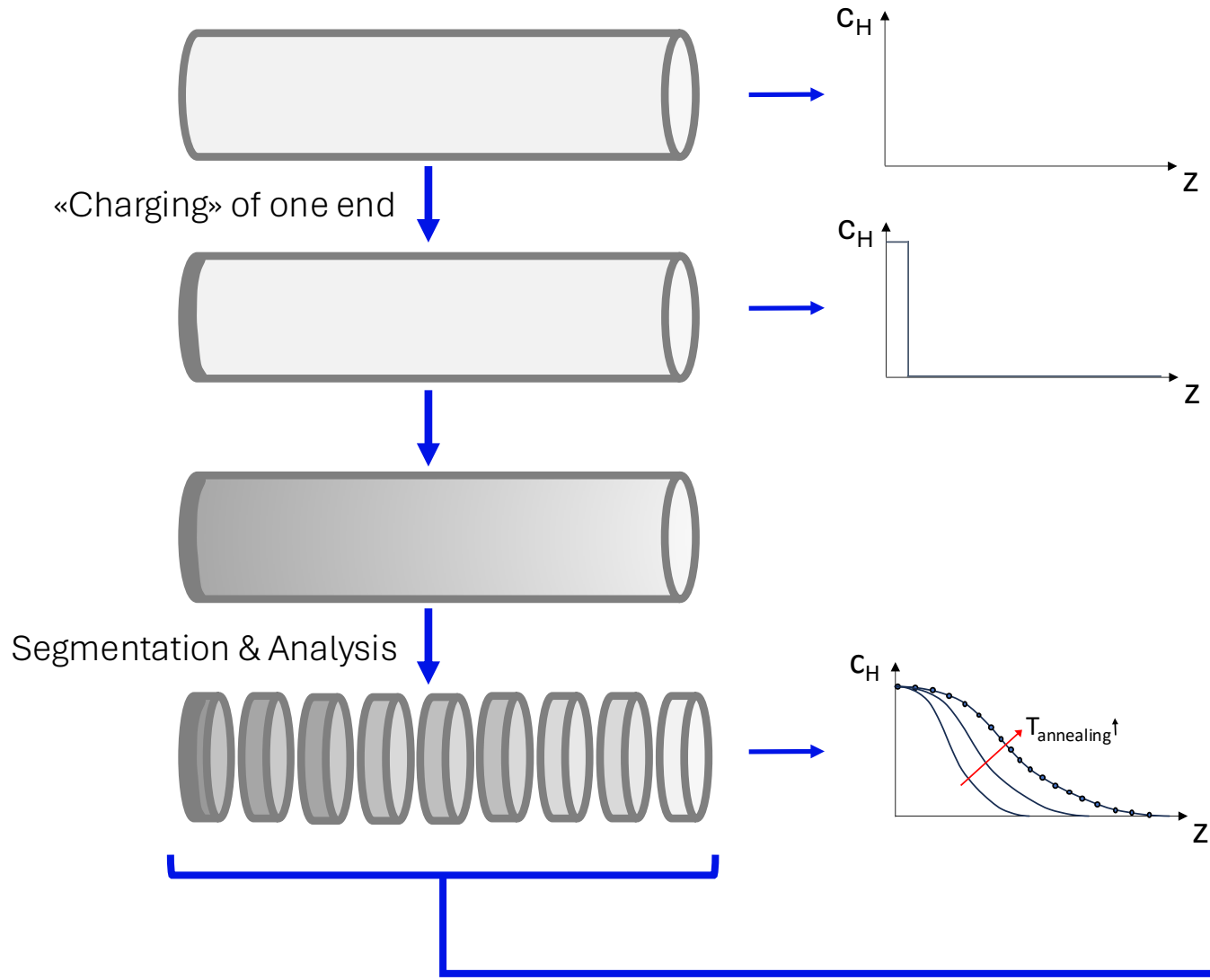


«Charged End» via electrochemical means (hydride layer)  $\Rightarrow$   
(semi-)infinite hydrogen source upon subsequent thermal treatment



S. Niedermeyer et al, Analysis of Axial Hydrogen Diffusion and Hydride Precipitation in Zirconium Alloy Nuclear Fuel Claddings, TopFuel, 2025, Oct 5-9, Nashville, TN

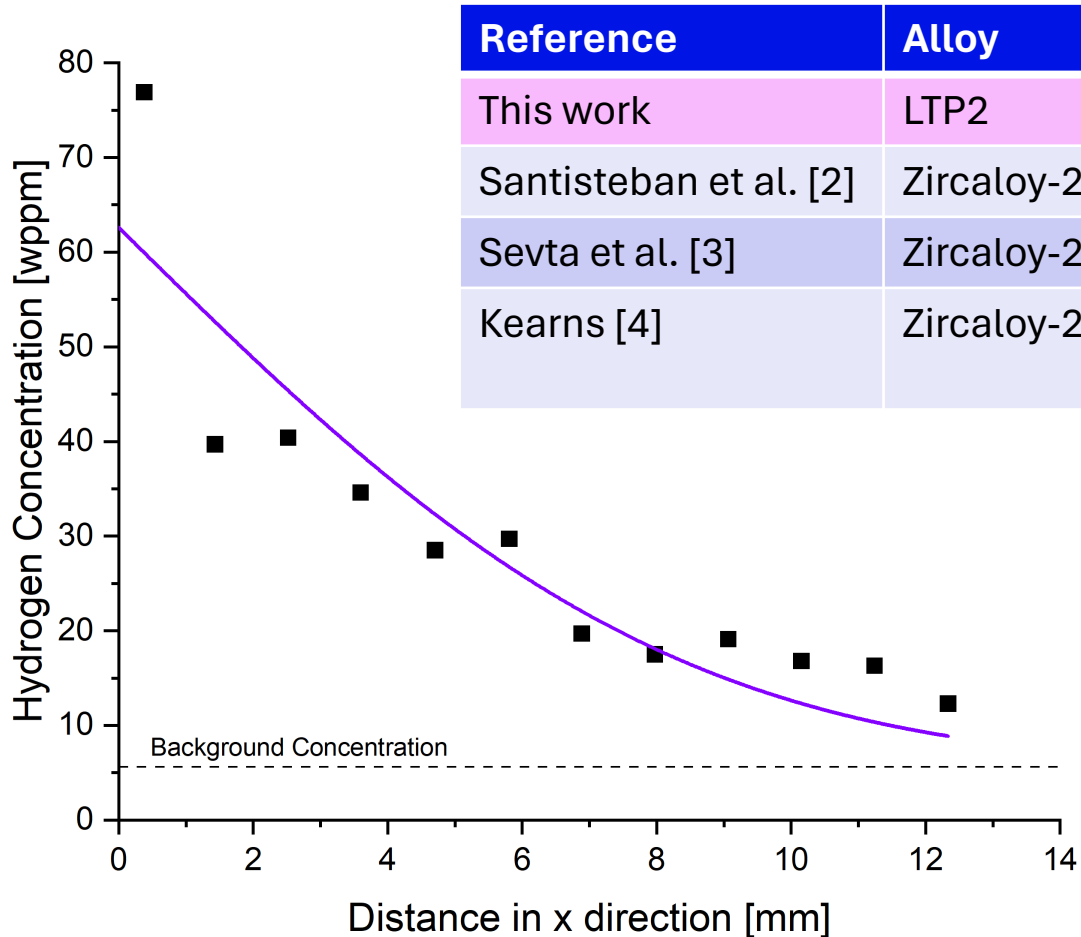
# Experimental Approach



- Hydrogen distribution:
- **Metallography:**  
Hydride morphology & distribution
  - **Hot Gas Extraction (HGE):**  
Total hydrogen content
  - **Neutron Imaging:**  
2D/3D visualization of hydrogen gradients

# Preliminary Results – Diffusion Experiments

Good agreement with literature: Zircaloy 2-based alloys at comparable temperatures.



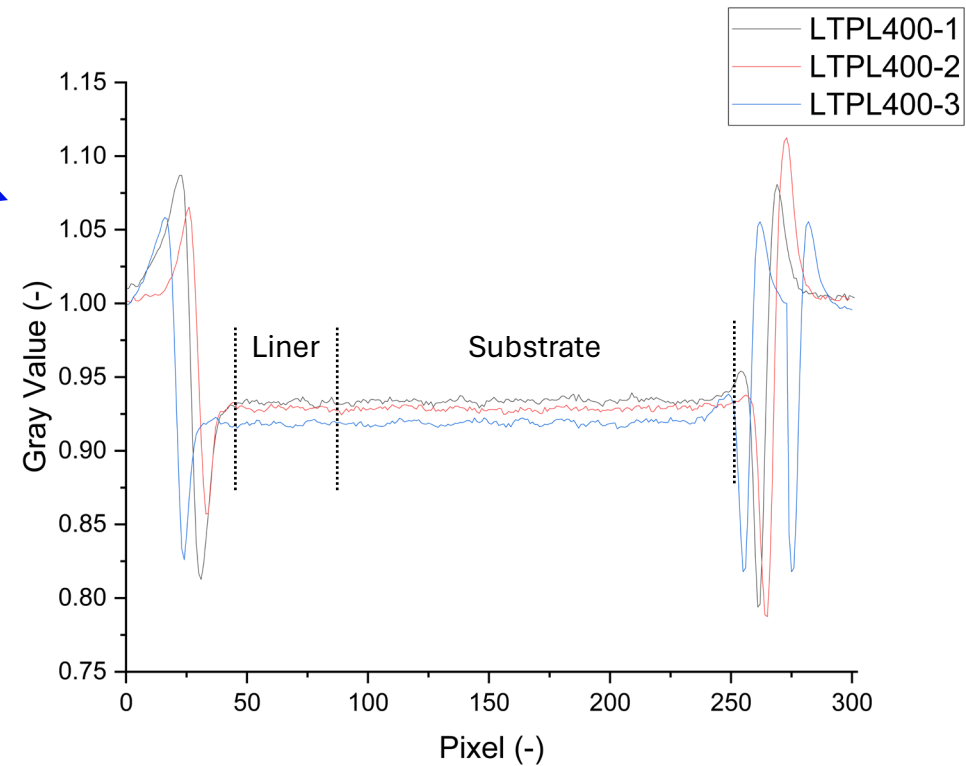
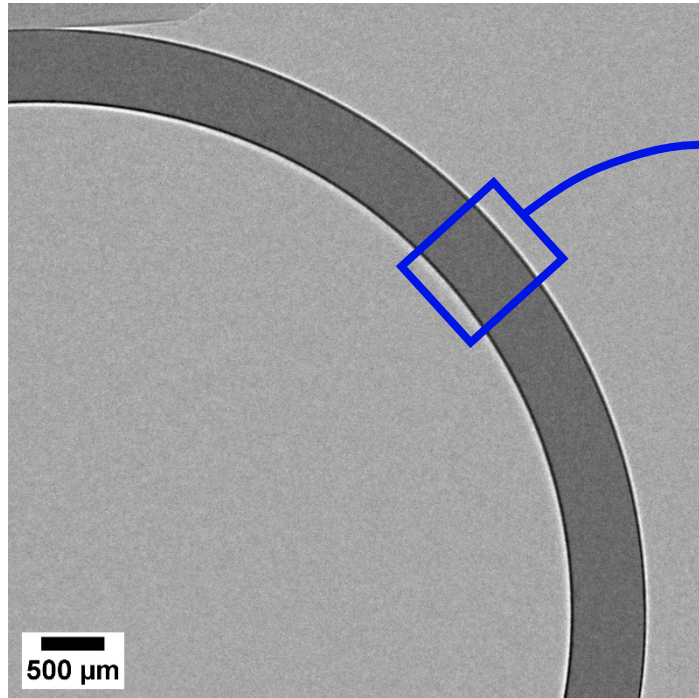
Reference	Alloy	Temperature	Diffusion Coefficient $D_H$
This work	LTP2	300 °C	$8.13 \times 10^{-11} \text{ m}^2/\text{s}$
Santisteban et al. [2]	Zircaloy-2 (various)	300 °C	$6 - 7 \times 10^{-11} \text{ m}^2/\text{s}$
Sevta et al. [3]	Zircaloy-2	300 °C	$4.25 \times 10^{-11} \text{ m}^2/\text{s}$
Kearns [4]	Zircaloy-2 (various)	335 °C	$7.3 \times 10^{-11} - 11.8 \times 10^{-11} \text{ m}^2/\text{s}$ (avg. $9.84 \times 10^{-11} \text{ m}^2/\text{s}$ )

- Diffusion experiments performed at different temperatures  $\Rightarrow$  enables determination of activation energy and pre-exponential factor via Arrhenius-type analysis according to

$$D_H = D_0 \times \exp\left(\frac{-E_a}{RT}\right)$$

- Diffusion experiments on liner cladding are completed and await analysis.

# Preliminary Results – HR-NI



- No heterogeneity in radial direction in (inner) liner cladding validates use of 1D diffusion equations.
- Quenched!
- Differences expected for slowly cooled sections.



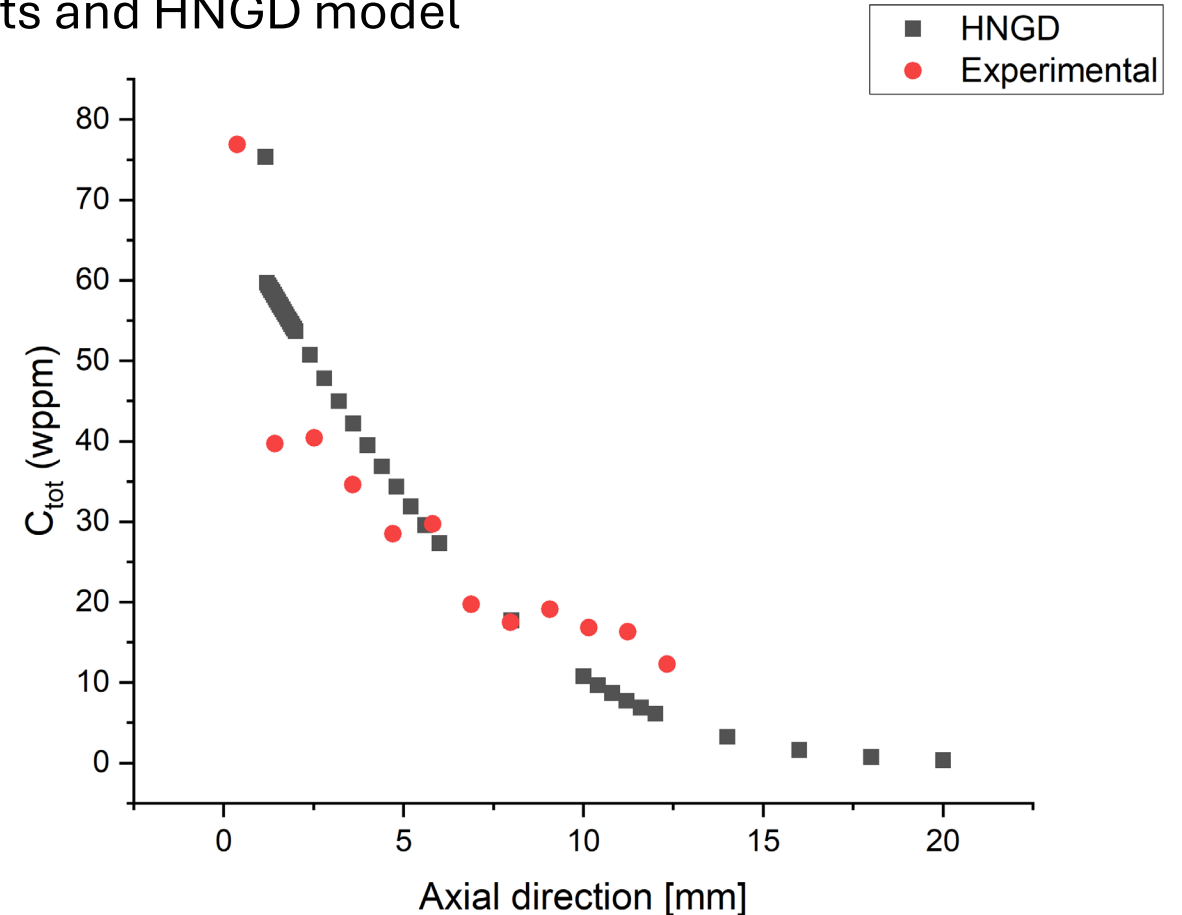
# Preliminary Results – Model Comparison

## Hydride Nucleation-Growth-Dissolution (HNGD)

- Hydride evolution by separating nucleation, growth, and dissolution
- Good agreement between experimental results and HNGD model

Simulation Parameter	Value
Hydride Layer Thickness	20 $\mu\text{m}$
Hydride Layer Concentration	17.600 wppm
Annealing Parameters	72 h @ 300 $^{\circ}\text{C}$
Cooling Rate	quench
Node Width	20 $\mu\text{m}$

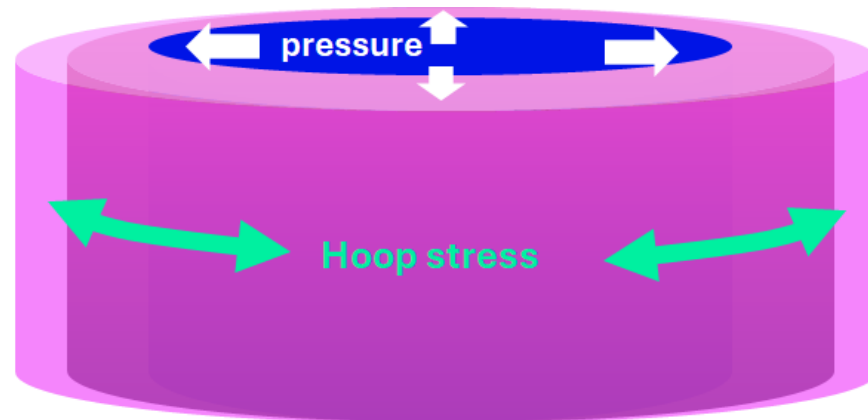
F. Passelaigue, E. Lacroix, G. Pastore, A.T. Motta, Implementation and Validation of the Hydride Nucleation-Growth-Dissolution (HNGD) model in BISON, Journal of Nuclear Materials 544 (2021) 152683, <https://doi.org/10.1016/j.jnucmat.2020.152683>



- Intro
- Axiality
- Creep
- Outlook

Understanding of cladding creep in respect to intermediate dry storage

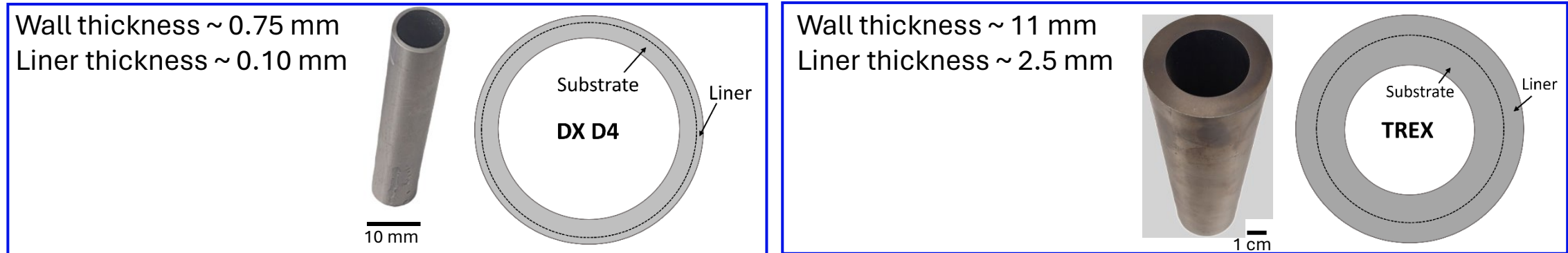
- Liner
  - Mechanical and chemical properties
  - Terminal solid solubility (TSS) for hydrogen
  - Texture/Microstructure
- Component properties



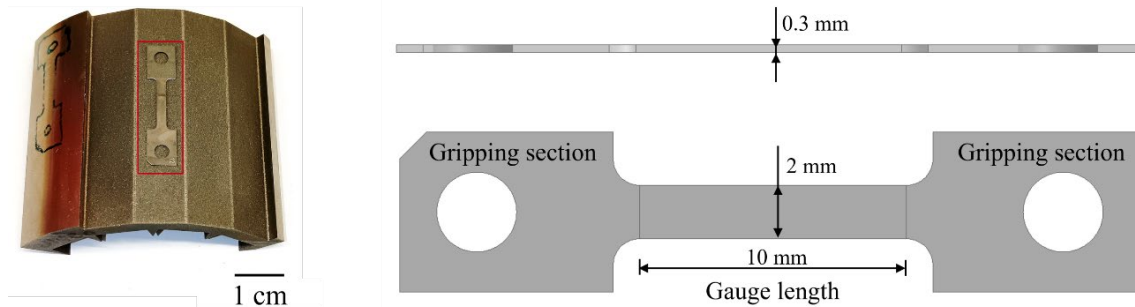
# Approach – use of pre-product TREX

Obtain, as far as, possible material data of individual parts of duplex cladding

- Final product DX D4 too small wall thickness to separate materials  $\Rightarrow$  use pre-product TREX



- Small samples can be machined out of the tube



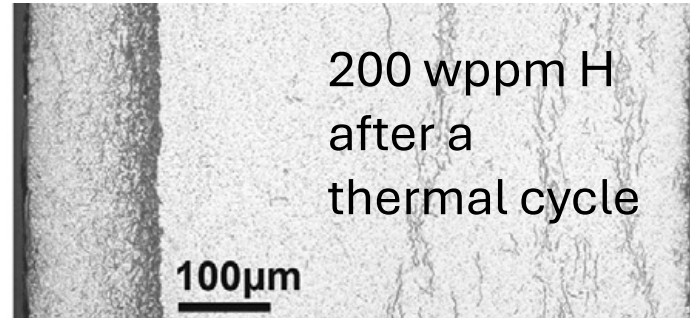
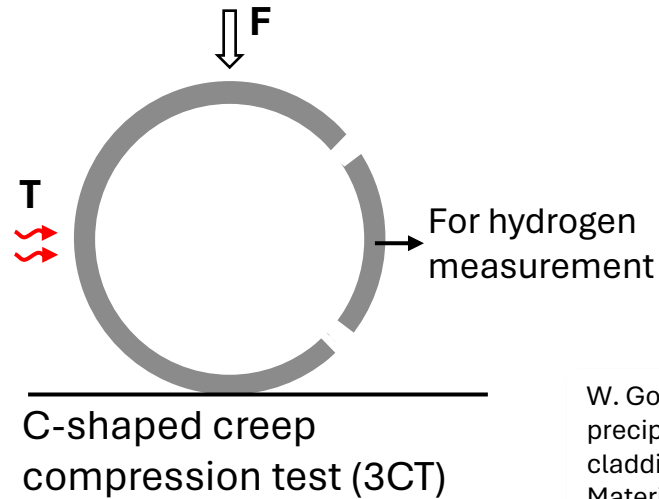
Liner and substrate dog-bone samples from TREX material

B. Buzzatti, Dry-Storage: Hydrogen Impact on Duplex Cladding, preliminary tests on mechanical properties, TopFuel, 2025, Oct 5-9, Nashville, TN

- TREX = DX D4 chemical composition of liner and substrate
- TREX  $\neq$  DX D4 thermomechanical treatment, mechanical properties, microstructure

# Approach – C-shape creep tests

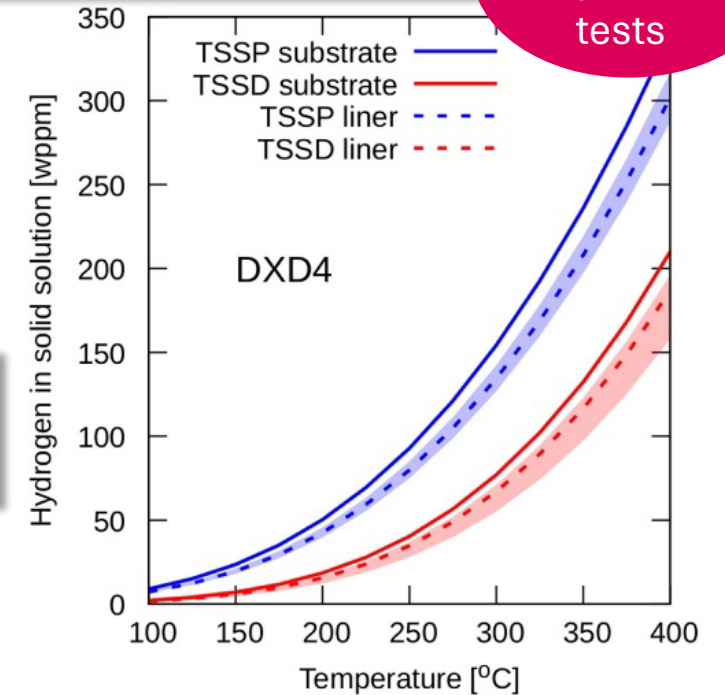
Perform creep tests on C-shape samples



W. Gong, P. Trtik, F. Ma, Y. Jia, J. Li, J. Bertsch, Hydrogen diffusion and precipitation under non-uniform stress in duplex zirconium nuclear fuel cladding investigated by high-resolution neutron imaging, *Journal of Nuclear Materials* 570 (2022) 153971, <https://doi.org/10.1016/j.jnucmat.2022.153971>

P. Konarski, C. Cozzo, G. Khvostov, H. Ferroukhi, Modeling of hydrogen behavior in liner claddings, *Journal of Nuclear Materials* 573 (2023) 154125, <https://doi.org/10.1016/j.jnucmat.2022.154125>

Confirmed by DSC tests



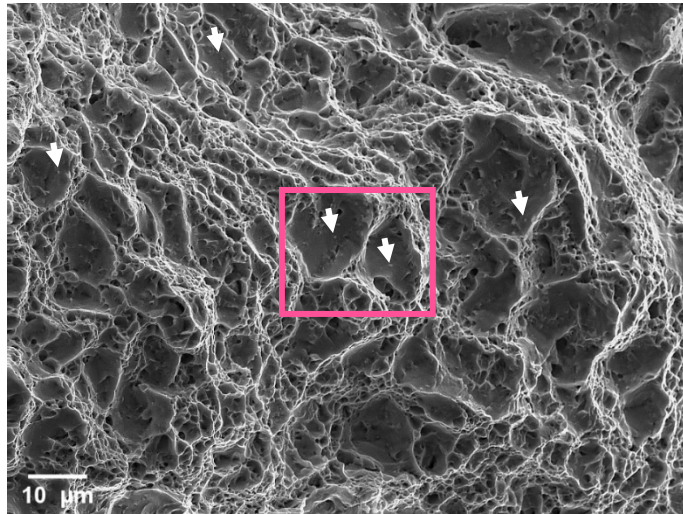
- Zry-4 and DX D4
- Hydrogenated or not, un-/irradiated, various temperatures
- Hydrogenation by gaseous process (in-house)
- Investigate hydrogen (re-)distribution with HR-NI
- Use FEM to link creep deformation and stresses, calculational feedback loop

- Hydrogen in solid solution accelerates creep, hydrides slow down creep
- Irradiation-induced hardening tends to reduce creep rate

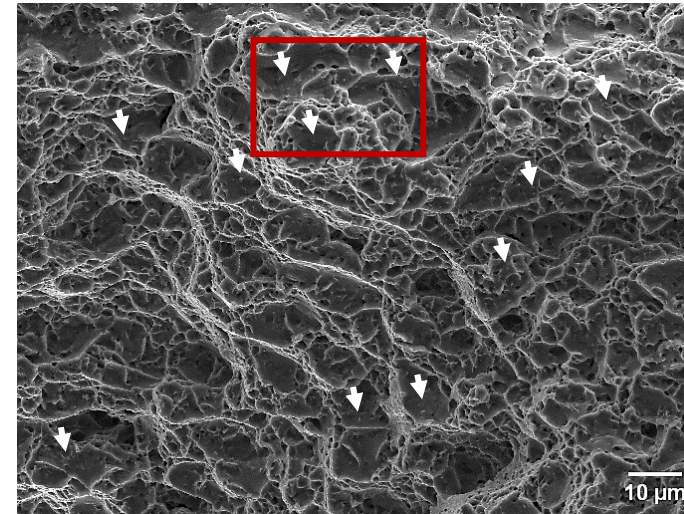
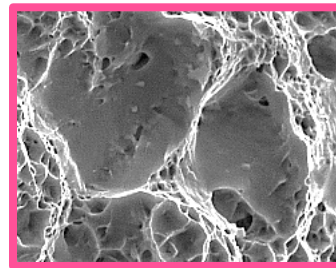
# First Results – TREX

## Dogbone tests:

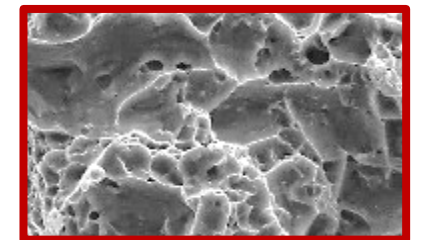
- Hydrogen (< 100 wppm) in TREX reduces both,  $R_{p0.2}$  and UTS
- At room temperature, crack initiation visible at  $Zr(Fe, Cr)_2$  precipitates – confirmed by EDS analyses



Substrate



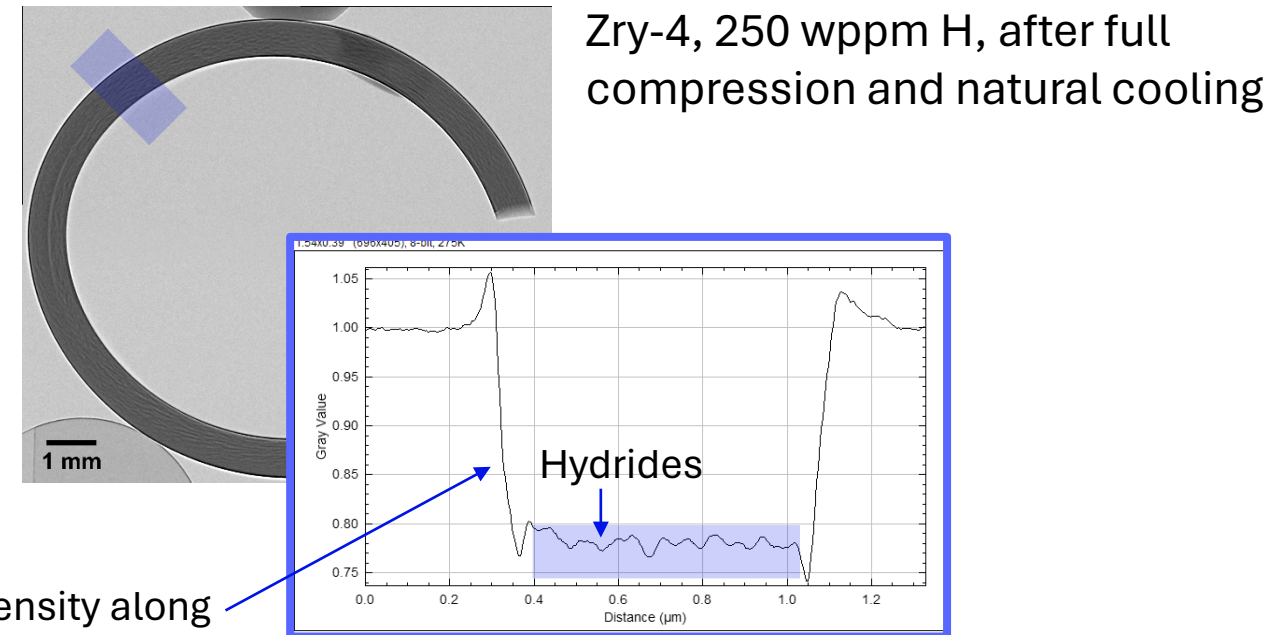
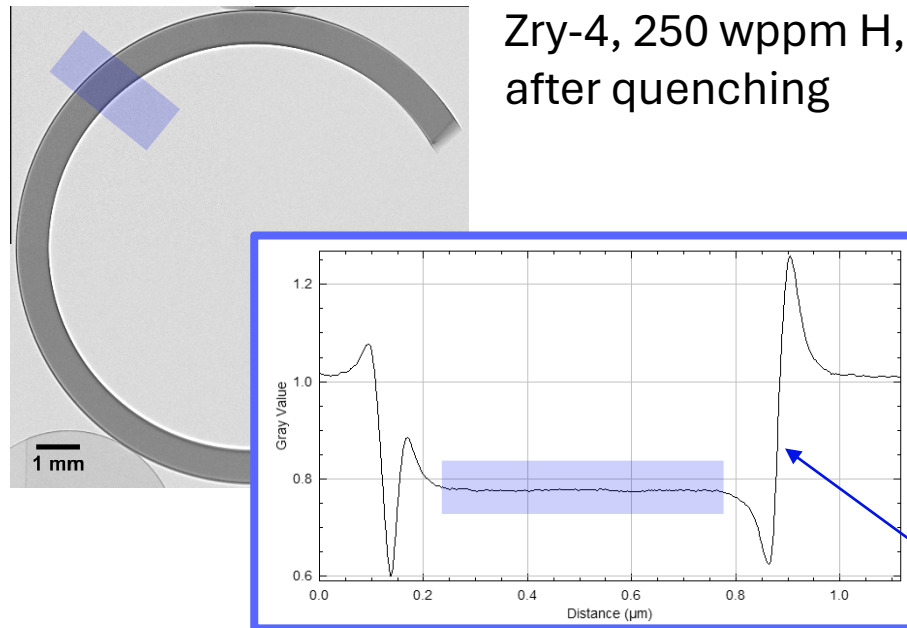
Liner



# First Results – 3CT Tests

## HR-NI C-shaped samples

- Imaging of DX D4 and Zr-4 as-received
- with 100 - 300 wppm of hydrogen



- Intro
- Axiality
- Creep
- Outlook

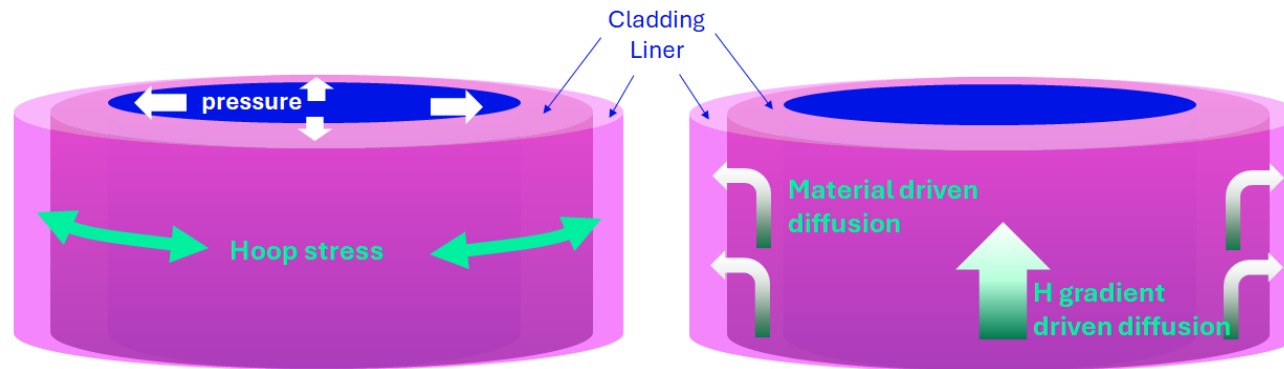


## Creep

- Continuation creep testing
- Implement FEM
- Irradiated Cladding

## Axial diffusion

- Different cladding materials
- Slow cooling analyses
- Irradiated cladding



# Take away messages ...

... liner cladding is specific for intermediate dry storage

... liner accumulates hydrides, influencing creep and axial H diffusion

... 2 PhD projects: axial hydrogen diffusion and creep of liner cladding

## My thanks go to

- BGZ for funding the axial diffusion PhD project
- swissnuclear for co-funding the creep PhD project
- Framatome for supplying test materials
- SINQ/Applied Materials Group

*Thank you for  
your attention*



**Apou Martial Kpemou**

ASNR

## **Dedicated investigation of secondary hydriding: experimental insights and modelling**

Secondary hydriding, which refers to the absorption of hydrogen by the cladding inner surface following high temperature oxidation, can occur during a LOCA (Lost of Coolant Accident) transient in case of cladding burst which allows steam ingress inside the fuel rod. This hydriding phenomenon results in high hydrogen, potentially leading to cladding material embrittlement. Many research institutes conduct semi-integral tests to study the cladding behaviour during a LOCA transient. These tests combine several coupled phenomena, making it challenging to perform a detailed analysis of the secondary hydriding phenomenon.

This paper aims at presenting the new and dedicated experimental protocol developed to finely characterize the secondary hydriding phenomenon under LOCA conditions.

Separate-effects tests were conducted with controlled geometries to better characterize the secondary hydriding phenomenon on fuel claddings. These tests allow investigating oxidation duration and temperature, gap size, pellet positioning inside the cladding, steam proportion, and cladding opening size and shape influence.

The developed protocol also encompasses a series of post-test examinations to evaluate the metallurgical transformations induced by oxidation, as well as hydrogen diffusion within the cladding. The protocol was specifically designed to provide data for code validation. Based on these tests, a modelling study was conducted, under axisymmetric conditions, enabling the simulation of the secondary hydriding phenomenon using the SHOWBIZ code.

The results obtained from both the experimental and modelling work conducted in this study provide valuable insight into the phenomenology of the phenomenon and help to better understand the observations reported on deformed cladding geometries from semi-integral tests.



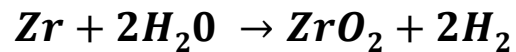
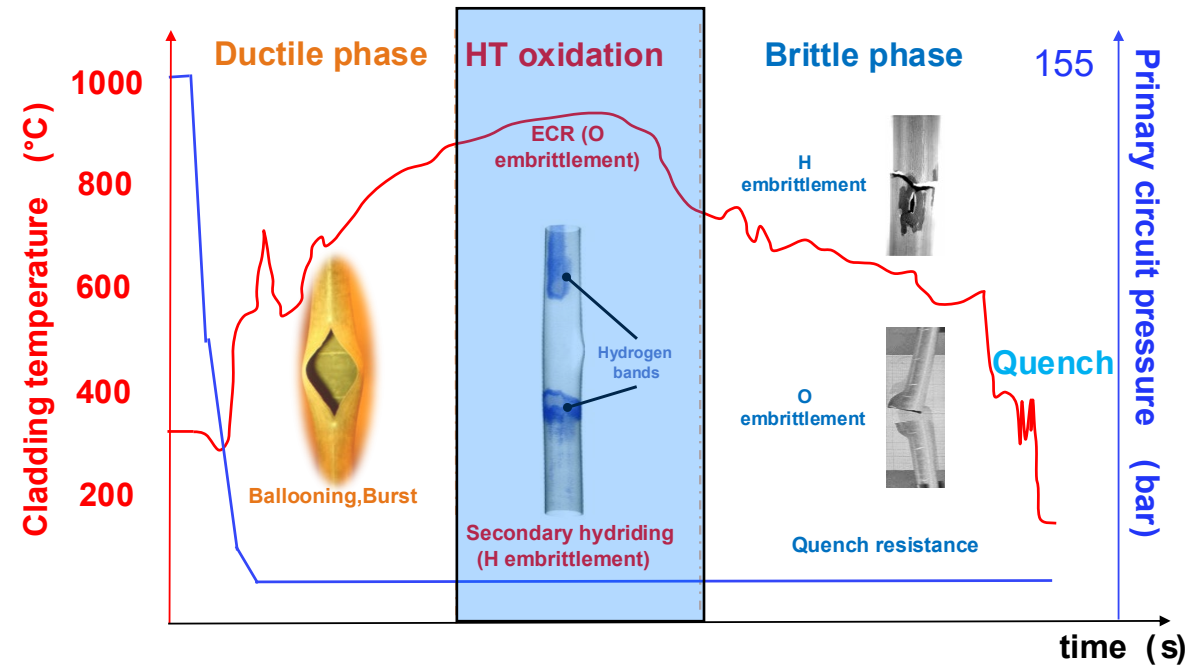
*[Stuckert et al., 2020, Grosse et al., 2006]*

30TH INTERNATIONAL QUENCH WORKSHOP (16 – 18 DECEMBER 2025)

# **DEDICATED INVESTIGATION OF SECONDARY HYDRIDING: EXPERIMENTAL INSIGHT AND MODELLING**

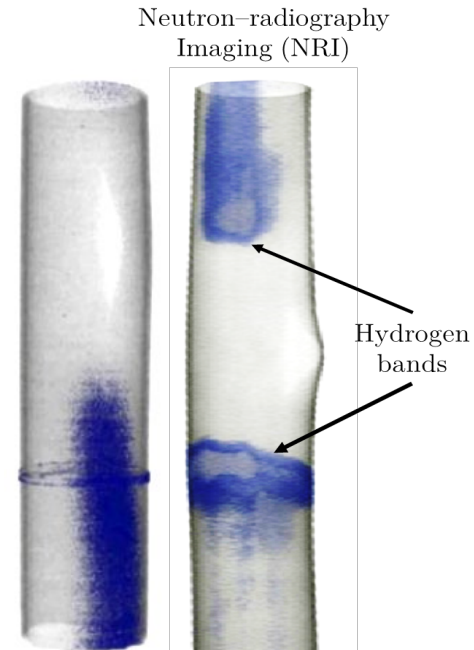
A. M. KPEMOU, S. GUILBERT, T. TAURINES, J. DESQUINES

## Steam High Temperature (HT) oxidation

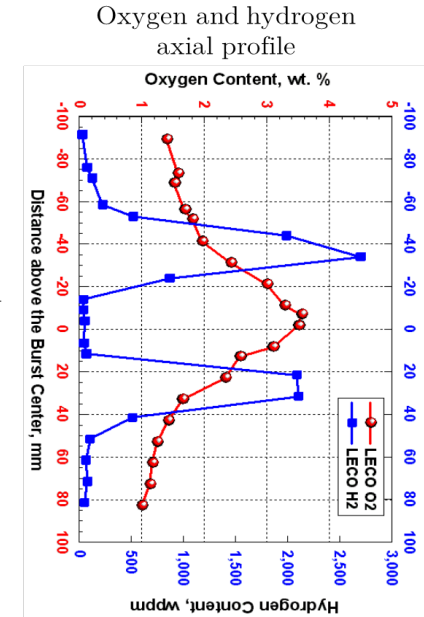


- Cladding is oxidised at high temperatures
- Hydrogen absorption at the inner cladding surface if burst (secondary hydriding phenomenon)

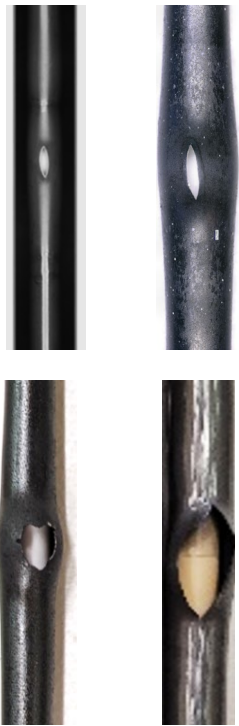
[Stuckert et al., 2020, Grosse et al., 2006]



[Billone et al., 2008]



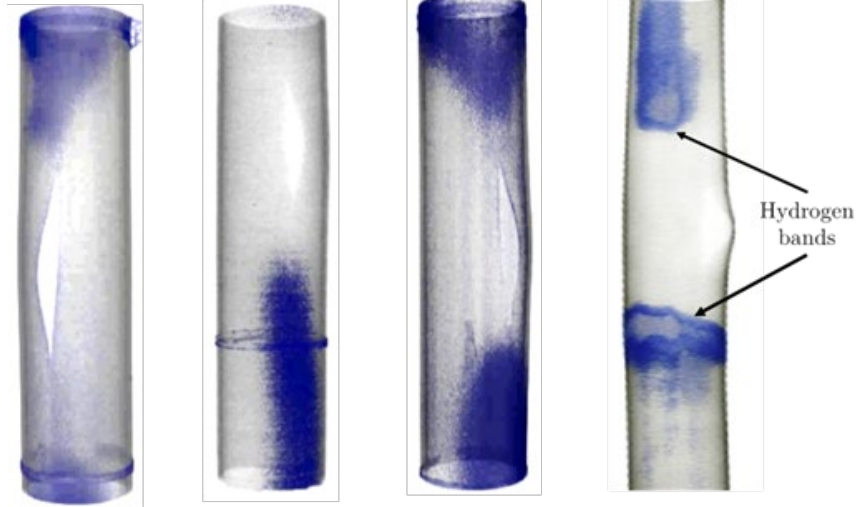
- Two hydrogen peaks located on both sides from the opening
- Heterogeneous hydrogen spatial distribution within the cladding



Cladding 3D geometries

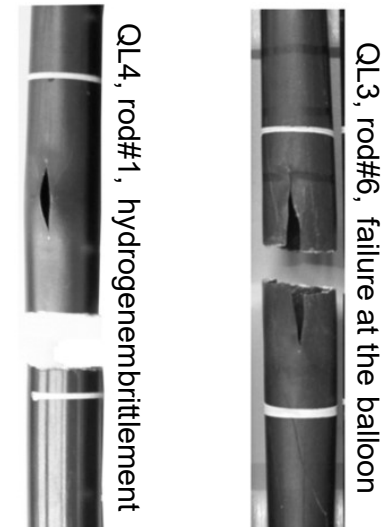
## High Temperature (HT) oxidation

[Stuckert et al., 2020, Grosse et al., 2006]



The **deformed geometry** influences the **secondary hydriding**

## Brittle phase (quench)



Cladding **embrittlement**

- The secondary hydriding is studied on deformed cladding geometry
- Studying key parameters influencing phenomenon in this configuration is complex

**New approach to allow characterising the secondary hydriding phenomenon with controlled geometries**



characterise the secondary hydriding phenomenon and its induced embrittlement on fuel claddings with controlled geometries

### Experimental characterisation of secondary hydriding

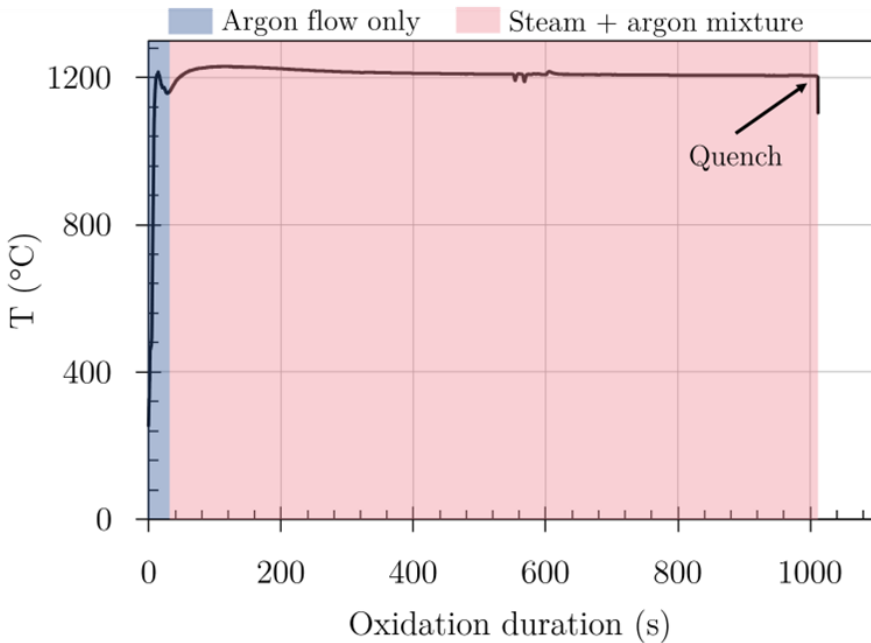
- New dedicated experimental protocol development
- Separate effects study of the phenomenon
- Data for code validation

### Modelling of the secondary hydriding phenomenon

- Modelling with SHOWBIZ\* code
- 1D axisymmetric modelling
- Parametric study of the phenomenon

\*SHOWBIZ: Studying Hydrogen and Oxygen Weakening Behaviour in Zirconium

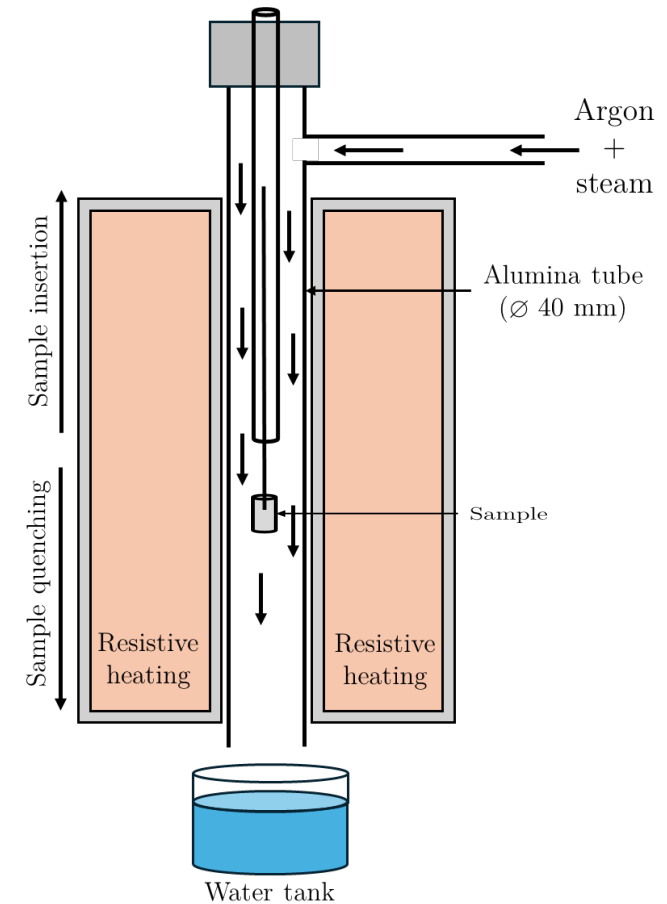
## The applied thermal transient



→ **Phase 1 in argon flow** to fill the sample with Ar and simulate rod gas filling before burst ( $T_{rate} > 50 \text{ °C/s}$ )

→ **Phase 2 in argon (50%) + steam (50%) flow**, to allow steam ingress in the cladding for the oxidation process

## Vertical furnace

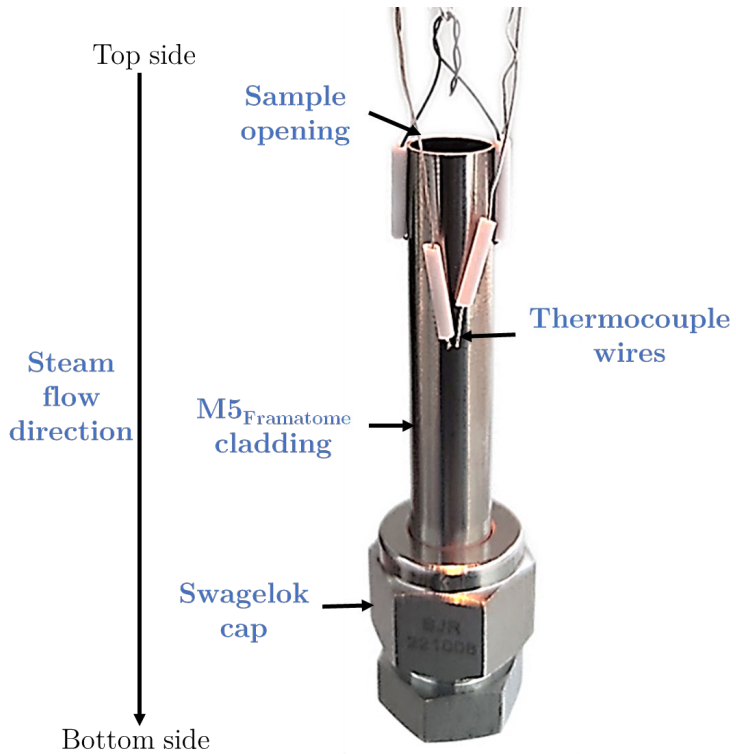


→ The cladding **ballooning** is not reproduced (non deformed cladding geometry)

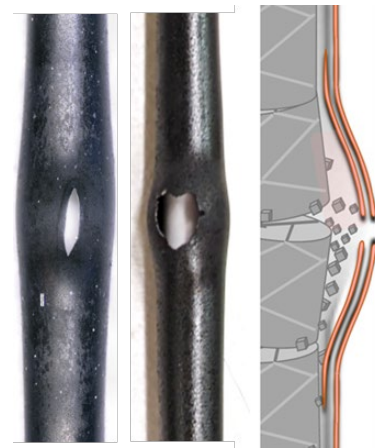
→ Tests are performed under **LOCA conditions** reproducing the **HT oxidation phase**



## SETs' sample geometry

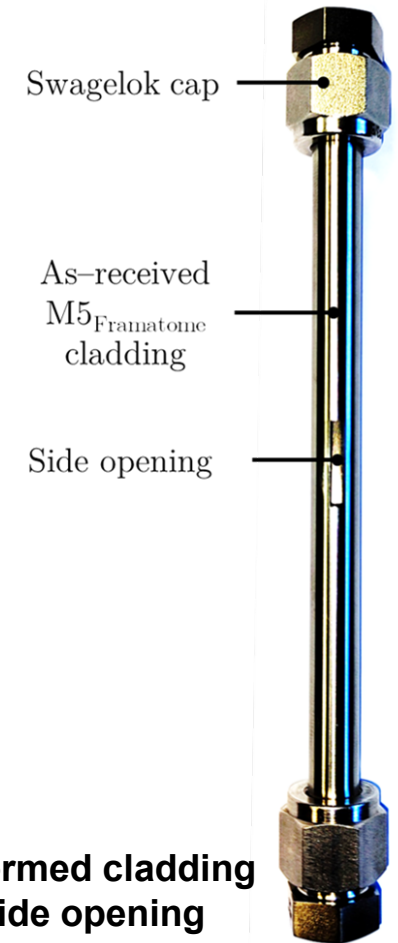


**Non deformed cladding with opening at the top**



**Conventional deformed cladding geometry**

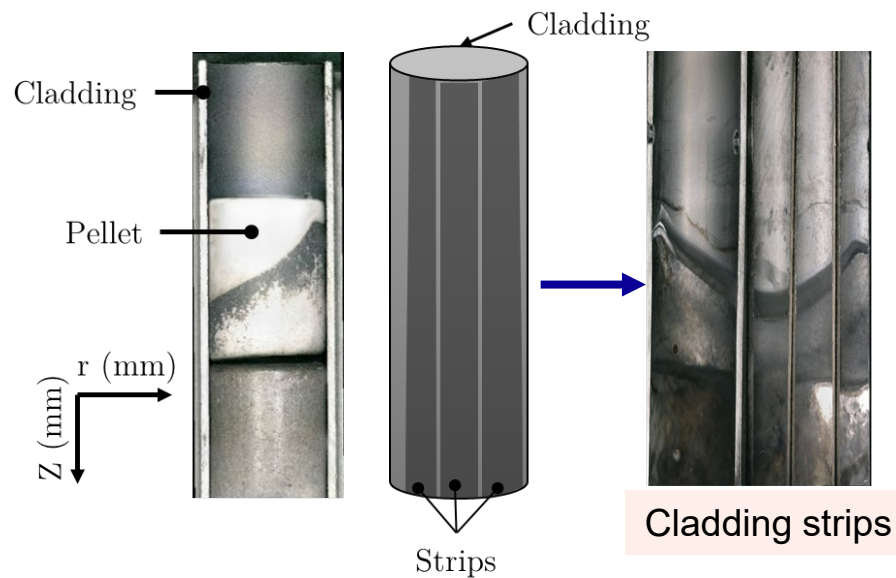
## SOTs' sample geometry



**Non deformed cladding with side opening**

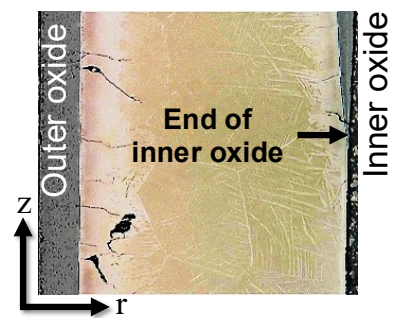
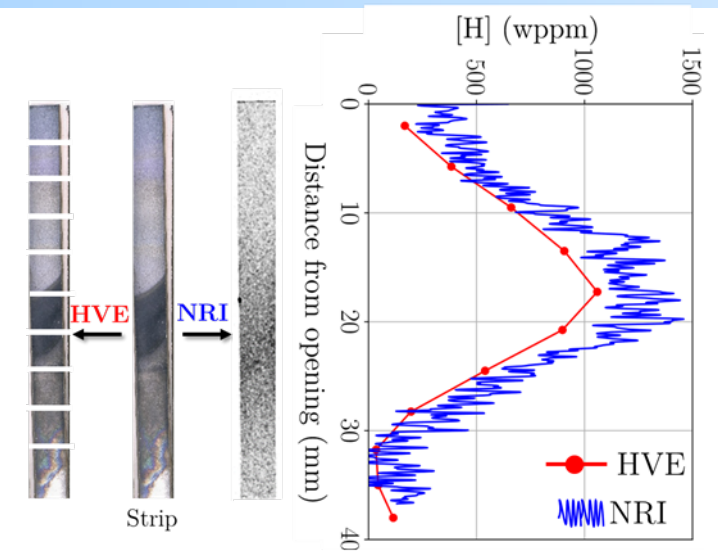
**Non-deformed cladding geometry for a better control of tests parameters**

# Experimental methods – Post-test characterisations

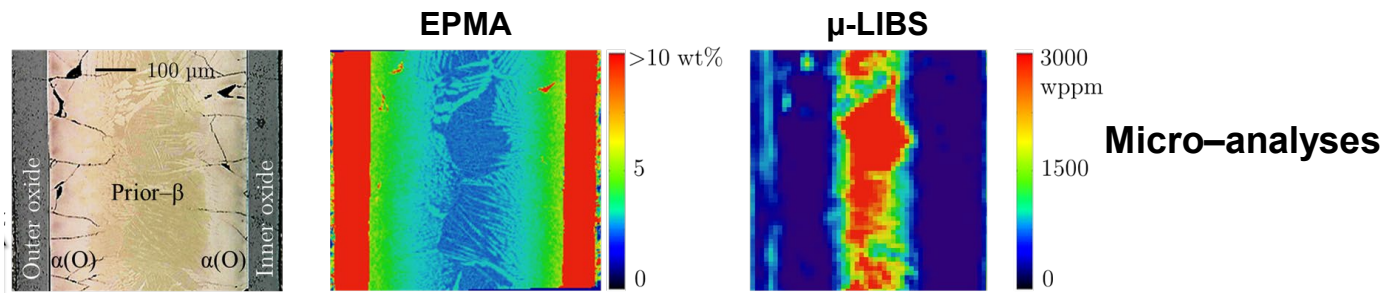


## Complementary H measurement techniques

- Hot Vacuum Extraction (HVE)
- Neutron Radiography Imaging (NRI)



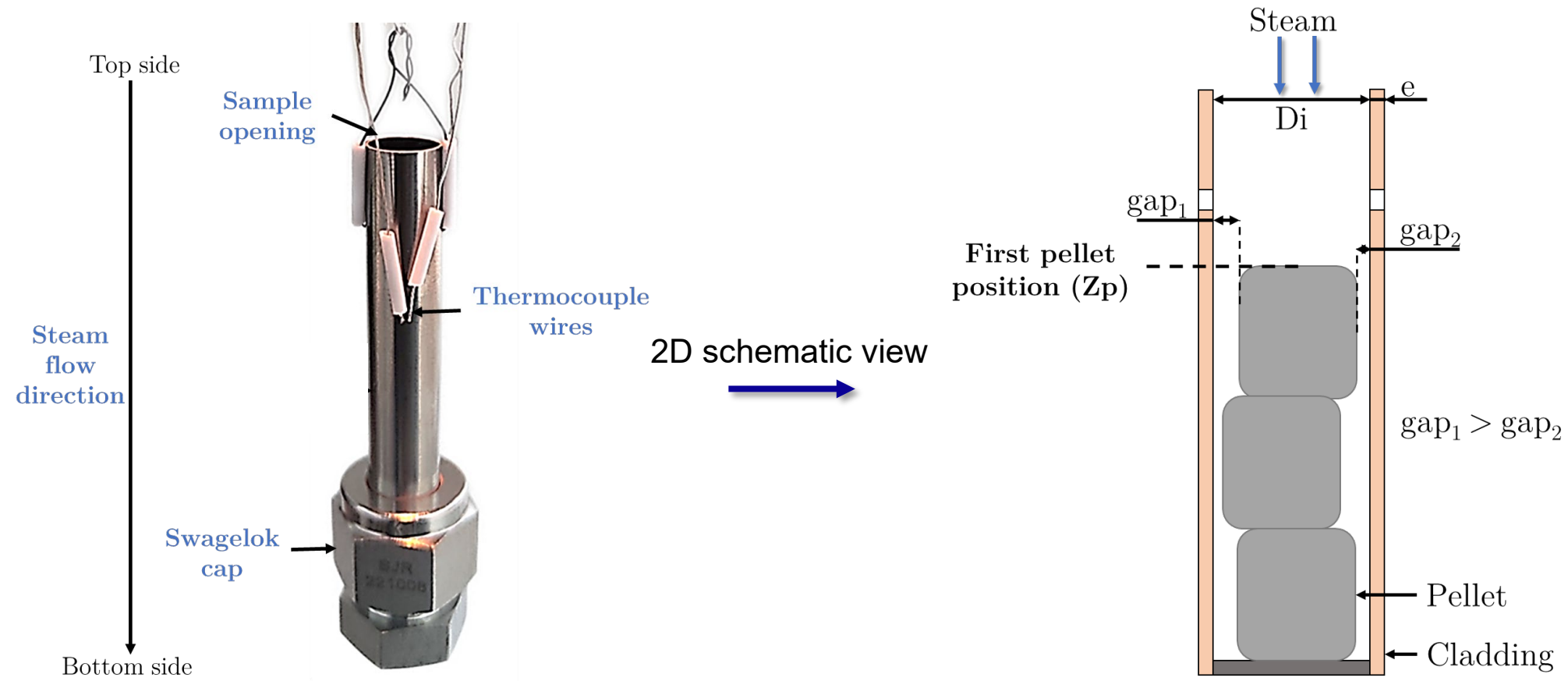
## Metallographic analyses



# 01 SEPARATE EFFECTS STUDY OF SECONDARY HYDRIDING (SETs)

Study of key parameters effects on secondary hydriding using a non-deformed cladding geometry with an opening at the top





- **Opening at the top side** of the sample (to allow axisymmetric steam ingress)
- **Free positioning** of stacked pellets inside the cladding
- **1D axisymmetric** modelling with well-defined boundary conditions

Influence of **several parameters:**

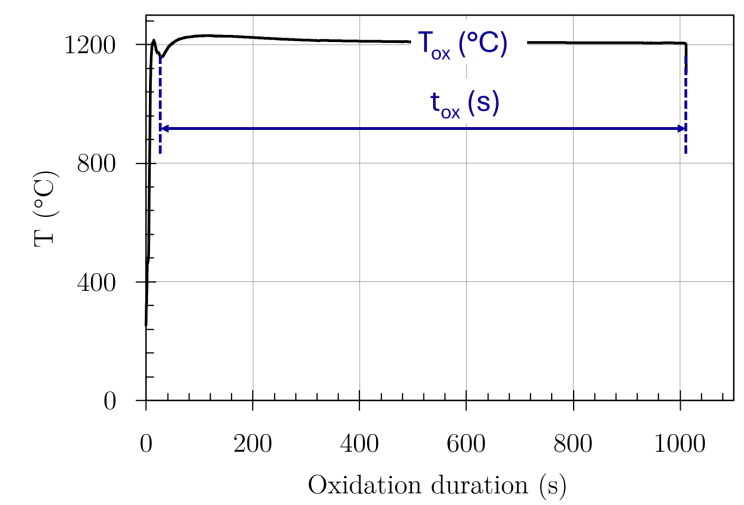
- Pellets positioning inside the cladding
- Oxidation temperature [1100°C – 1200°C] and duration [100s – 1400s] (\*\*)
- Average gap size [80 μm, 130 μm, 230 μm] (\*\*)
- Opening size [2 mm, 4 mm] (\*\*)
- pre-oxide layer [6 μm, 8 μm, 12 μm] (\*\*)
- Steam partial pressure

(\*\*) Modelling sensitivity study performed

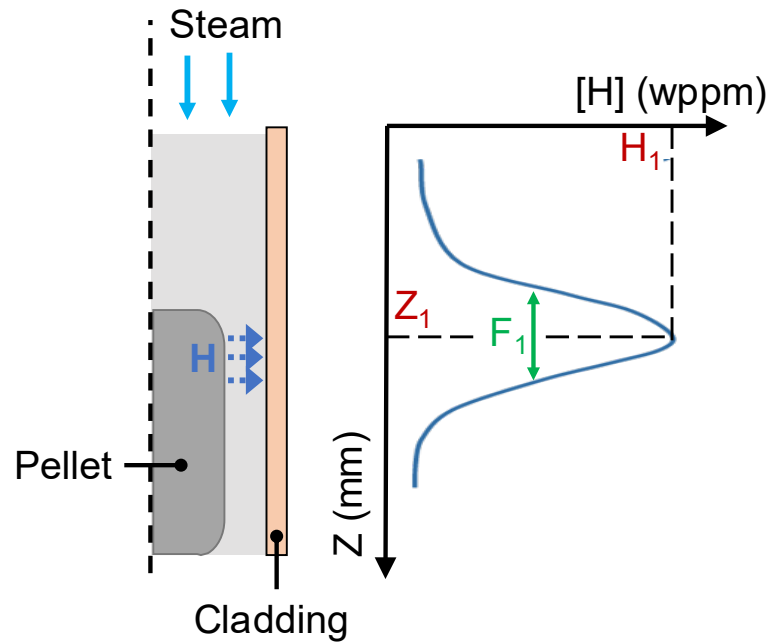
Results published in [A.M. KPEMOU et al., 2025]



Oxidation duration and temperature

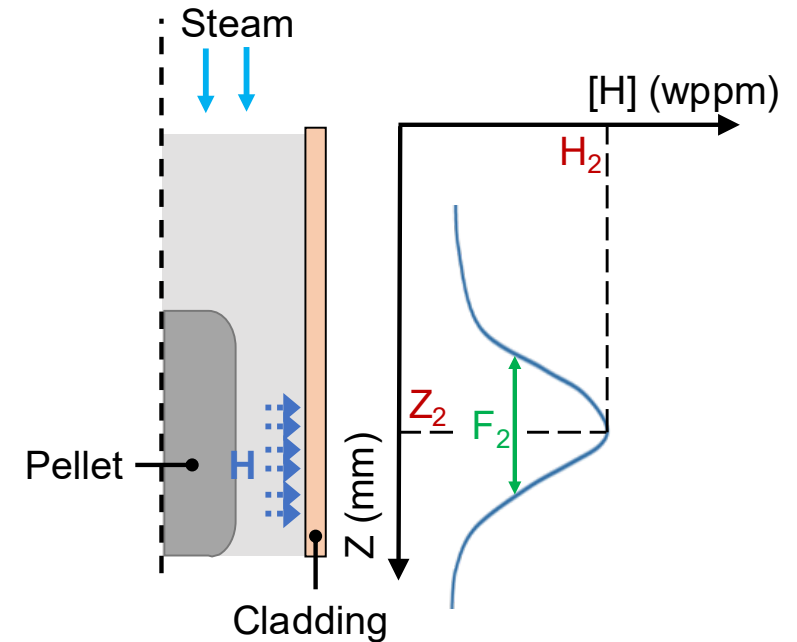


A.M. Kpemou, S. Guilbert, J. Desquines, T. Taurines, M.C. Baietto, B. Normand, J. Soulacroix, A. Ambard, F. Bourlier, A new approach to investigate secondary hydriding phenomenon on M5 Framatome clads under high-temperature LOCA conditions, J. Nucl. Mater. 603 (2025) 155462. <https://doi.org/10.1016/j.jnucmat.2024.155462>.



When the local gap increases (few  $\mu\text{m}$ )

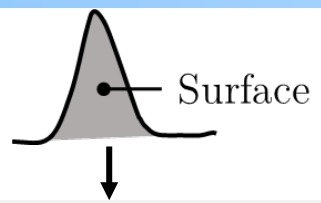
$$Z_1 < Z_2 \text{ and } H_2 < H_1$$



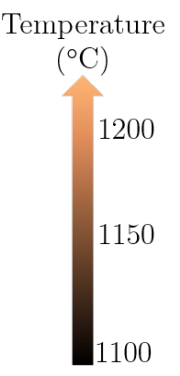
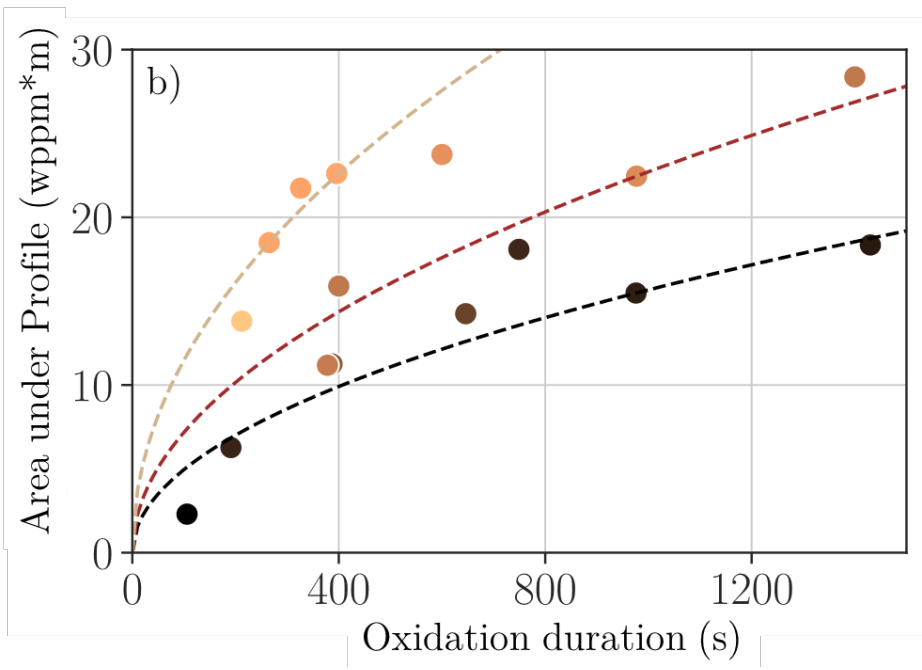
- **Gases transport** in the gap is **reduced**
- **H-peak** is **near the first pellet** position
- H-profile exhibits a **narrow profile**

- **Gases transport** in the gap is **facilitated**
- **H-peak** shifts about **few mm** along the pellet
- H-profile exhibits a **wider profile**

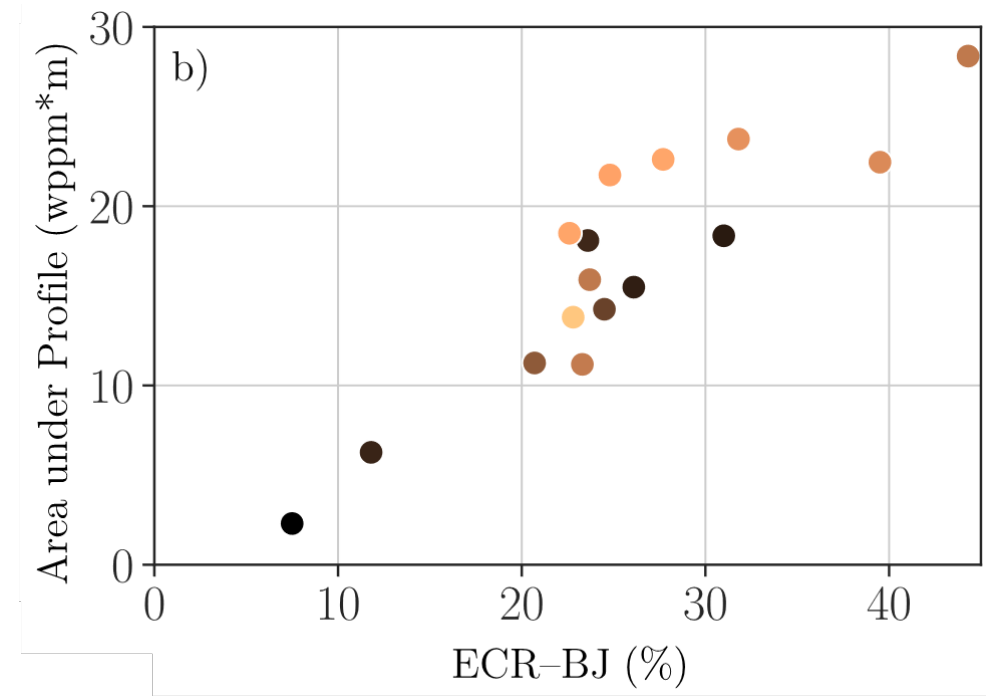
Local gap closure induce closeness of hydrogen peaks on irradiated fuel rods compare to unirradiated  
 [Nagase and Fuketa, 2006]



Evolution of the **overall** H content

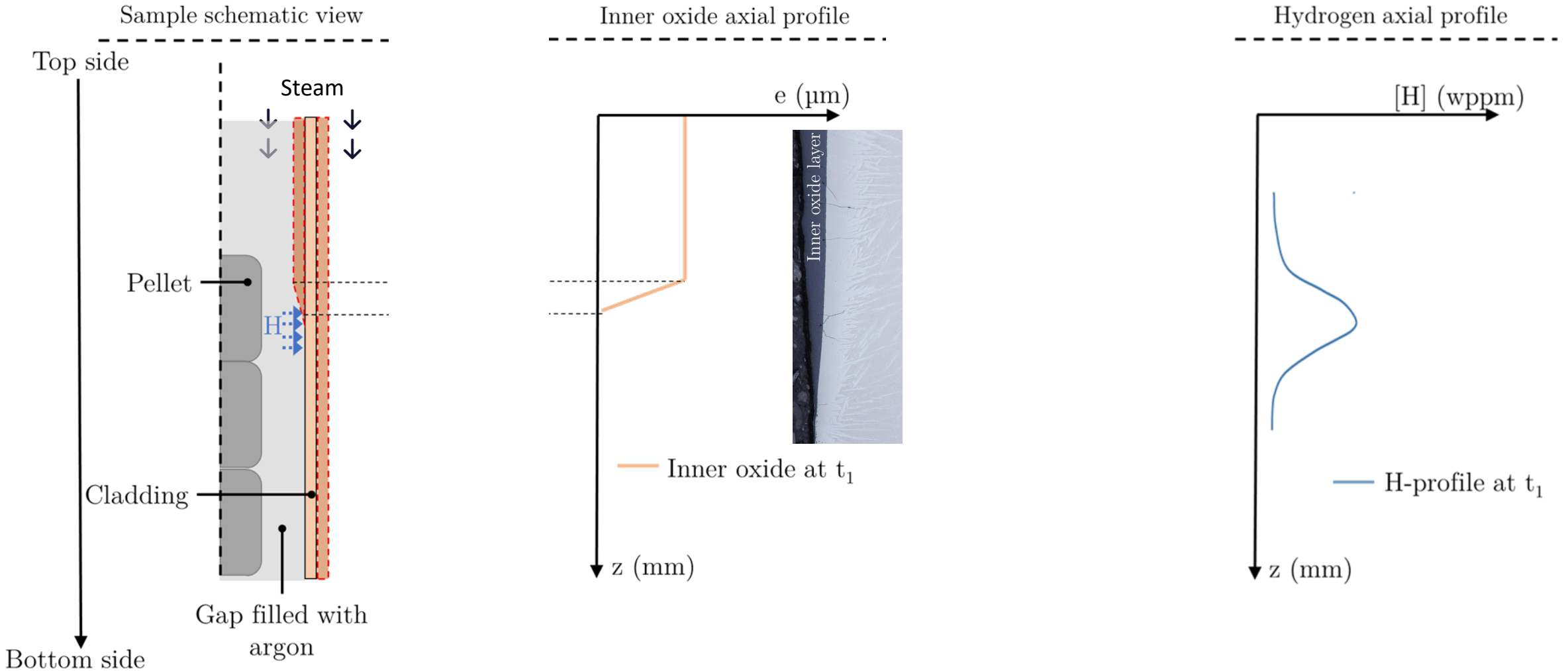


Corresponding  
ECR



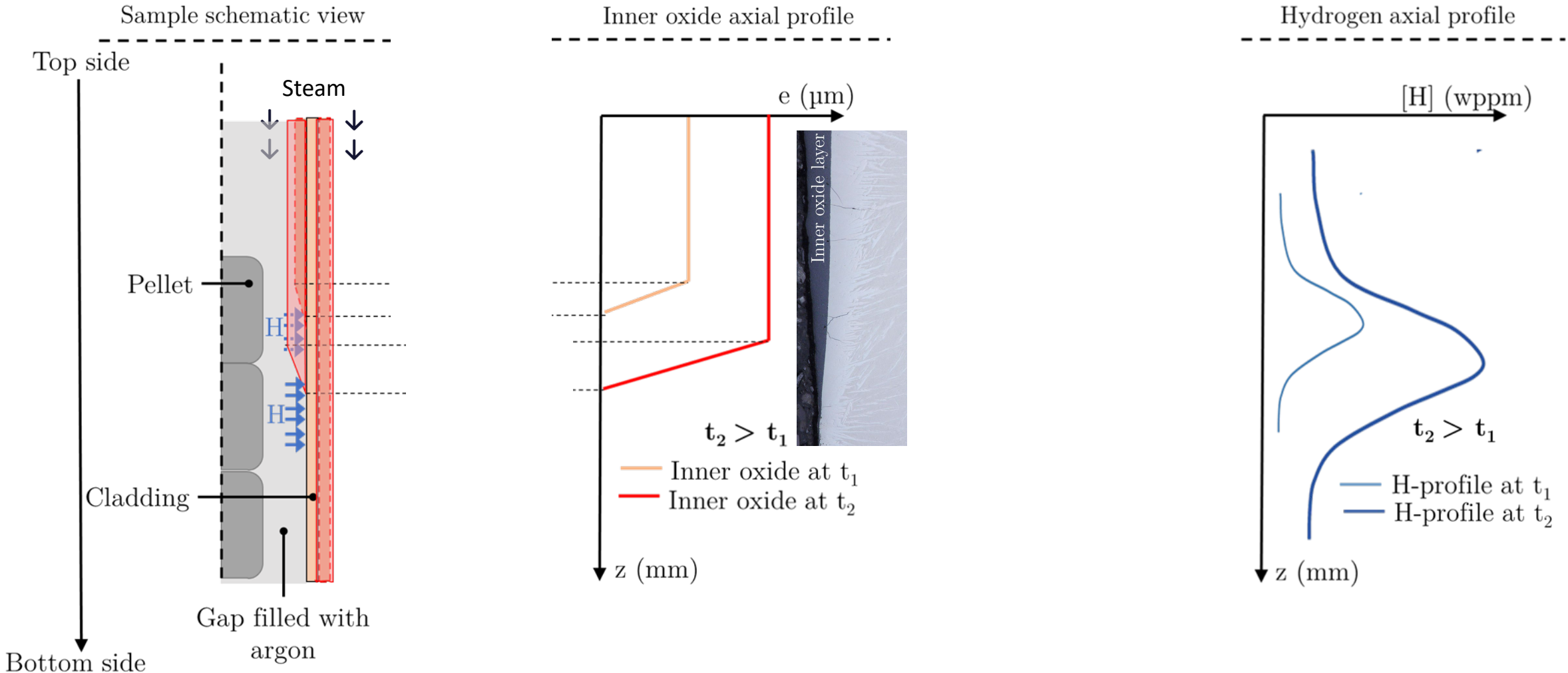
- The total H content increases with respect to the duration (parabolic trend) and the temperature
- The total hydrogen content increases linearly with the cladding ECR degree

Secondary hydriding based on SETs' results

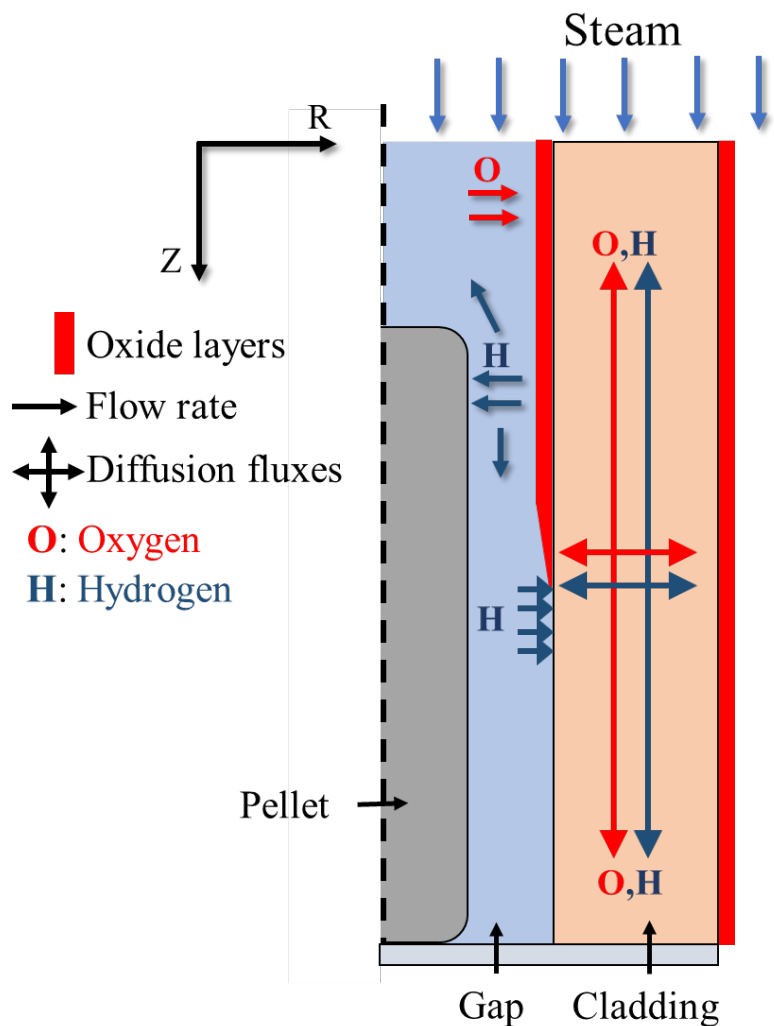




Secondary hydriding based on SETs' results



The current understanding of the phenomenon was used to support the modelling work



**1D axisymmetric** modelling with the **SHOWBIZ\*** software

**Gases transport (steam, filling gas, hydrogen...)**

- 1D axisymmetric modelling of the pellet and the gap
- Steam, hydrogen and argon transport in the gap
- Advective (Darcy + Poiseuille) and diffusive laws

**Chemical reactions**

- Cladding inner and outer oxidation reaction
- Hydrogen absorption (Sievert law where the oxide layer is thinner than 0.5  $\mu\text{m}$ )

**2D diffusion in the cladding**

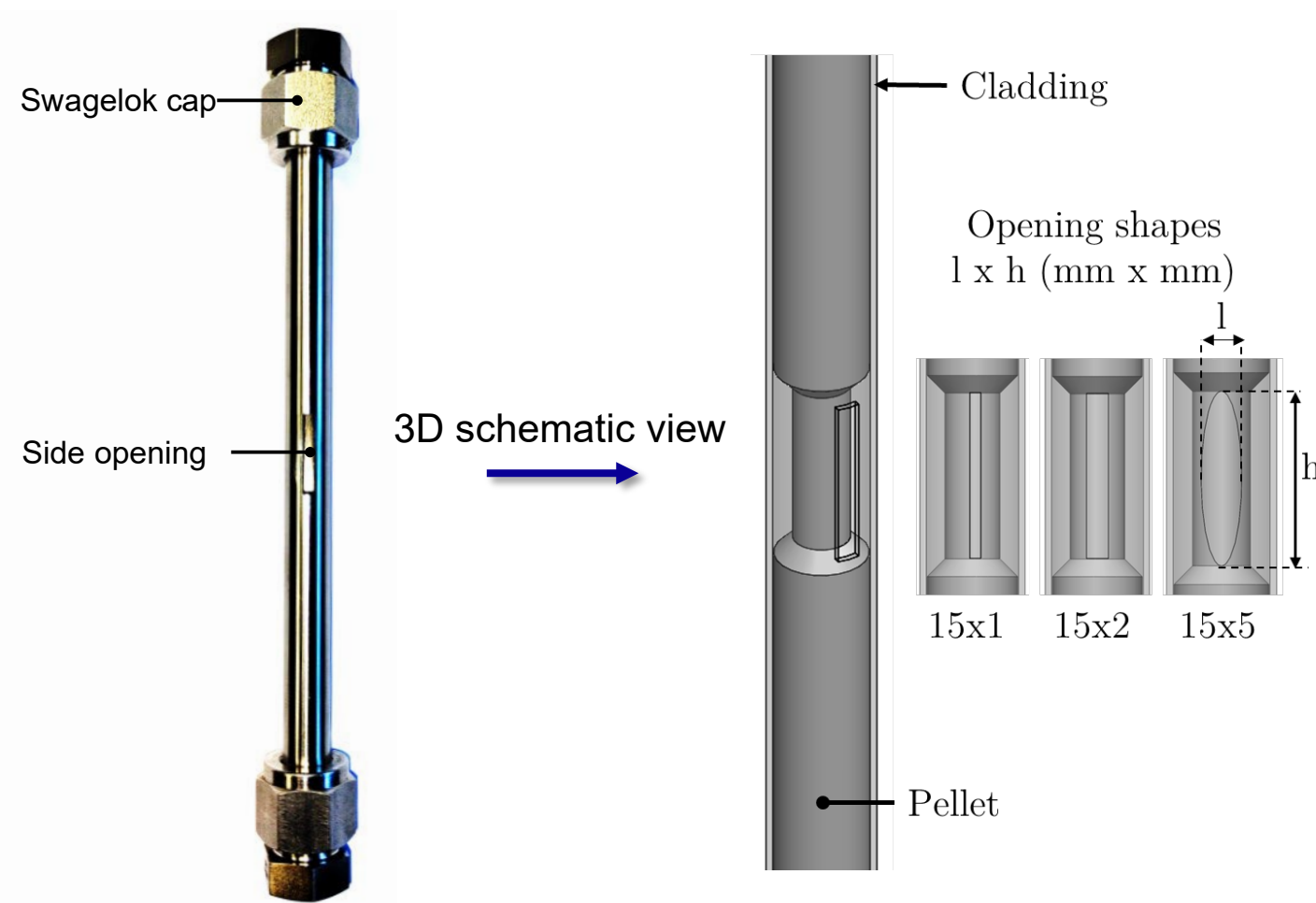
- Oxygen and hydrogen diffusion within the material
- Cladding metallurgical transformation due to the oxidation ( $\text{ZrO}_2$  and  $\alpha(\text{O})$ )

- Simulated results' trends were found consistent with experimental results
- Refinements of the modelling “boundary conditions are needed (Overestimation of the H uptake)

## 02 SECONDARY HYDRIDING ON SAMPLE WITH A SIDE OPENING (SOTs)

Study of different opening shape and size effects on the secondary hydriding phenomenon using non-deformed sample with a side opening







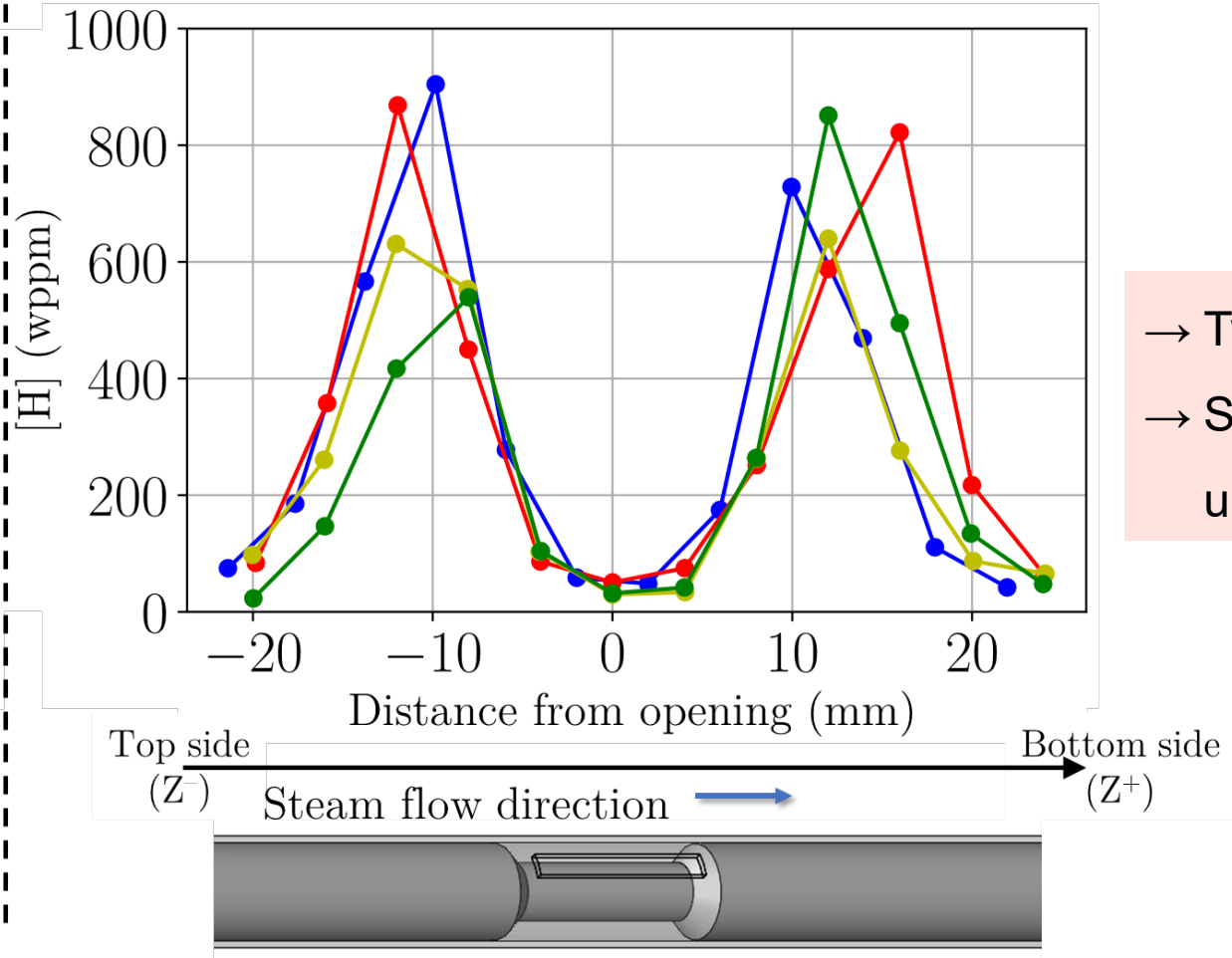


Oxidation tests on non-deformed claddings  
with different burst opening geometry and size  
 $T_{ox} : 1160 \text{ }^\circ\text{C}$   
 $t_{ox} : 300 \text{ s}$   
ECR-BJ : 18.5 – 19.5 %

- Non-deformed cladding with side-opening
- Single centred alumina pellet inside the cladding

Axial hydrogen profiles following the oxidation tests

- 
 Sample ID : **Rec\_1**  
 Shape: Rectangular  
 Dimensions: 15x1 (Hxl)  
 Curve: —
- 
 Sample ID : **Rec\_2**  
 Shape: Rectangular  
 Dimensions: 15x2 (Hxl)  
 Curve: —
- 
 Sample ID : **Ova\_1**  
 Shape: Oval  
 Dimensions: 15x5 (Hxl)  
 Curve: —
- 
 Sample ID : **Ova\_2**  
 Shape: Oval  
 Dimensions: 15x5 (Hxl)  
 Curve: —

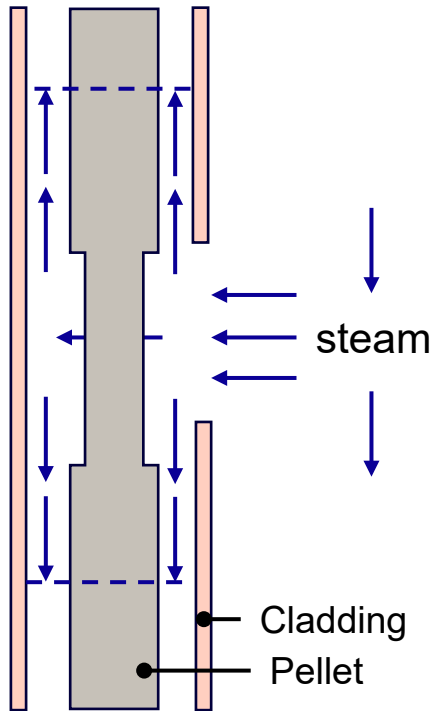


→ Two symmetrical hydrogen peaks  
 → Steam transport inside the cladding uniform on either side of the opening

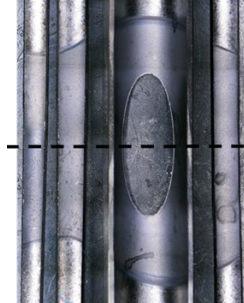
Results confirmed the so called “M-shape” profile following hydrogen absorption related to the secondary hydriding



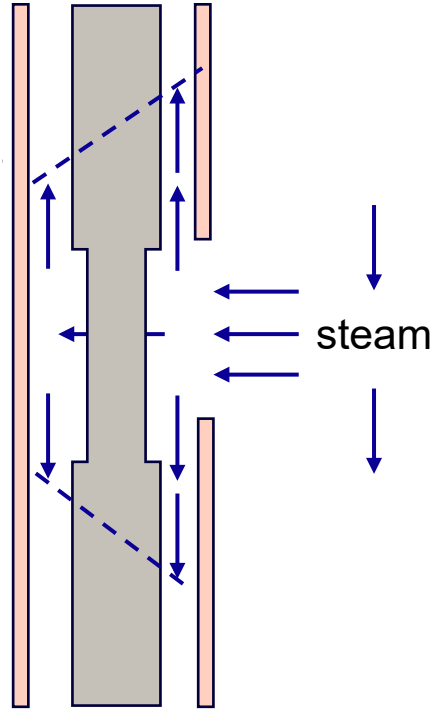
Rectangular opening



Homogeneous steam transport inside the cladding



Oval opening



Heterogeneous steam transport inside the cladding

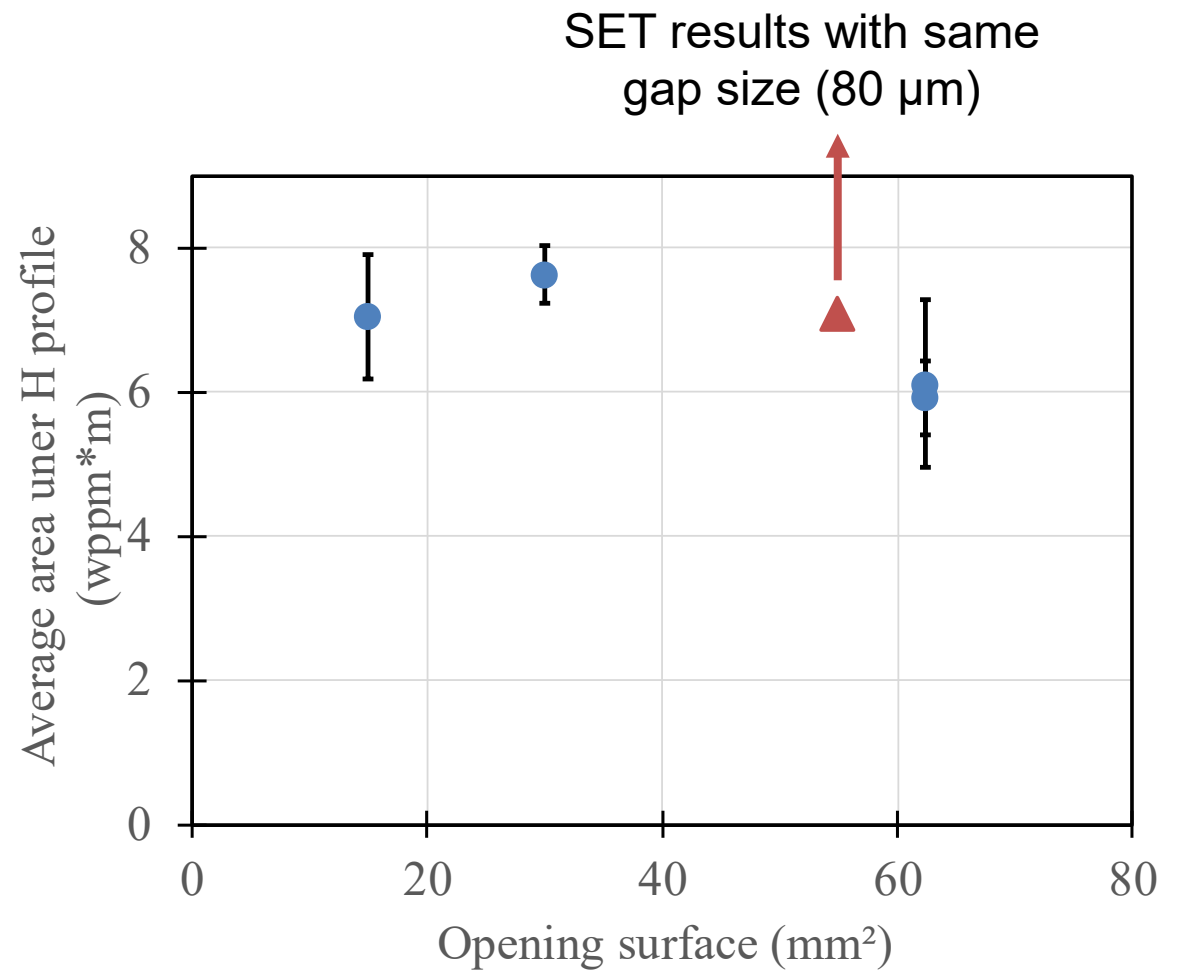
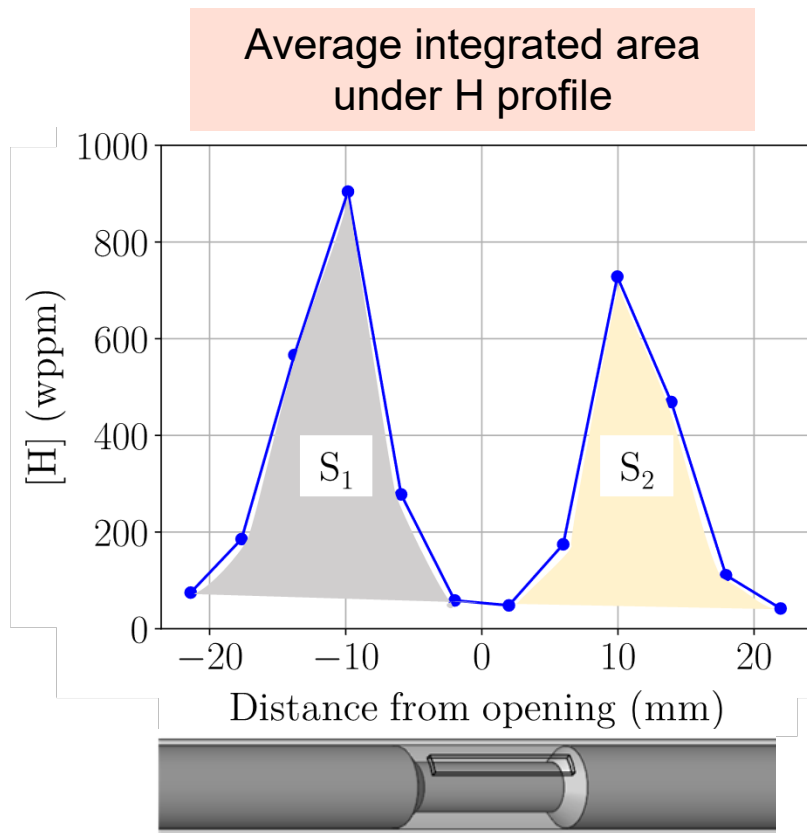
Could explain why

Reported NRI data



[Stuckert et al., 2020, Grosse et al., 2006]

→ Steam transport is enhanced near the opening depending on the burst geometry



- No significant influence of opening size on the total H content (too large opening size ? )
- The obtained H content with SOTs is coherent with the SETs results

## Experimental and modelling characterisation of secondary hydriding

- The **novel and dedicated experimental protocol on undeformed claddings** allowed to **reproduce secondary hydriding**
  - The **effects of several parameters** were evidenced
  - The phenomenon was **finely characterised**, and the obtained results were used for **modelling work**
  - A **1D axisymmetric modelling** of the phenomenon and **sensitivity studies** were carried out
- The obtained data help understand the reported data on semi-integral tests (irradiated and unirradiated materials)
  - The obtained data served as basis for modelling purposes and for code validation



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**Thank you for your  
attention!**

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**Raimon Pericas**

ISS

## **Expanding the Capability of the ASTST VER3.5 System Thermal Hydraulic and SCDAPSIM Modeling Options to Support the Fukushima Daiichi Decommissioning R&D Analysis and Assessment**

Immediately after the accident at Fukushima Daiichi, Innovative Systems Software, and other members of the international SCDAP Development and Training Program (SDTP) started an assessment of the possible core/vessel damage states of the Fukushima Daiichi Units 1-3. The assessment included a brief review of relevant severe accident experiments and a series of detailed calculations using RELAP/SCDAPSIM. The calculations used a detailed RELAP/SCDAPSIM model of a representative BWR plant provided by the Comision Nacional de Seguridad Nuclear y Salvaguardias, the Mexican Nuclear Regulatory Authority. The initial assessment was originally presented to the International Atomic Energy Agency on March 21st, 2011 to support their emergency response team and later to our Japanese colleagues to support their Fukushima Daiichi specific analysis and model development activities. Additional calculations were performed using RELAP/SCDAPSIM to help refine the certainties in the thermal hydraulic boundary conditions including potential failures in the reactor coolant system leading to the depressurization of Units 1 and 3. However, those calculations were limited to the in-vessel phase of the accidents, since at that time very little was known about the conditions of vessel failure and relocation of material into the reactor cavity.

Starting in 2020, with the help of our colleagues in Japan and Europe, a new integrated BEPU code, ASYST, was created as part of a new ASYST Development and Training Program (ADTP). It was intended as a framework for our program members to extend the capabilities of RELAP/SCDAPSIM to include more advanced system thermal hydraulics modeling options including the ability to model the RCS and containment during severe accident conditions. Two main versions of ASYST are being developed. ASYST VER4.x focuses on advanced fluid and reactor systems. VER3.x focuses on the improvement of SCDAPSIM modeling options for LWRs and PHWRs. For our activities related to Fukushima Daiichi decommissioning R&D, ASYST VER3.5 is being extended to enable end-to-end BWR severe-accident analysis from in-vessel degradation through ex-vessel behavior. As described in more detail in the presentation, the modeling extensions (a) enable multiple COUPLE meshes so the reactor lower head and reactor cavity are modeled simultaneously; (b) implement a vessel creep-rupture failure trigger that opens a break coupling the lower plenum and reactor cavity thermal hydraulic volumes and initiates the slumping of the in-vessel debris into the cavity; (c) add configurable debris–water interaction/breakup options in the cavity; (d) incorporate the RELAP/SCDAPSIM/MOD4 FPTRAN.

The image features a blue-bordered banner with a world map background. The text 'SDTTP' is written in large, blue, stylized letters with a white outline on the left side. To its right, the text 'ADTTP' is written in large, green, stylized letters with a white outline. A white rectangular box with a black border is positioned in the upper right area of the banner, containing black text.

**SDTTP**

Development of best estimate methods  
for reactor and advanced fluid systems  
safety analysis and training

**ADTTP**

Expanding the Capability of the ASYST VER3.5  
System Thermal Hydraulic and SCDAPSIM  
Modeling Options to Support the Fukushima  
Daiichi Decommissioning R&D Analysis and  
Assessment

Dr. Raimon Pericas and Dr. Chris Allison  
Innovative Systems Software (ISS)  
30th Int. QUENCH Workshop  
16-18 Dec. 2025 Karlsruhe, Germany

# Outline I

## \* Background

- \* Benchmarking of BWR modeling options using CORA BWR electrically heated experiments, PBF-SFD and LOFT in-pile experiments and TMI-2.
- \* Early assessment of influence of uncertainties in over TH boundary conditions on fuel melting and relocation.
- \* Long time collaboration with Mexican Laguna Verde NPP (BWR type) and Fukushima Daiichi post accident activities.

## \* Extension of ASYST VER3.5 SCDAPSIM modeling options (improvements to de code).

- \* Latest improvements on ASYST VER3.5.

# Outline II

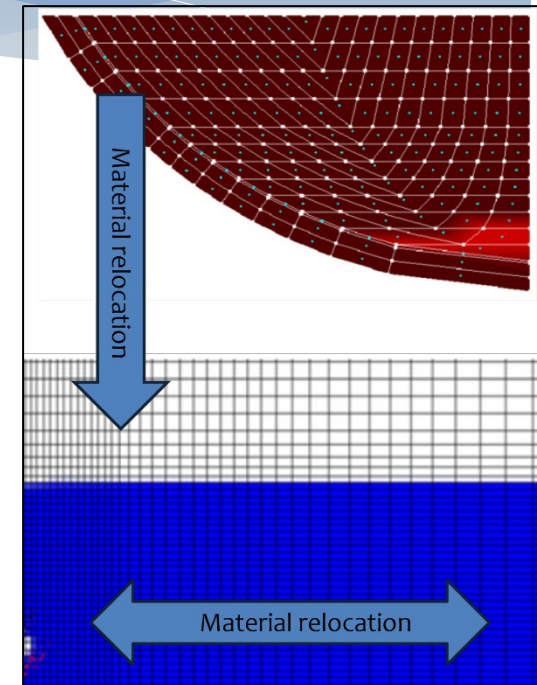
- \* Expansion of BWR input models for model assessment and sensitivity analysis (improvements of the BWR existing models)
  - \* Improving plant and facility representations with the existing capabilities of the code.
- \* Expansion of advanced GUI and IUA (integrated uncertainty analysis) to support model verification, analysis of results, and integrated sensitivity studies (adds on to the code)
  - \* Adding new capabilities to the code
  - \* Different analysis approach (Integrated Uncertainty Analysis)

# Extension of ASYST VER3.5 SCDAPSIM modeling options

- \* Enable use of **multiple detailed 2D Finite Element mesh (FE)** porous media regions
- \* Implement **vessel creep rupture** failure of lower head and initiation of lower head debris into reactor cavity
- \* Add **debris-water interaction**/breakup in cavity options
- \* Incorporate FPTRAN detailed **fission product transport** and deposition models for TH volumes in RCS and containment
- \* Develop **standardized interfaces** to couple to external modules or codes for containment and source term analysis

# Detailed 2D FE porous media models to describe behavior of **lower plenum debris/vessel** – reactor cavity

- Heat conduction
    - 2D finite element
    - gap resistance (solid/melt)
    - 1D model at crust boundary perimeter
  - Molten pool behavior
    - Transient natural circulation
    - **Interactions with vessel wall**
    - **MCCI Melt Coolability and Concrete Interaction (TBD)**
- \* **Creep rupture failure of vessel wall**
  - \* **Material relocation**
    - \* **Relocation of upper plenum structures**
    - \* **Relocation of core component materials**
    - \* **Molten pool slumping**
  - \* **Ex-vessel flooding - Flooding**



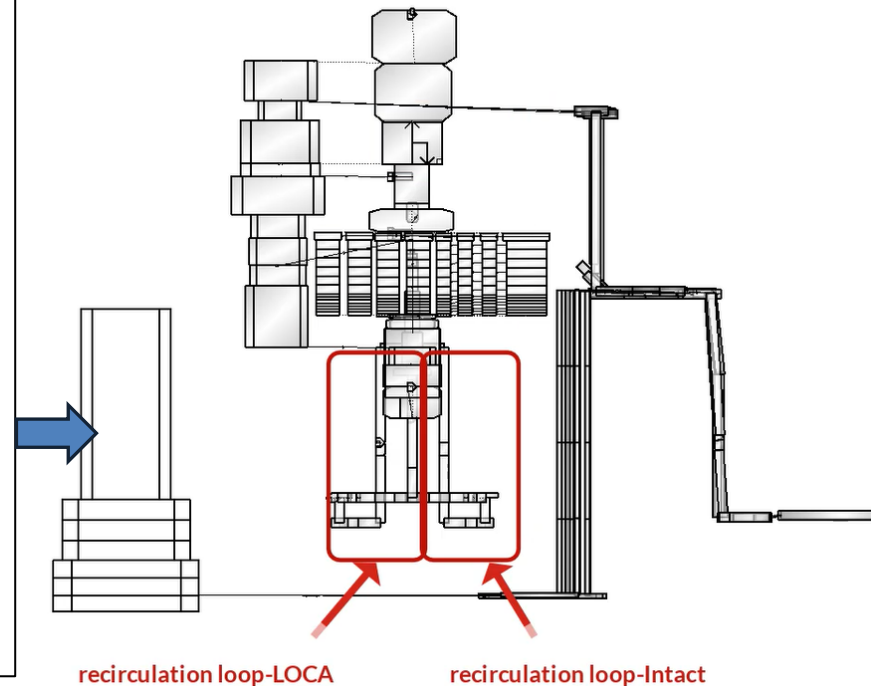
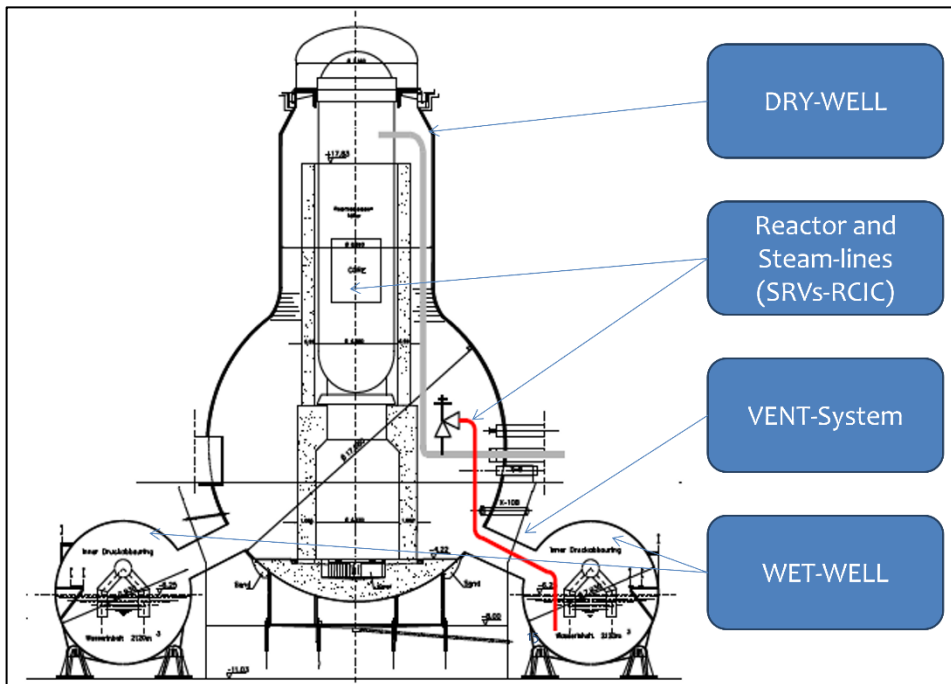
# Expansion of BWR input models for model assessment and sensitivity analysis

- \* **Extension of original BWR full plant model** to include representative passive cooling systems for Units 1-3, containment thermal hydraulics system to perform sensitivity studies on water addition to vessel and containment and FP transport and deposition
- \* **Adjusting the model** from Laguna Verde to Fukushima Daiichi like type reactor.
- \* **Development of representative BWR core/LP/vessel/reactor cavity models** for comparisons to TMI-2 results and sensitivity studies on core TH modeling and late phase fuel relocation into lower plenum and reactor cavity
- \* **Development of representative BWR fuel and CBCB assembly input model** for benchmarking against CORA BWR and PBF-SFD in-pile experiment results and assembly-specific sensitivity studies

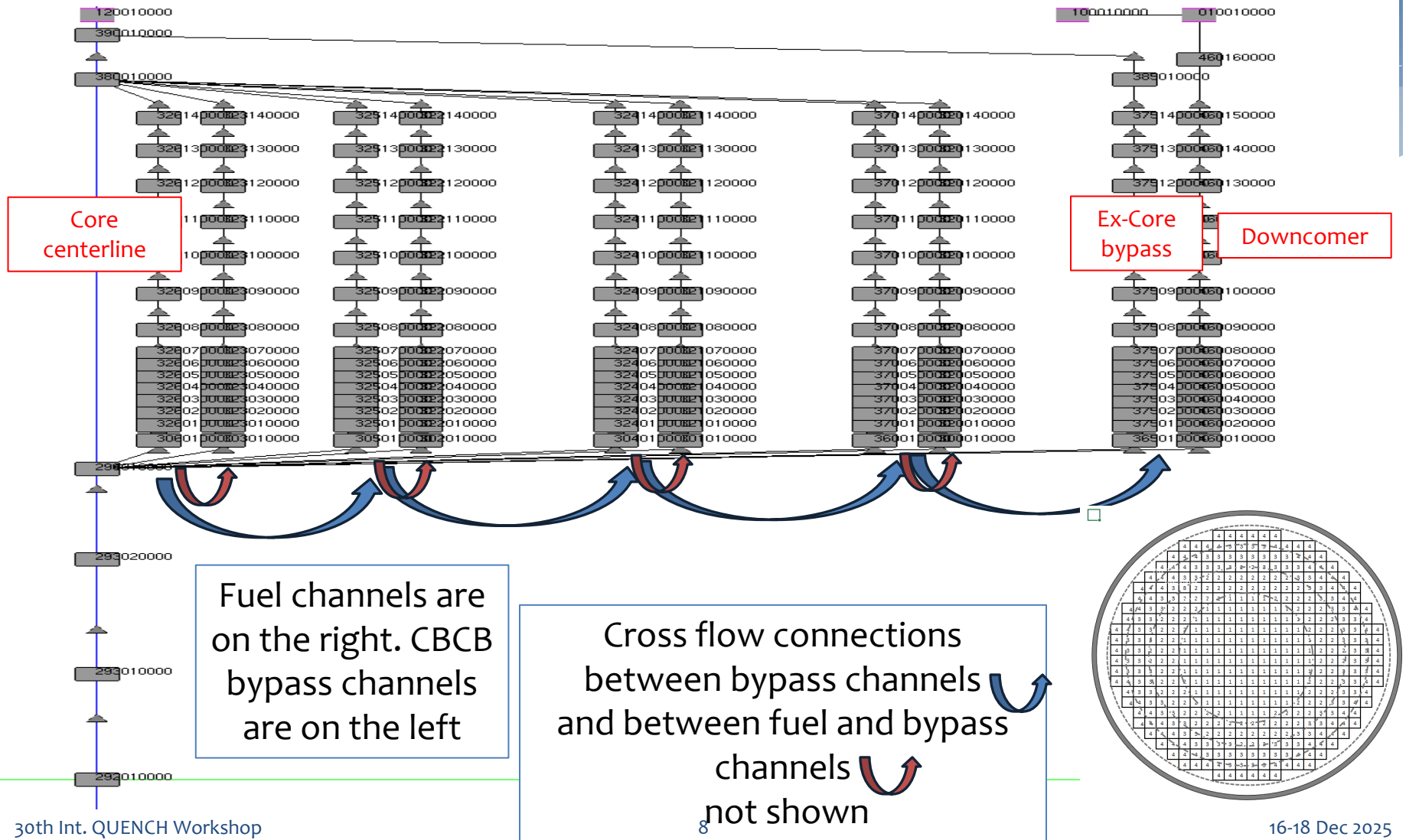


# Extensions of original BWR plant model to evaluate passive cooling system influence, initial PCS failure, and containment response

## RHYS – ASYST Display

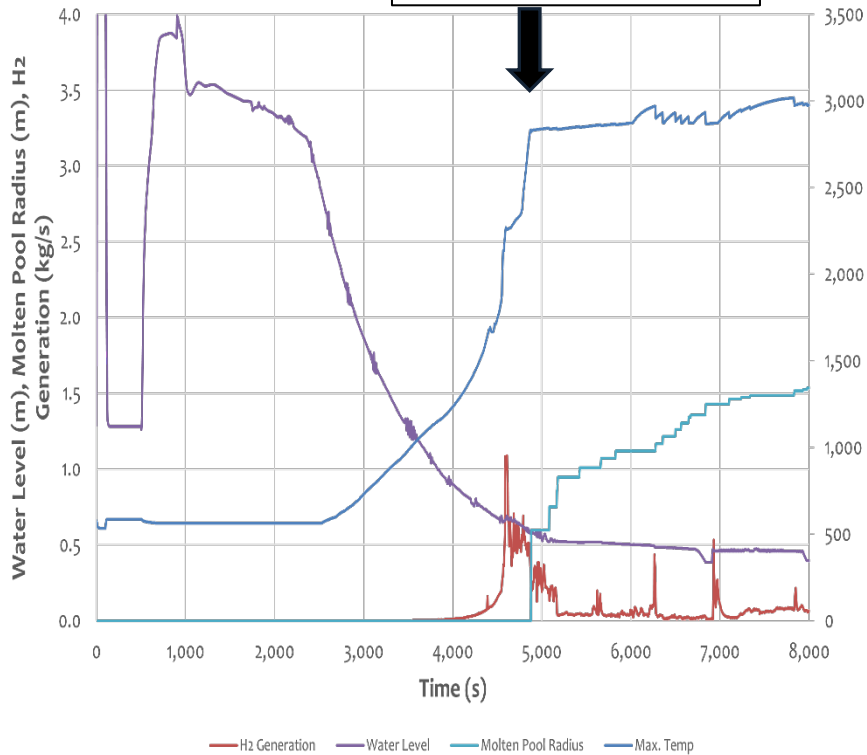


# Develop improved core input model with more realistic channel box/control blade (CBCB) thermal boundary conditions



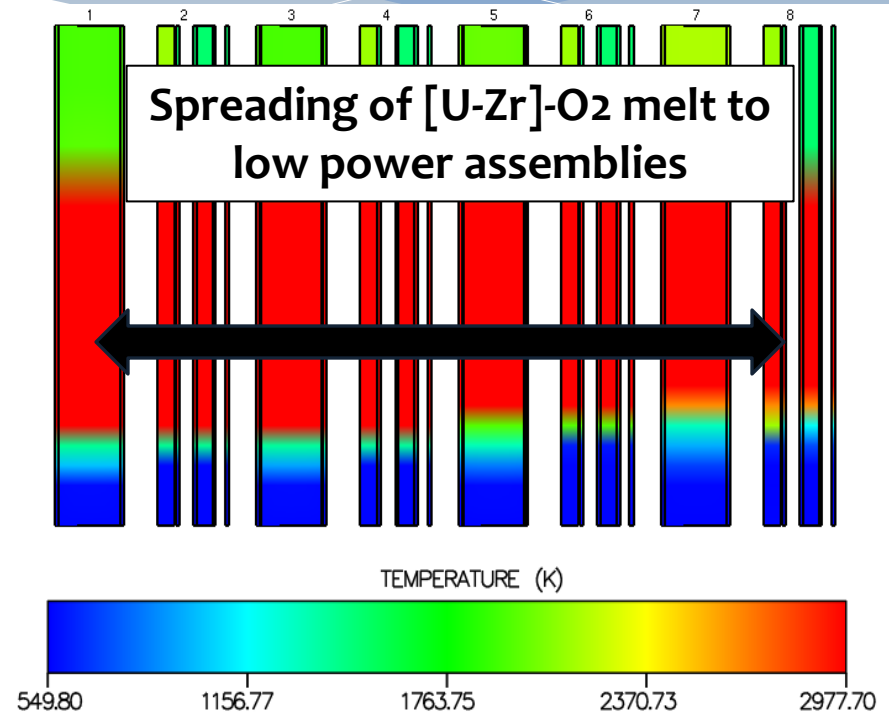
# Example- Results from improved BWR core input model – Impact of 1700 K channel box failure

**[U-Zr]-O<sub>2</sub>  
molten pool  
formation**



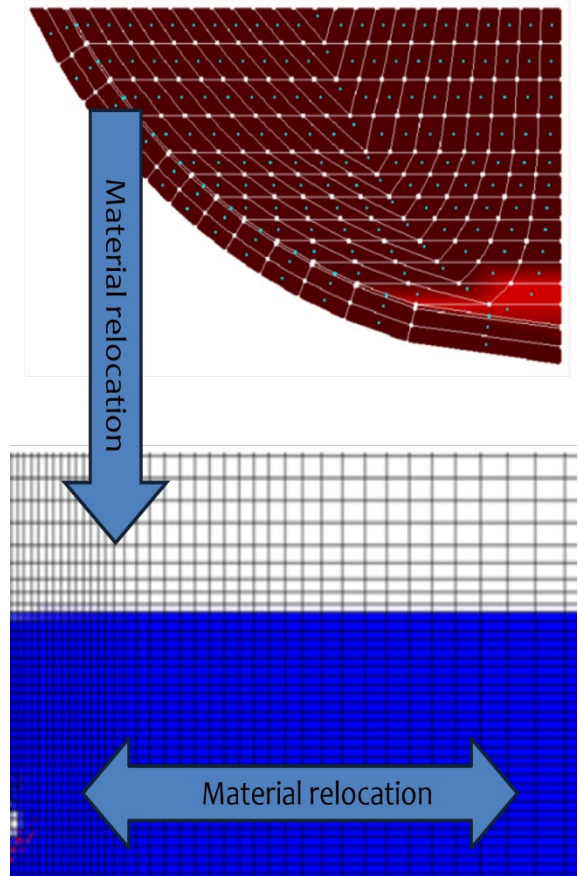
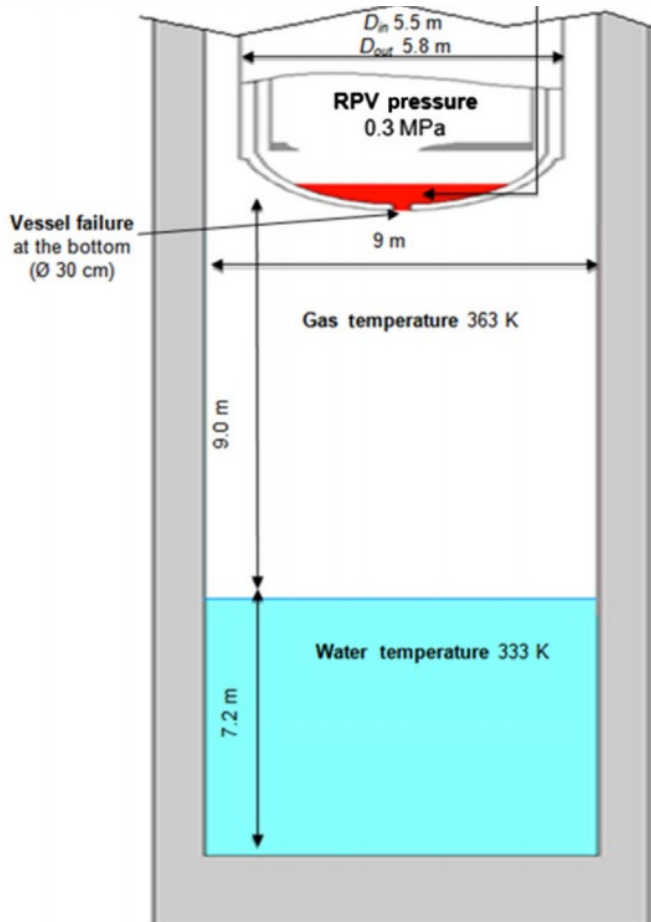
Hi Power

Lo Power

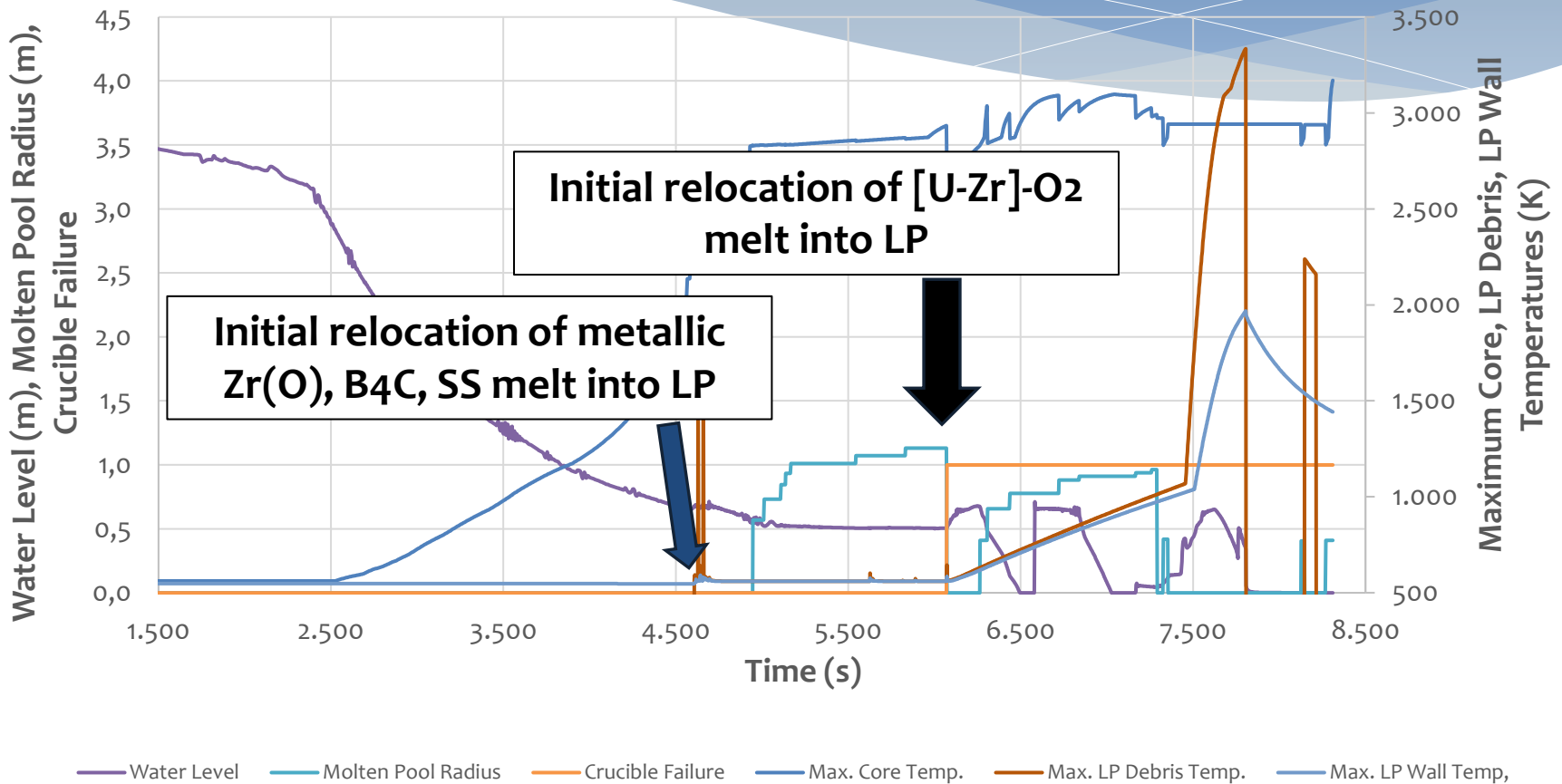


Representative core  
temperatures at  
8000s

# Extension of input model for vessel failure and melt relocation into reactor cavity



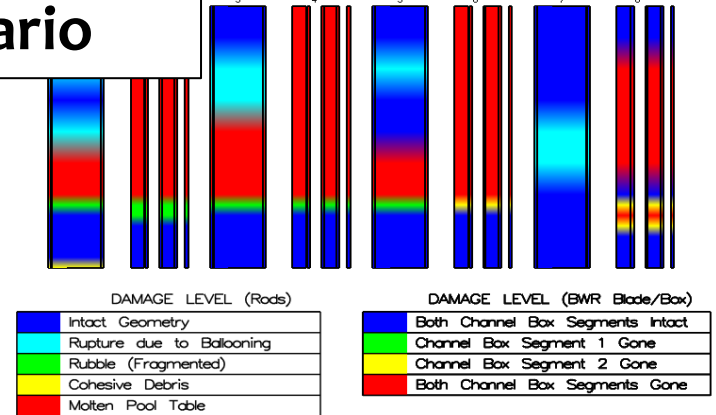
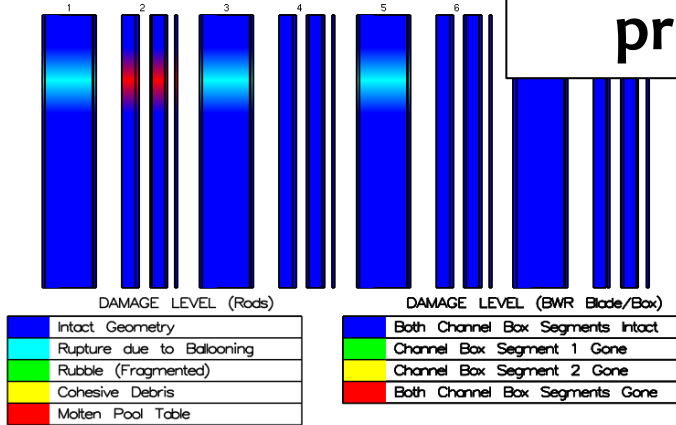
# Expansion of advanced GUI Results from BWR core with 2D lower plenum porous media model – Hi Pressure scenario



# Interactive Adv3Dgui SCDAP display for hi pressure scenario

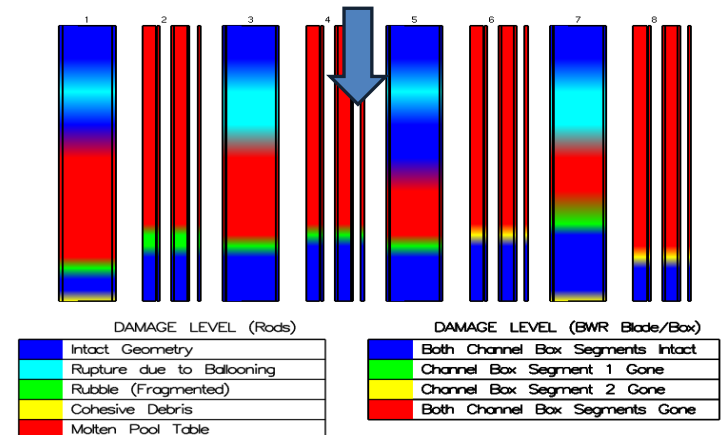
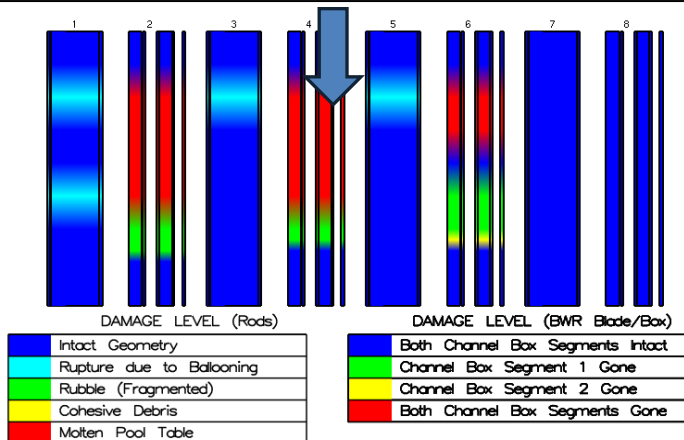
4600s

6000s



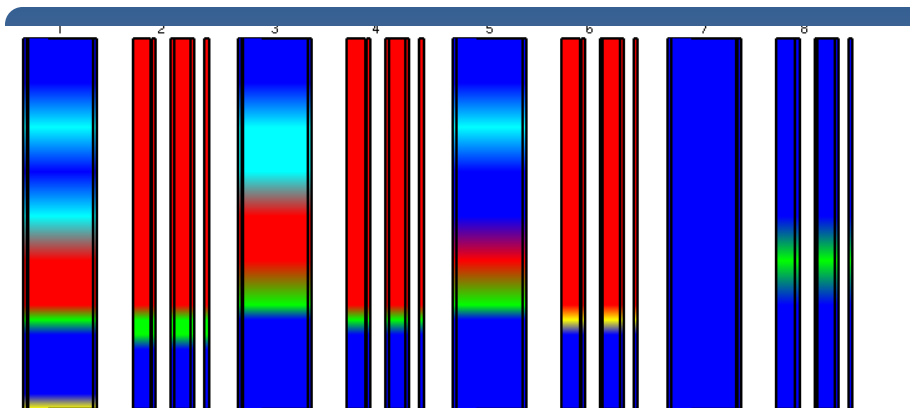
## Initial melting and relocation of channel box and control blade

## Initial relocation of [U-Zr]-O<sub>2</sub> melt into LP



4800s

7300 s

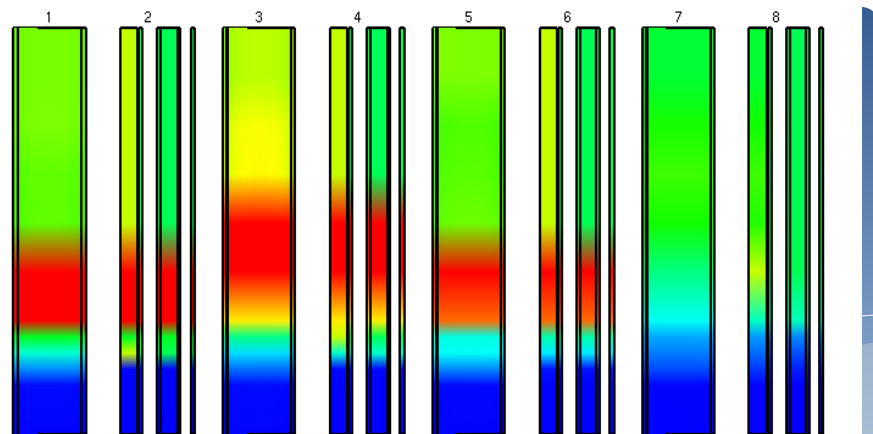


DAMAGE LEVEL (Rods)

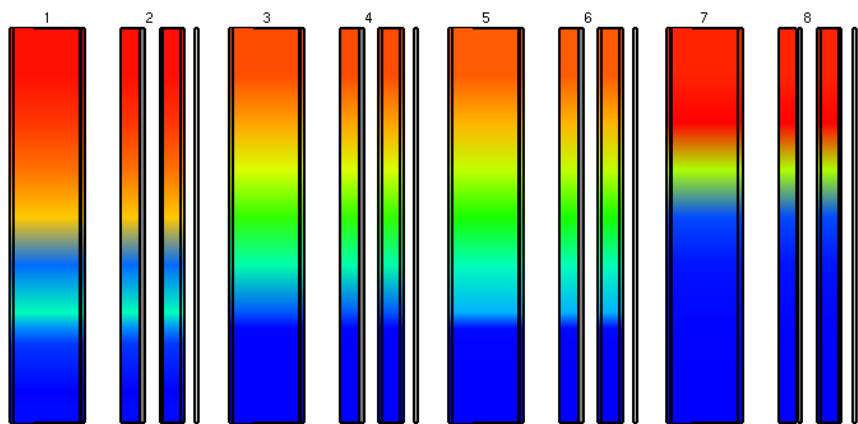
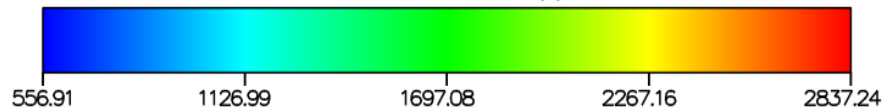
DAMAGE LEVEL (BWR Blade/Box)

Blue	Intact Geometry
Cyan	Rupture due to Ballooning
Green	Rubble (Fragmented)
Yellow	Cohesive Debris
Red	Molten Pool Table

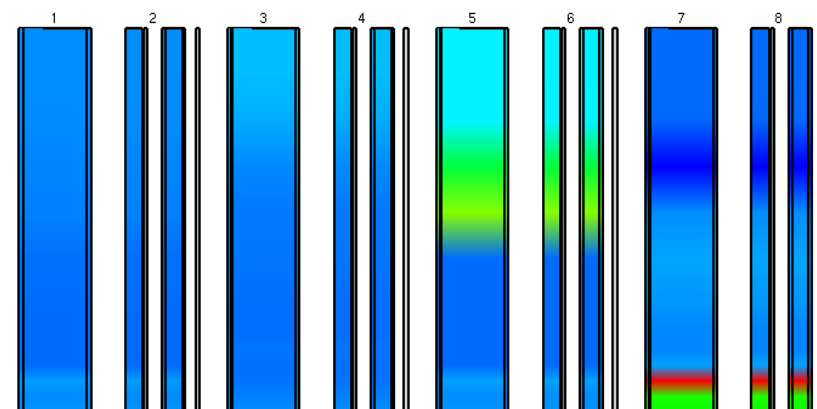
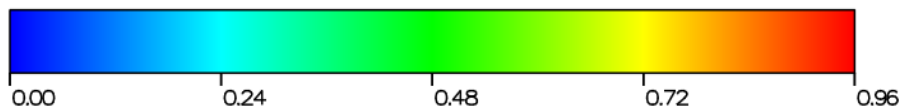
Blue	Both Channel Box Segments Intact
Green	Channel Box Segment 1 Gone
Yellow	Channel Box Segment 2 Gone
Red	Both Channel Box Segments Gone



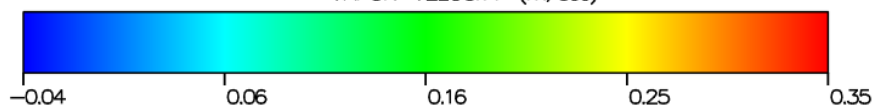
TEMPERATURE (K)



NONCONDENSABLE MASS FRACTION



VAPOR VELOCITY (m/sec)

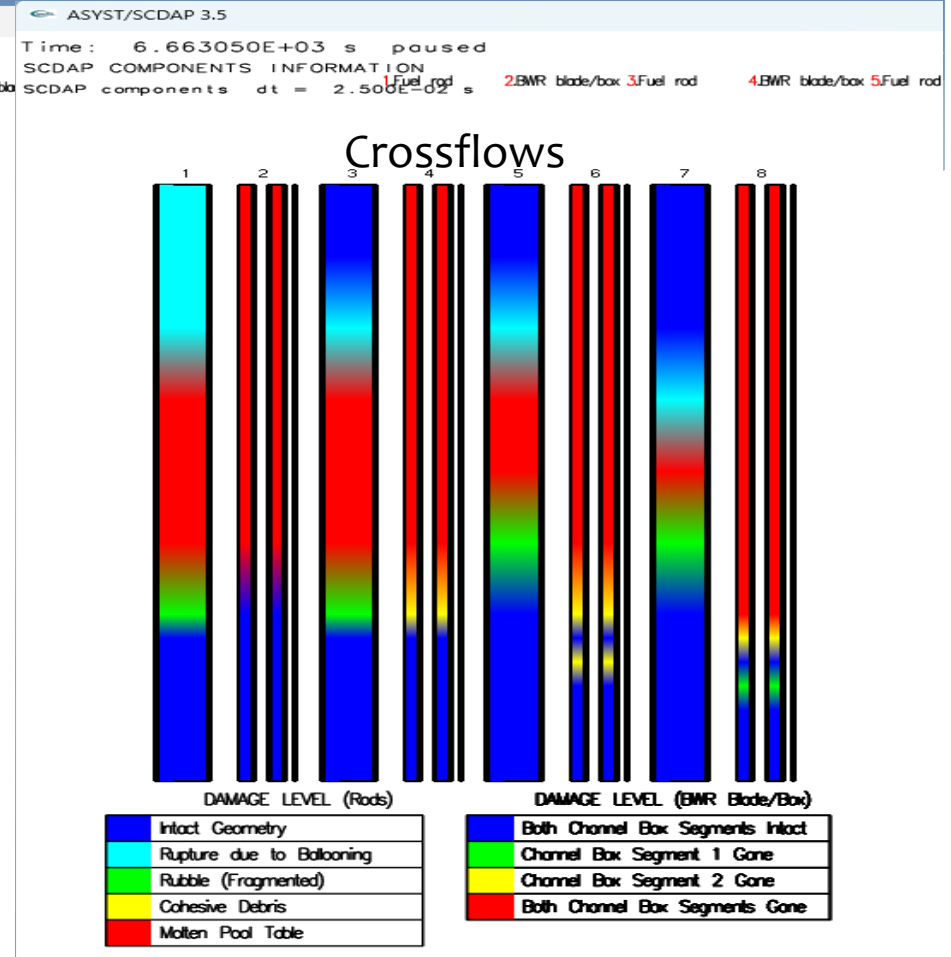
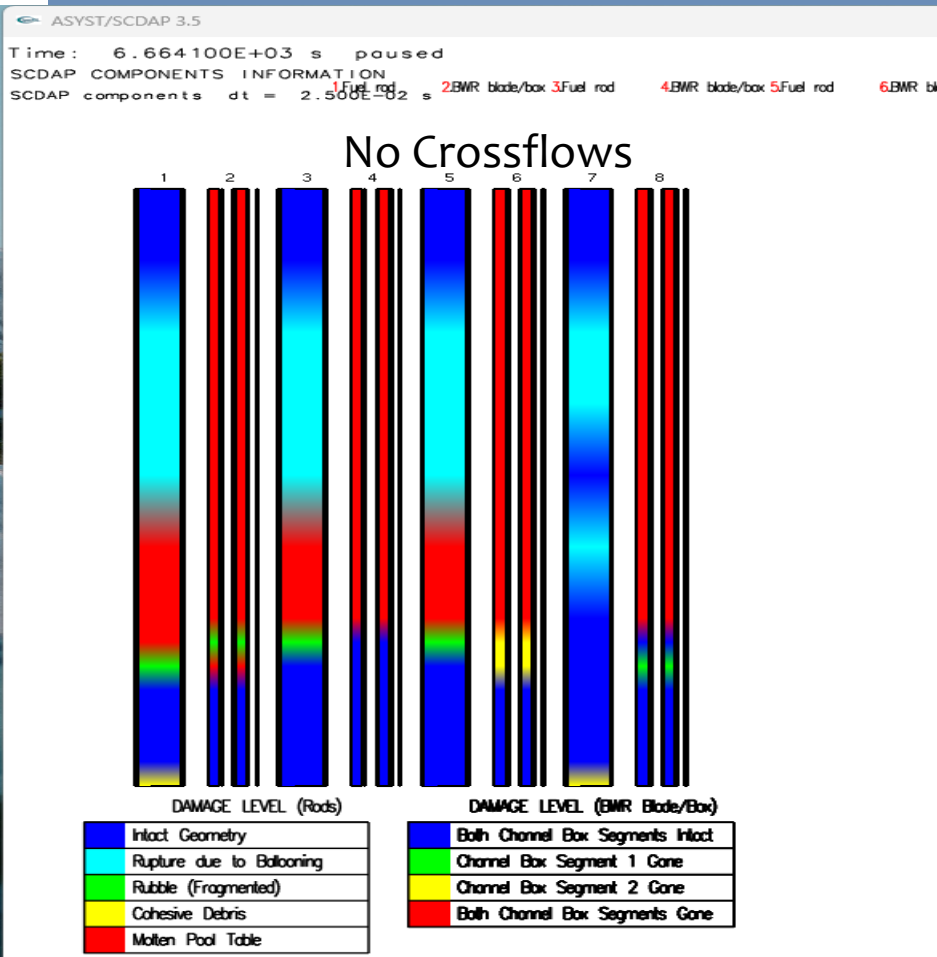


# Influence of horizontal crossflows with fuel channel failure at 1700K

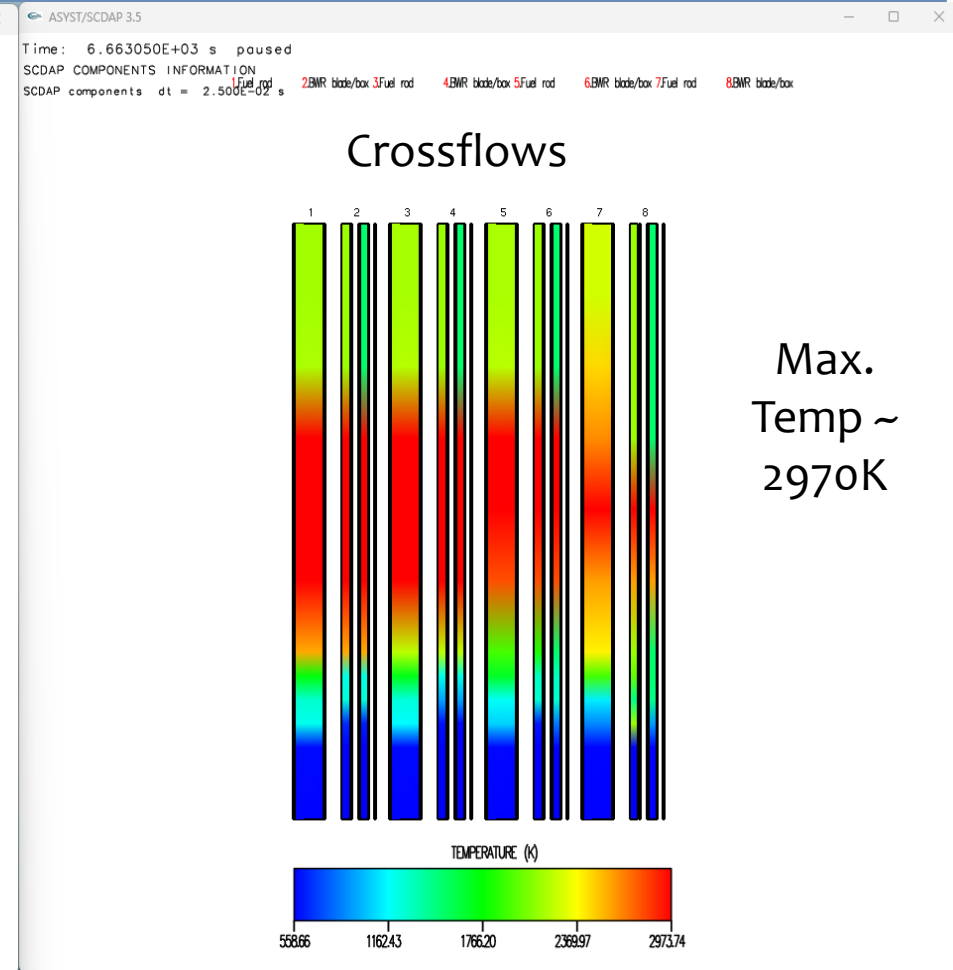
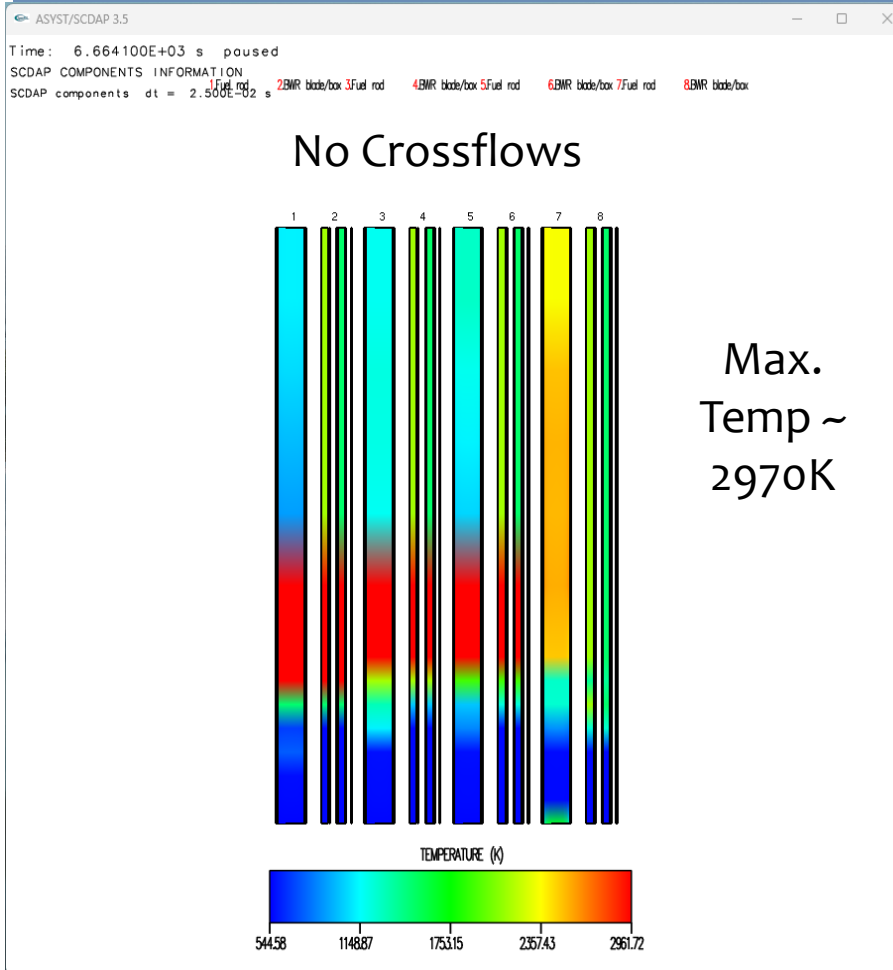
- \* Reduction in horizontal crossflows have minimal impact on overall global parameters but can impact axial and radial distributions with core and relocation of melts into lower plenum
  - \* Bounding case with crossflows set to zero
    - \* Increases peak temperatures in higher power channels
      - \* Decreases the time for the initial relocation of molten metallics (Zr, SS, B<sub>4</sub>C) into the lower plenum
      - \* May increase the amount of molten metallics in lower plenum prior to molten fuel relocation
    - \* Decreases the rate of radial spreading of the molten pool to the outer lower power fuel assemblies
    - \* May significantly delay the relocation of the molten fuel into the LP



# Influence of horizontal crossflows with fuel channel failure at 750K – Core damage level at 6660 s – Peak temperatures ~ 2970 K

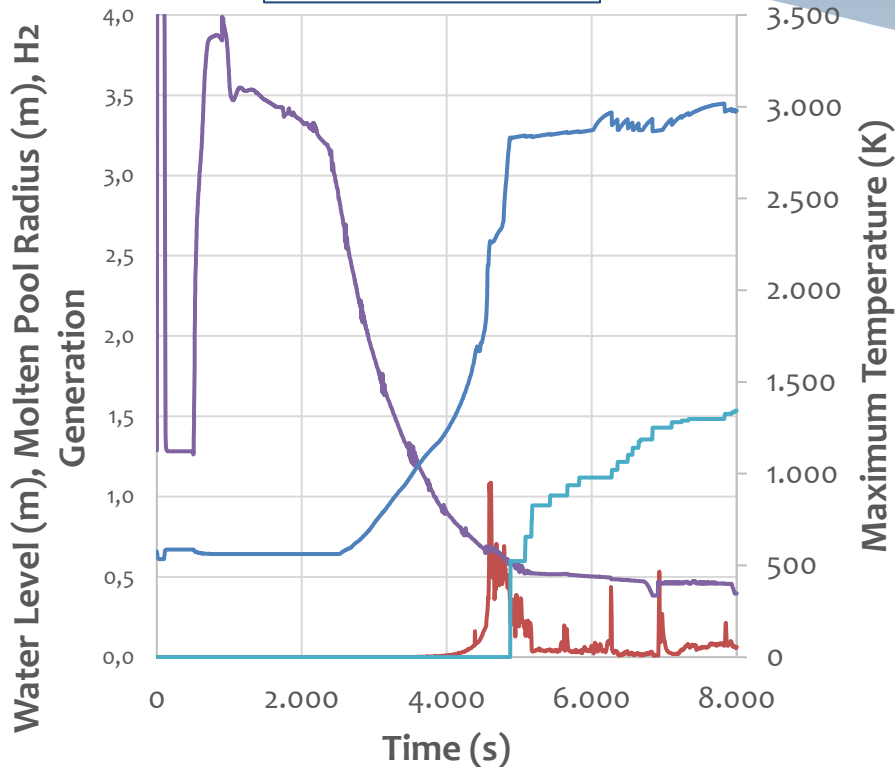


# Influence of horizontal crossflows with fuel channel failure at 750K – Core temperatures at 6660 s – Peak temperatures at 6660 s – Peak temperatures ~ 2970 K

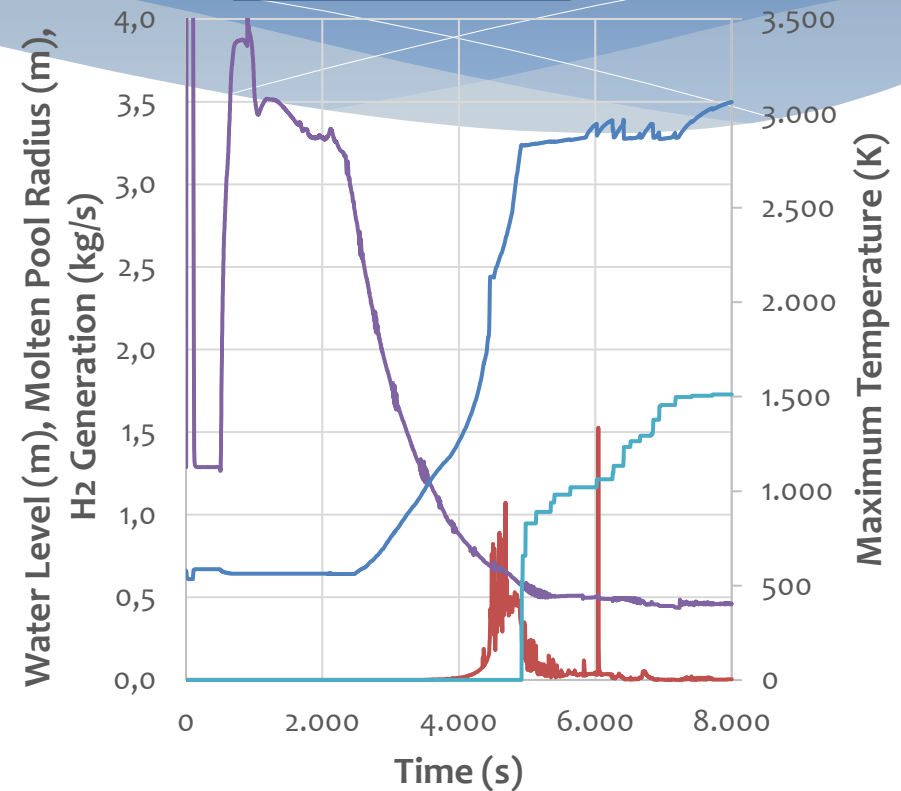


# Influence of changes in horizontal crossflow – 1700 K channel failure

Crossflow



No Crossflow

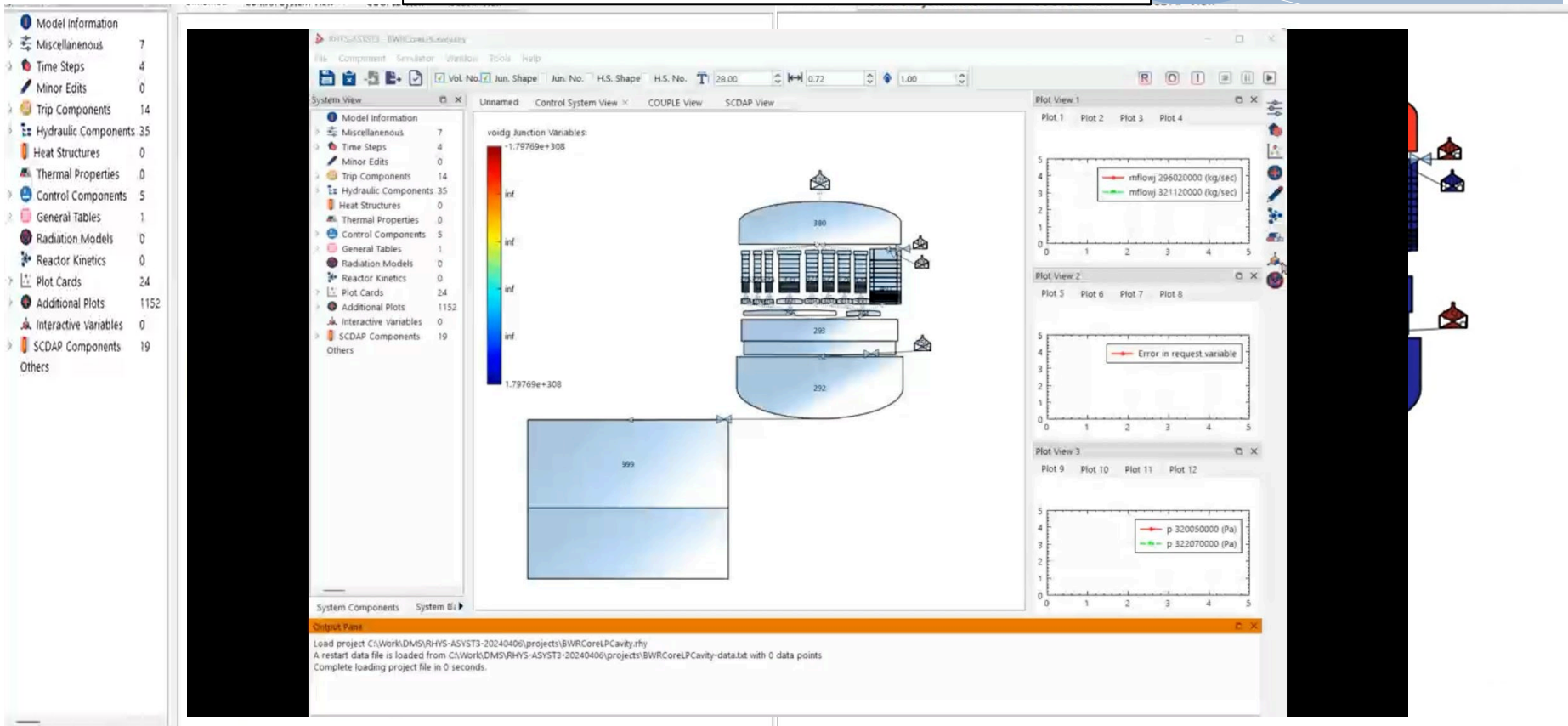


— H2 Generation — Water Level — Molten Pool Radius — Max. Temp

— H2 Generation — Water Level — Molten Pool Radius — Max. Temp

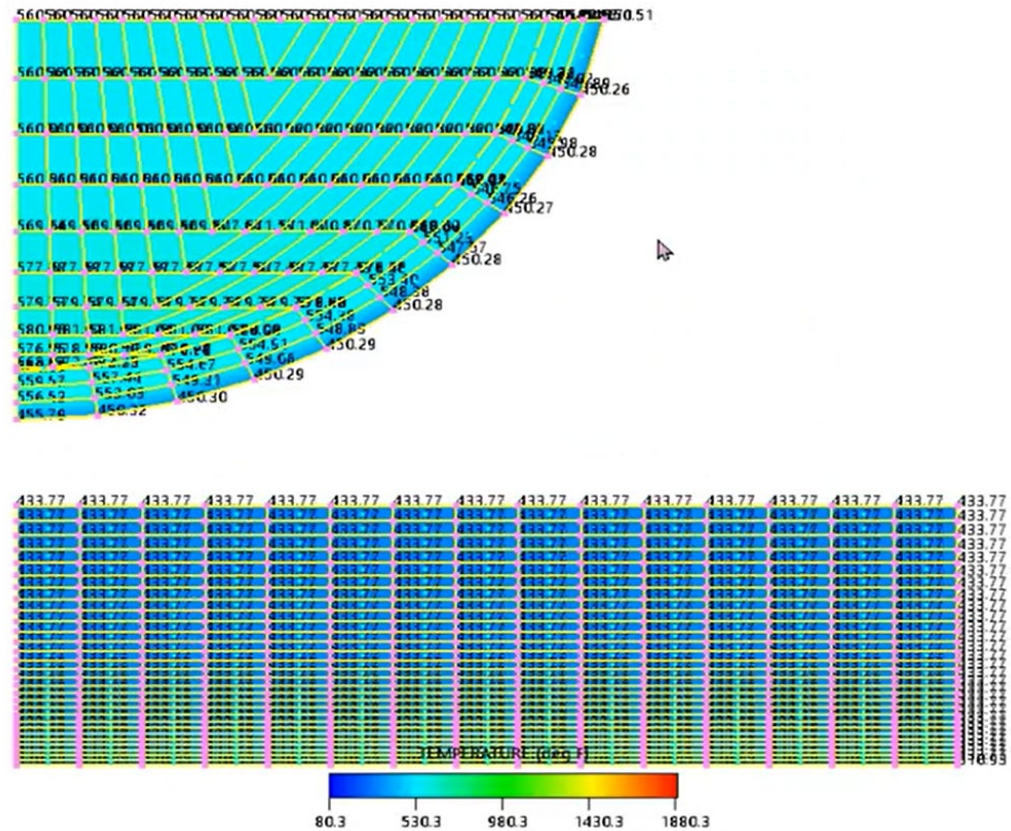
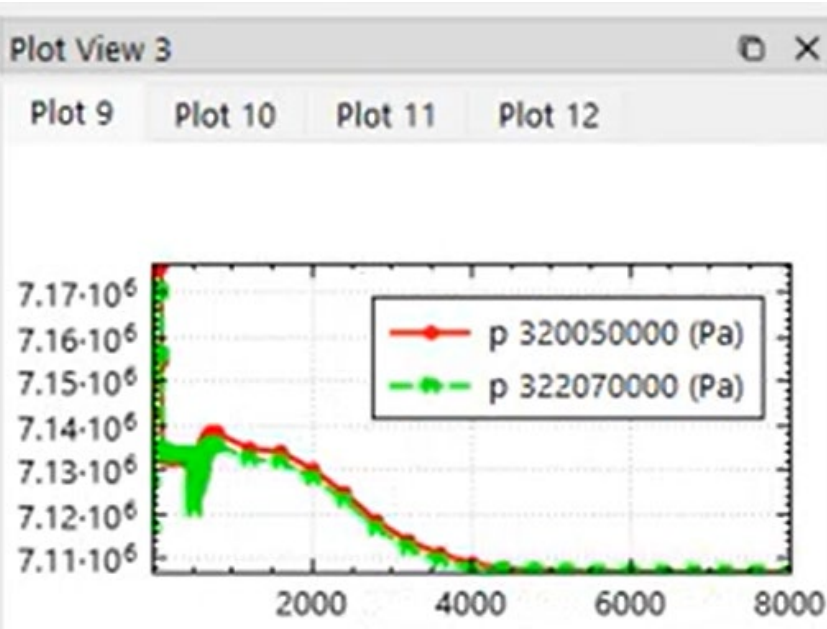
# BWR core with 2D lower plenum and reactor cavity porous media model

## Interactive RHYS desktop GUI



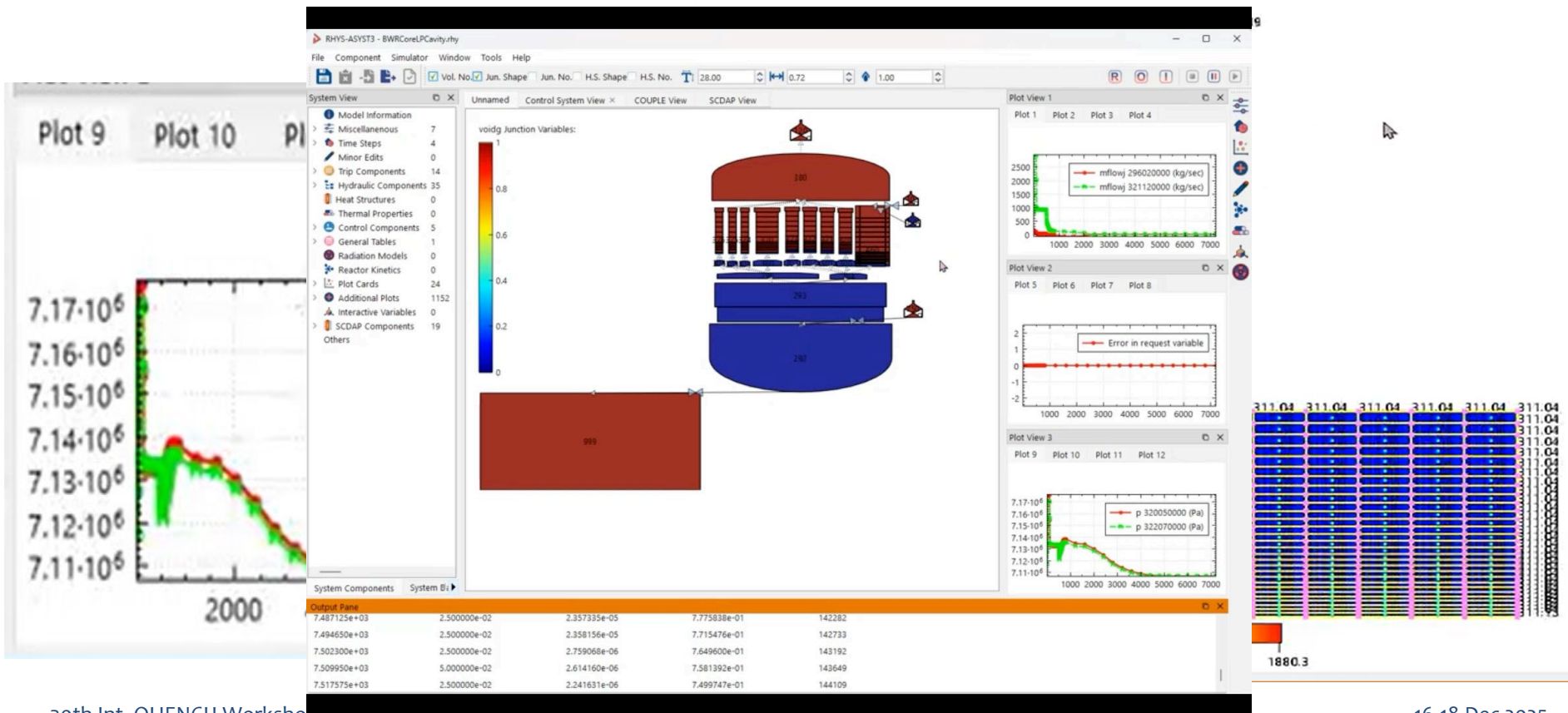
# BWR core with 2D lower plenum and reactor cavity porous media model

Interactive RHYS desktop GUI running depressurization scenario



# BWR core with 2D lower plenum and reactor cavity porous media model

Interactive RHYS desktop GUI running depressurization scenario



# Conclusions

- \* Adding capabilities ex-vessel for the ASYST platform allows us to perform a broader analysis of the severe accident scenarios.
  - \* Ex-vessel phenomena and Fission Product transport...
- \* New visualization tools allow us to have a better comprehension of the overall behavior of the modeled system.
  - \* Combination of the accurate modelling and the visualization tools allow us to see for example the influence horizontal crossflows.
  - \* RHYS platform allows overall and Realtime viewing of the calculations
- \* Alive project on nuclear modelling
  - \* Continuously improving platform. Large community worldwide members using and improving the platform in many areas of expertise.
    - \* Adding the Integrated Uncertainty Analysis package possibility as an example.

# Thank you for your attention

Dr. Raimon Pericas and Dr. Chris Allison  
Innovative Systems Software (ISS)  
30th Int. QUENCH Workshop  
16-18 Dec. 2025 Karlsruhe, Germany





**Gregor T. Stahlberg**

RUB

## **Analysis of the COAL Reflooding Experiments: Recent Simulations with AC<sup>2</sup>**

The validation of system codes for Loss-of-Coolant Accident (LOCA) scenarios, particularly those involving fuel rod deformation, requires rigorous benchmarking against experimental data to ensure reliable safety assessments. The primary objective of this work is to present the simulation results of selected COAL experiments using the AC<sup>2</sup>-ATHLET code, developed by GRS gGmbH, within the framework of the OECD-NEA ISP-53 benchmark.

The numerical analysis was performed at the Plant Simulation and Safety Group (PSS) at Ruhr-Universitaet Bochum (RUB). The modeling strategy employs a 1D lumped parameter approach to represent the thermal-hydraulic behavior of the test facility. The nodalization approach was maintained identical between the post-test analysis of the intact bundle (B0) and predictions of the deformed bundle (B2). This approach establishes a consistent basis for future investigations of B2 – beyond the scope of the current work – to directly assess the code's capability to predict the impact of flow blockage and ballooned rods without prior case-specific tuning.

The assessment strategy presented here focuses on the transient reflooding phase of the intact bundle under varying system pressures. While the simulation captures the key physical phenomena and demonstrates plausible system behavior, the results highlight specific sensitivities. In the high-pressure scenarios (20 bar), the code shows satisfactory agreement with experimental data. However, at lower pressures (3 bar), deviations regarding the quench front progression and peak cladding temperatures are observed.

Although the efficient single-channel approximation achieved satisfying agreement with the experimental data, the potential of a parallel channel model to resolve radial temperature gradients could be investigated. This extension would possibly capture flow deviations induced by the ballooned regions and complement the successful validation already achieved.

### **Acknowledgement**

This work was carried out within the framework of the WGAMA WGFS ISP-53, whose support and collaboration have been instrumental in the successful completion of this research.

Responsibility for the content lies with the authors.

The results were obtained using the GRS software package AC<sup>2</sup> 2023.



**RUB**

**RUHR-UNIVERSITÄT BOCHUM**

## **Analysis of the COAL Reflooding Experiments: Recent Simulations with AC<sup>2</sup>**

**Gregor T. Stahlberg, Marco K. Koch**

30<sup>th</sup> International QUENCH Workshop | RUB PSS | 2025 | KIT, Karlsruhe

**PSS** Plant Simulation and Safety  
Prof. Dr.-Ing. Marco K. Koch

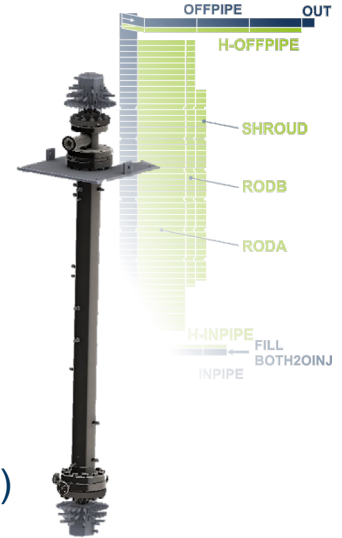
# AGENDA

- Introduction
- Modeling
- Results
- Summary



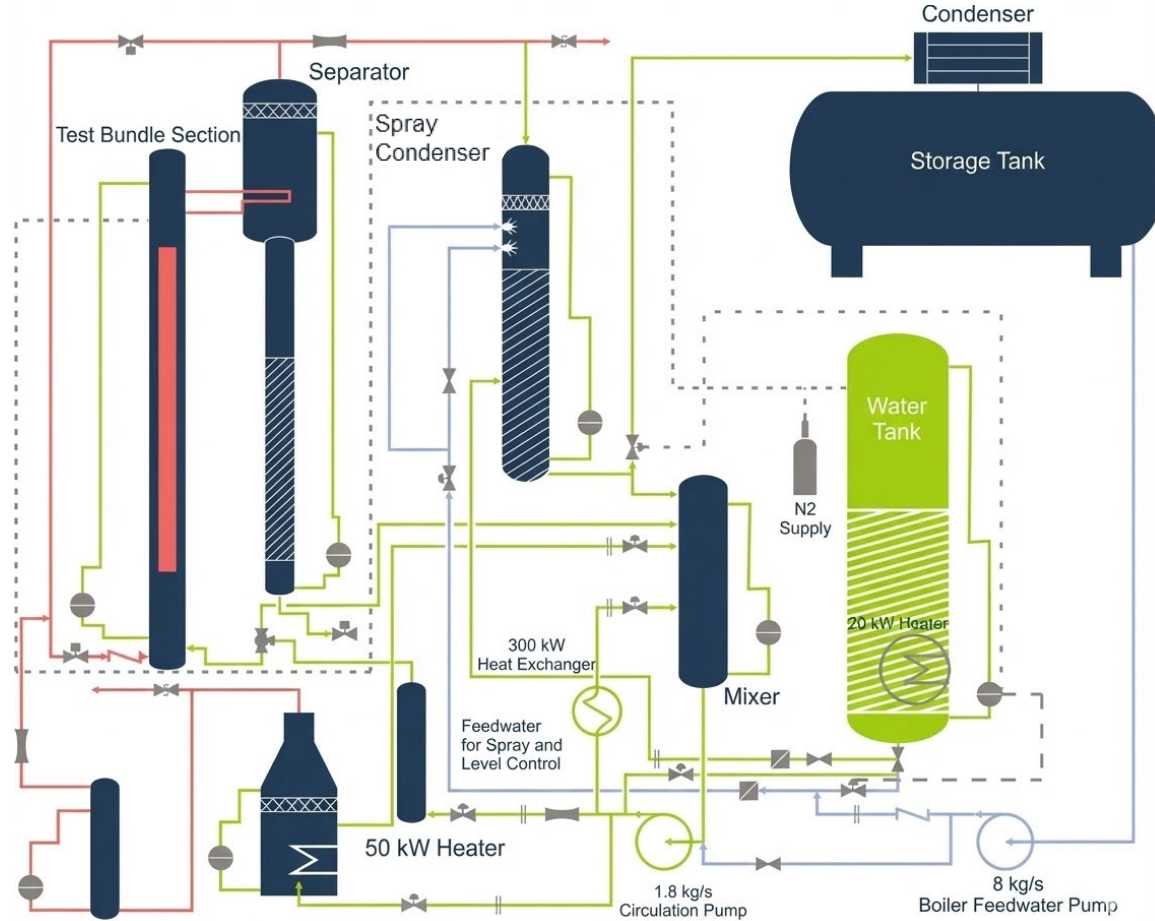
# INTRODUCTION

- **Framework:** OECD-NEA ISP-53 led by ASNR, France
  - International Standard Problem (ISP) to benchmark safety codes
  - 🎯 Increase confidence in code validity for safety assessments
  - International cooperation (more than 12 countries)
- **Experimental Setup:** COAL test facility
  - Focus on reflooding experiments under LOCA conditions
  - Geometry: 7x7 electrically heated rod bundles (simulating PWR 17x17 design)
- **Project Phases**
  - Open Phase B0: Simulation of undeformed rods for „calibration“ of input deck
  - Blind Phase B2: Simulation of deformed ("ballooned") rods **without** prior knowledge of exp. results
  - Open Phase B2: Simulation of deformed ("ballooned") rods **with** all exp. data



# INTRODUCTION

## Test facility



# INTRODUCTION

## Test facility

### ■ Facility & Conditioning

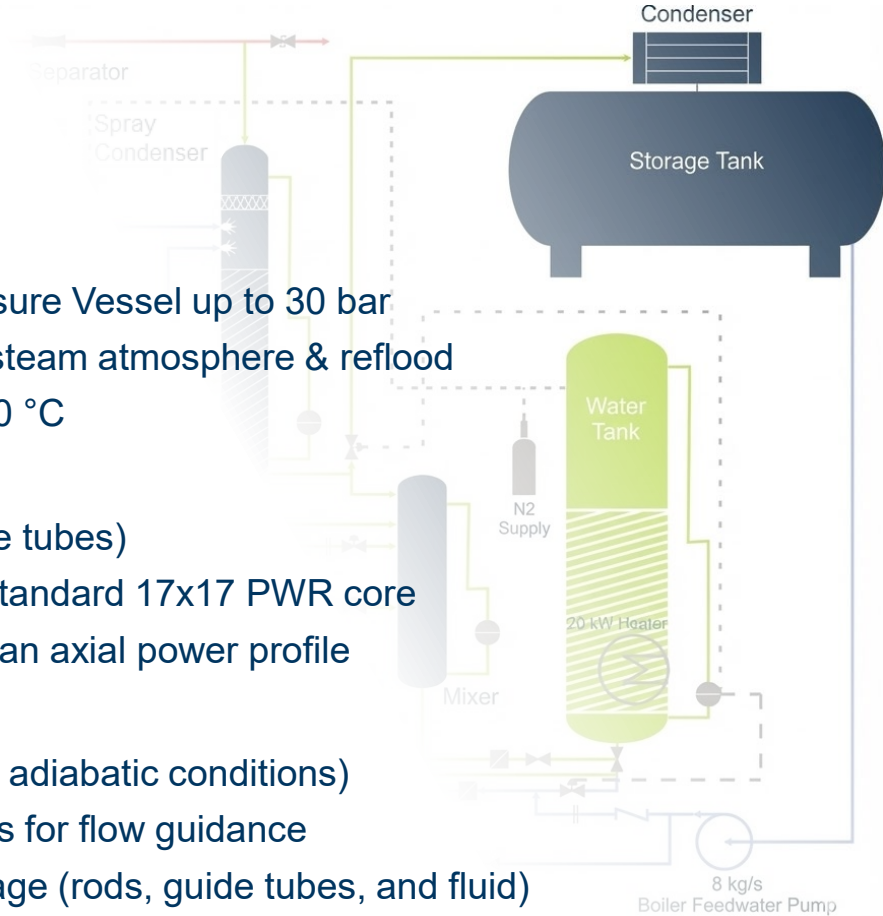
- Pressure Vessel: Simulates PWR Reactor Pressure Vessel up to 30 bar
- Test Conditions: Simulation of scenarios within steam atmosphere & reflood
- Initialization: Electrical pre-heating of rods to 300 °C

### ■ Test Bundle Geometry

- Configuration: 7x7 array (46 heater rods, 3 guide tubes)
- Representation: Corresponds to a section of a standard 17x17 PWR core
- Heating Profile: 3.0 m active heated length with an axial power profile

### ■ Components & Boundary Conditions

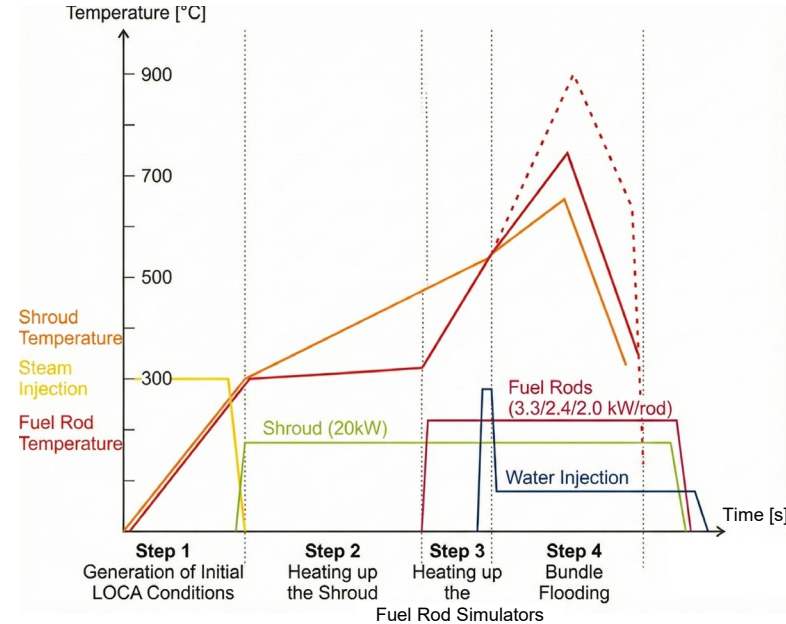
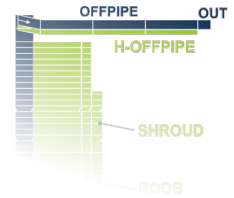
- Shroud: Actively heated flow channel (simulates adiabatic conditions)
- Grids: Includes 2 spacer grids and 4 mixing grids for flow guidance
- Instrumentation: Extensive thermocouple coverage (rods, guide tubes, and fluid)



# INTRODUCTION

## Schematic overview of the sequence

- Experimental Sequence:
  - **Step 1:** System preheating ( $\sim 300^{\circ}\text{C}$ ) with steam injection, initial LOCA conditions
  - **Step 2:** Shroud is electrically heated (20 kW) to increase boundary temperatures
  - **Step 3:** Rod Heating Power is applied to the fuel rod simulators, causing a rapid temperature rise
  - **Step 4:** Water injection begins; rod temperatures peak and subsequently drop as quenching occurs
  - End of Sequence
- Simulations include all above mentioned phases

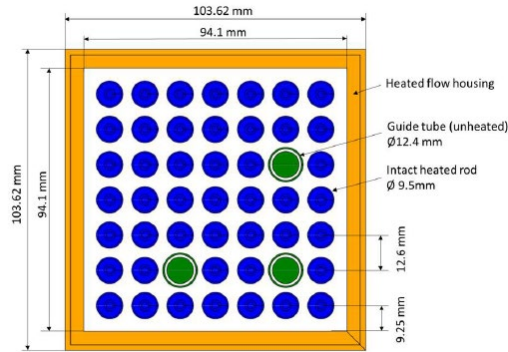


# INTRODUCTION

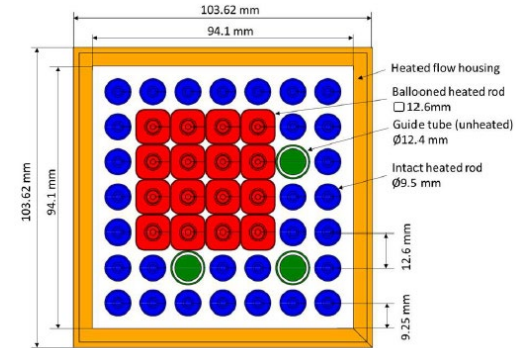
## Status Quo

- Experiments on flow blockage, local power increase through blockages
- Reflooding of a fuel rod bundle in the event of a loss-of-coolant accident
- Data set with AC<sup>2</sup>-ATHLET completed, tested and prospectively further developed
  - Intact Bundle, B0
  - Deformed Bundle, B2

Intact  
Bundle



Deformed  
Bundle





# MODELING

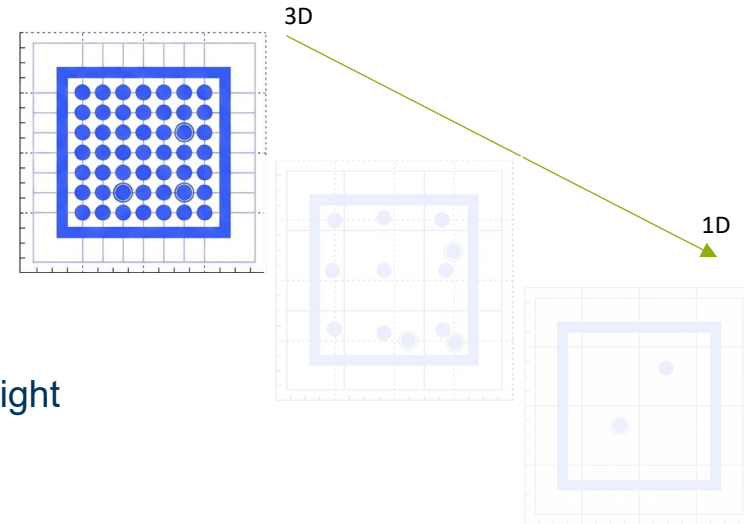
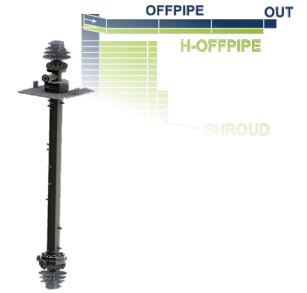
## Strategies: Balancing Precision and CPU Cost

### ■ Simulation Objectives

- Capture main reflooding phenomena
- If possible, reproduce “3D” effects (e.g., radial temperature gradients, flow deviation around ballooned regions)

### ■ Possible Modelling Approaches

- Sub-channel 3D Modelling
  - Coarse 3D Modelling (Clustered)
  - 1D Modelling (Lumped)
- Detailed resolution of the geometry
  - Con: High CPU cost (up to days) vs. detailed flow insight



# MODELING

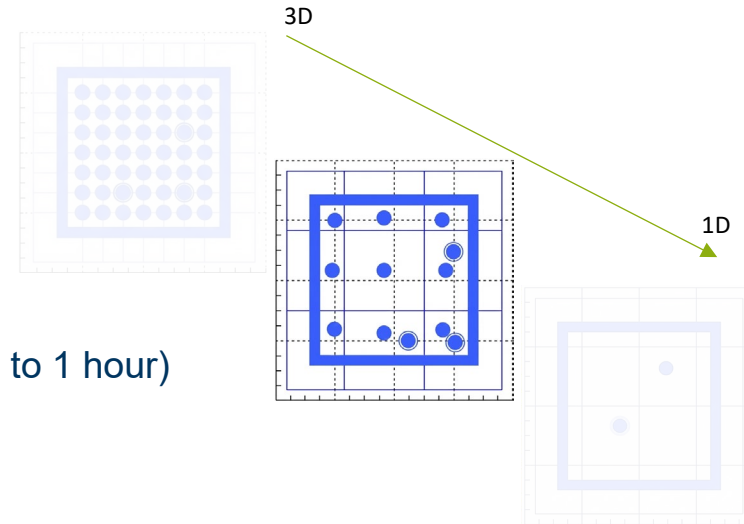
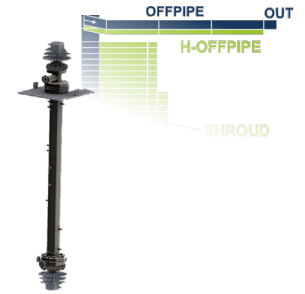
## Strategies: Balancing Precision and CPU Cost

### ■ Simulation Objectives

- Capture main reflooding phenomena
- If possible, reproduce “3D” effects (e.g., radial temperature gradients, flow deviation around ballooned regions)

### ■ Possible Modelling Approaches

- Sub-channel 3D Modelling
- Coarse 3D Modelling (Clustered)
- 1D Modelling (Lumped)
  - Grouping several sub-channels/rods into clusters
  - Pro: Captures radial trends with reasonable effort (up to 1 hour)
  - Relevance: Often used to balance accuracy



# MODELING

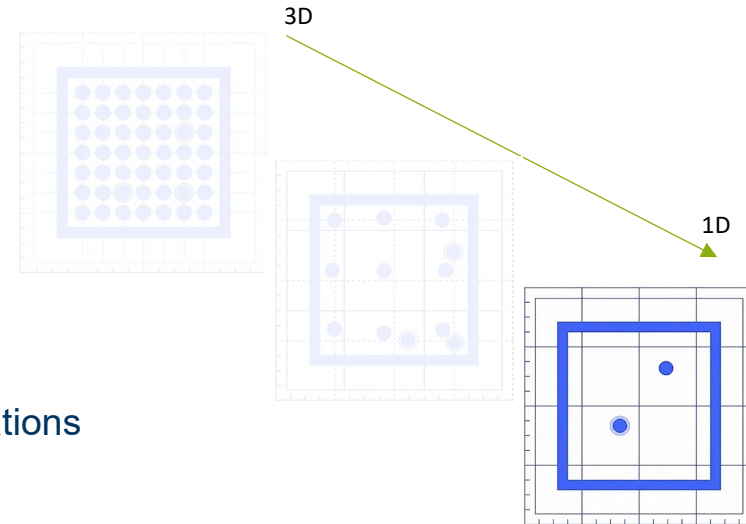
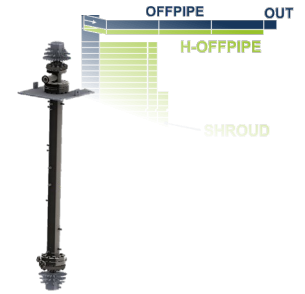
## Strategies: Balancing Precision and CPU Cost

### ■ Simulation Objectives

- Capture main reflooding phenomena
- If possible, reproduce “3D” effects (e.g., radial temperature gradients, flow deviation around ballooned regions)

### ■ Possible Modelling Approaches

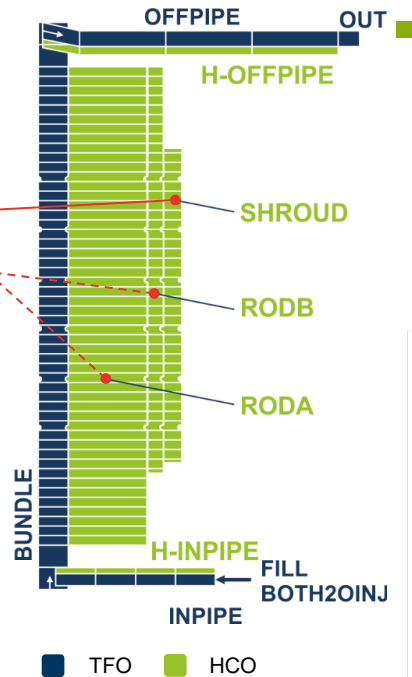
- Sub-channel 3D Modelling
- Coarse 3D Modelling (Clustered)
- 1D Modelling (Lumped) ← **used for this work!**
  - Averaging relevant components each into one object
  - Pro: Very fast calculations (minutes)
  - Con: Underestimates radial profiles + local flow deviations



# MODELING

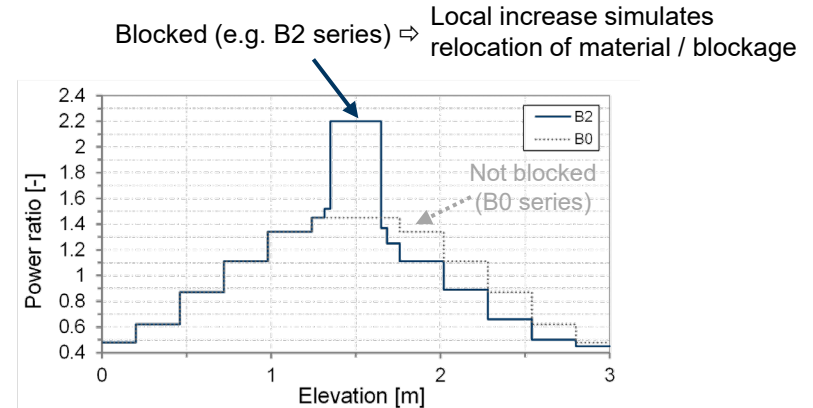
## AC<sup>2</sup> Data Set Development

- 1D-Module of ATHLET representing flow path
- Relevant components:
  - Shroud, spacer grids
  - Weighted fuel rod (RODA) and guide tube objects (RODB)
  - For experiments with deformed rods additional objects are implemented
- Components are modeled as multilayer structures (e.g. Shroud, RODs)



## Boundary Conditions & Power Profile

- Pressure, Temperature
- Axial Power Profile
- Electric Power



# MODELING

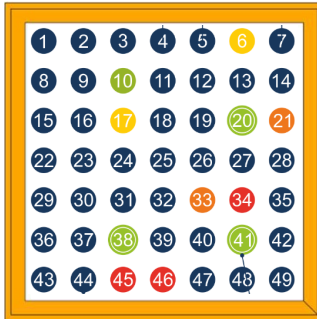
## Selected COAL-B0 Boundary Conditions

Parameter	B0-03-50	B0-20-17
Pressure	3 bar	20 bar
Inflow	50 kg/m <sup>2</sup> /s (0,269kg/s)	17 kg/m <sup>2</sup> /s (0,089kg/s)
Temperature of Quenchwater	74 °C	192 °C
Power per rod	3,3 kW	2,0 kW
Shroud power	20 kW	20 kW

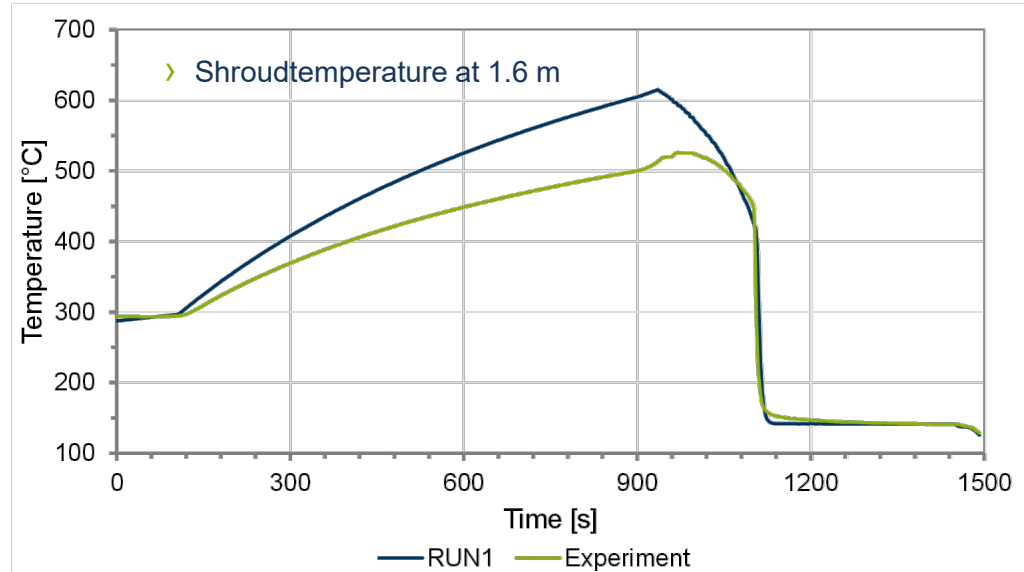
# RESULTS

## B0-03-50: Selected Results

- Scenario at low pressure (3 bar) with 0,269 kg/s reflooding rate
  - Rod power at 3.3 kW
  - › Shroud temperature is qualitatively calculated but overestimated ( $\sim 610^{\circ}\text{C}$ )
  - › Timing is captured closely



Bundle Configuration



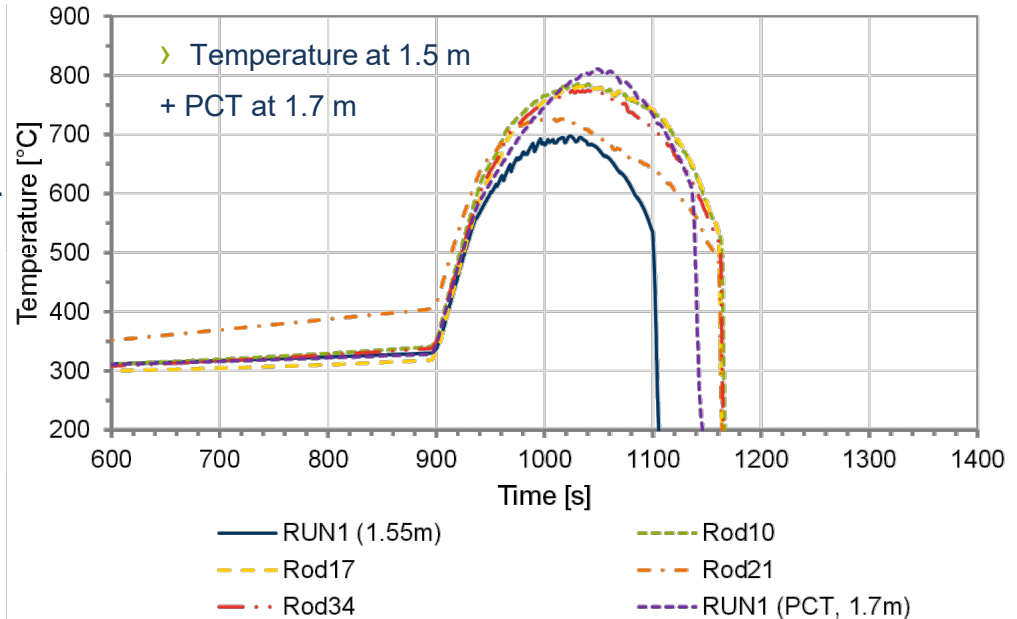
# RESULTS

## B0-03-50: Selected Results

- Scenario at low pressure (3 bar) with 0,269 kg/s reflooding rate
  - Rod power at 3.3 kW
    - › Calculated rod temperatures reach max. 810°C at 1.7 m and 700°C at 1.5 m
    - › Simulation shows axial shift: simulation data at 1.7 m match experimental data at 1.5 m, possibly due to delayed quenching



Bundle Configuration



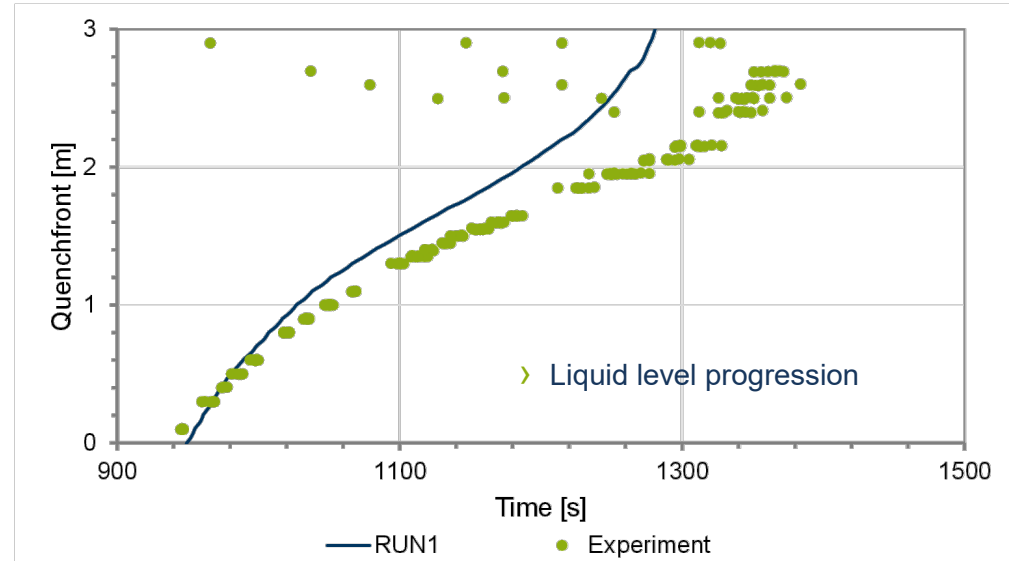
# RESULTS

## B0-03-50: Selected Results

- Scenario at low pressure (3 bar) with 0,269 kg/s reflooding rate
  - Rod power at 3.3 kW
  - › After reaching local plateau, the bundle is eventually fully quenched
  - › Simulation captures initial rise but overpredicts subsequent water column rise



Bundle Configuration

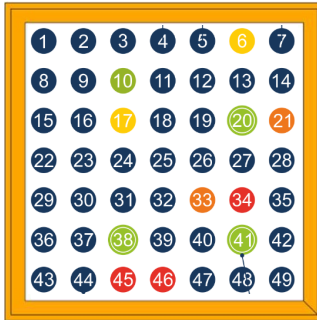




# RESULTS

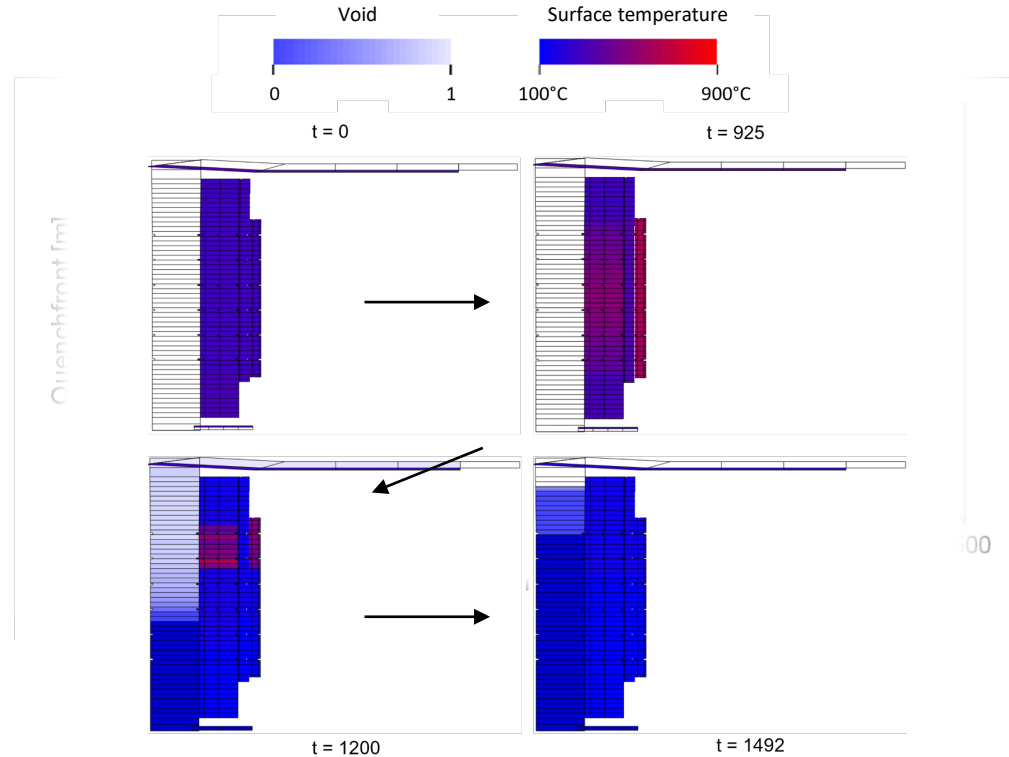
## B0-03-50: Selected Results

- Scenario at low pressure (3 bar) with 0,269 kg/s reflooding rate
  - Rod power at 3.3 kW
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Bundle Configuration

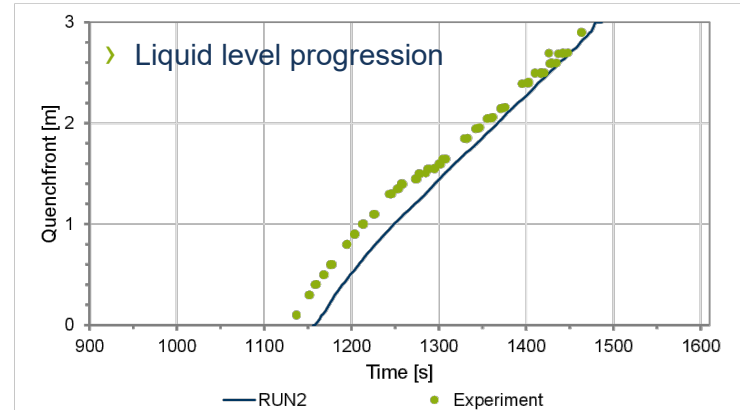
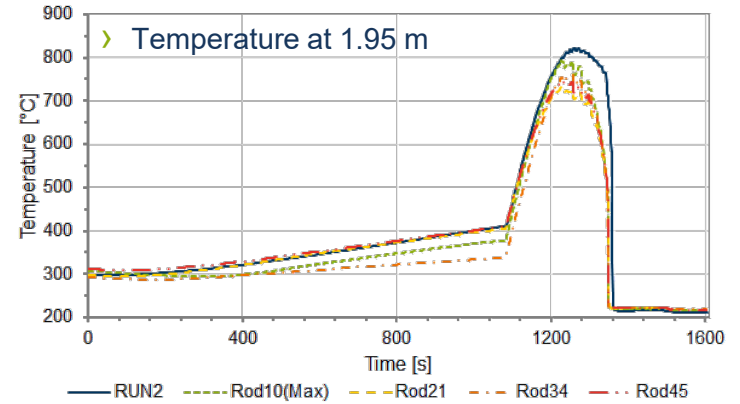
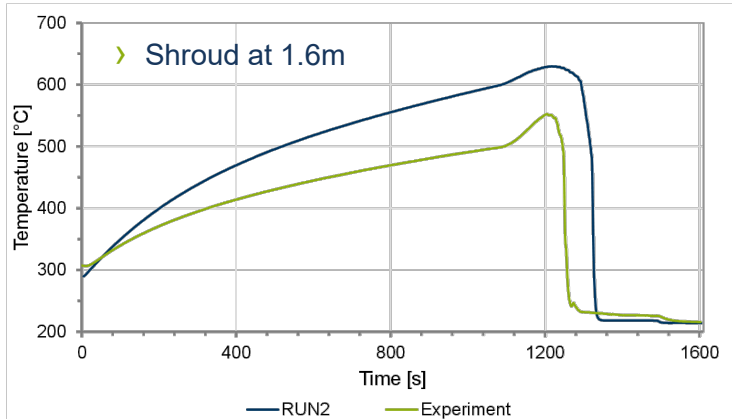
## B0-03-50 key events visualized



# RESULTS

## B0-20-17: Selected Results

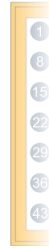
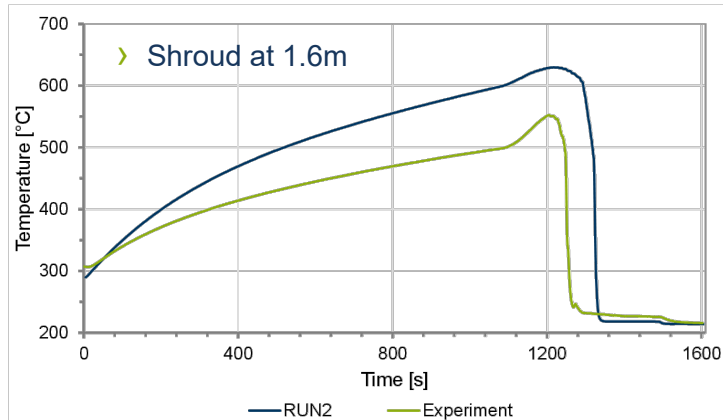
- Scenario at higher pressure (20 bar) and lower reflooding rate (0,089 kg/s)
  - Lower rod power at 2 kW
  - Bundle is fully quenched
  - Rod temperatures reach max. 820°C



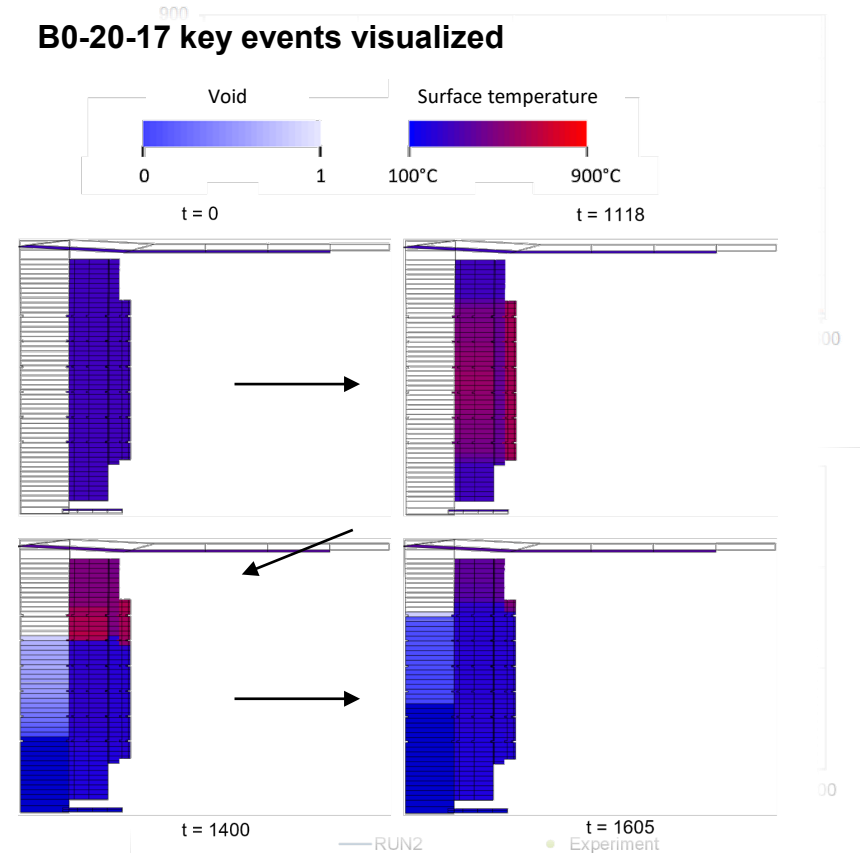
# RESULTS

## B0-20-17: Selected Results

- Scenario at higher pressure (20 bar) and lower reflooding rate (0,089 kg/s)
  - Lower rod power at 2 kW
  - Bundle is fully quenched
  - Rod temperatures reach max. 930°C



## B0-20-17 key events visualized



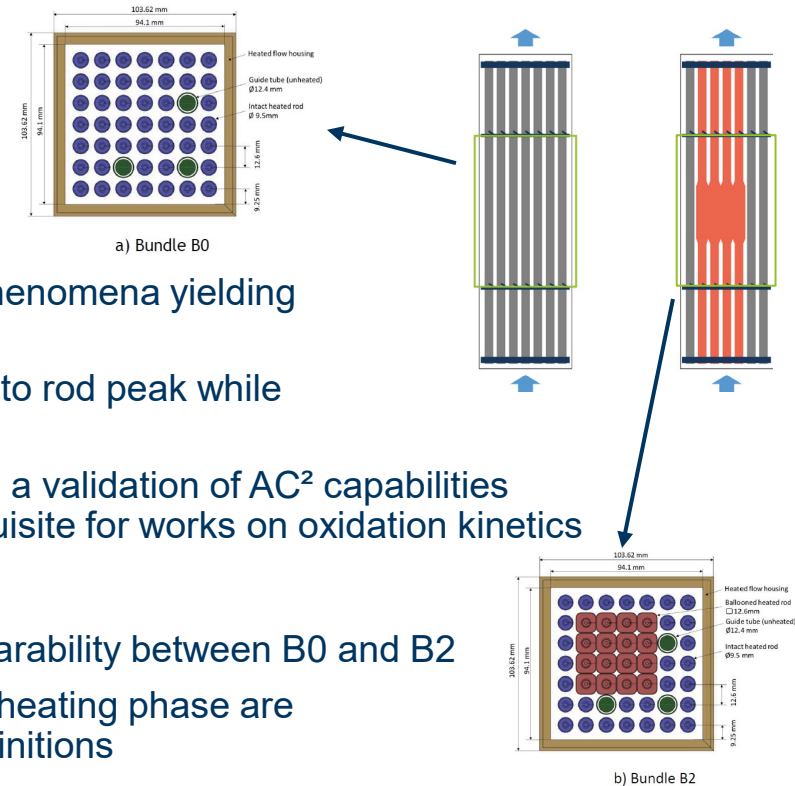
# SUMMARY

## ■ Simulation Results

- Transient Response: ATHLET captures key physical phenomena yielding plausible behaviour throughout the reflooding phase
- Steady-State Agreement: Satisfactory agreement prior to rod peak while deviations are observed during the heating phase
- Like Quench-Experiments, these experiments serve as a validation of AC<sup>2</sup> capabilities to predict cladding temperatures accurately – a prerequisite for works on oxidation kinetics

## ■ Modelling Strategy & Outlook

- The current nodalization is maintained to ensure comparability between B0 and B2
- Model Refinement: The observed discrepancies in the heating phase are identified as limitations of the 1D-approach and BC definitions
- Investigating a multi-channel model (parallel channels) is recommended to investigate to possibly improve the radial temperature profile; additionally, sensitivity studies regarding shroud heater positioning and initial BC are advised to further enhance accuracy



# REFERENCES

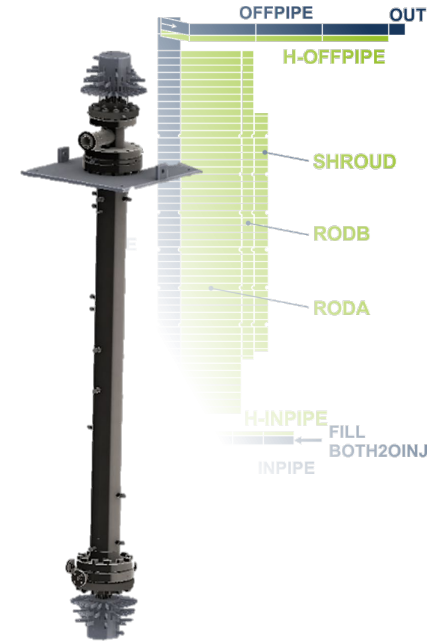
- [NEA24] Nuclear Energy Agency: *WGAMA ISP-53*, 2025, Available at: [https://www.oecdnea.org/jcms/pl\\_92672/wgama-isp-53](https://www.oecdnea.org/jcms/pl_92672/wgama-isp-53)
- [REP15] Repetto, G., et al.: *The R&D PERFROI project on Thermal mechanical and thermal hydraulics behaviors of a fuel rod assembly during a Loss Of Coolant Accident*, NURETH-16, American Nuclear Society, Chicago (IL), 2015.
- [REP17] Repetto, G., et al.: *Core Coolability in loss of coolant accident: the coal experiments investigating the thermal hydraulics of a rod bundle with blocked area during the reflooding*, NURETH-17, American Nuclear Society, Xi'an, China, 2017.
- [REP22] Repetto, G., et al.: *COAL Experiments investigating the reflooding of a 7 x 7 rods bundle during a loss of coolant accident thermalhydraulics results*, NURETH-19, Brüssel, Belgien, 2022.
- [REP23] Repetto, G., et al.: *COAL Experiments investigating the reflooding of a 7 x 7 rods bundle during a loss of coolant accident: effect of a partially blocked area with ballooned rods*, NURETH-20, Washington, USA, 2023.
- [REP24] Repetto, G., et al.: *COAL reflooding experiments during a loss of coolant accident: Effect of the water flow rate, the pressure and the rod power with ballooned rods*. Nuclear Engineering and Design, Volume 429, 2024.

# ACKNOWLEDGEMENT

This work was carried out within the framework of the WGAMA WGFS ISP-53, whose support and collaboration have been instrumental in the successful completion of this research.

Responsibility for the content lies with the authors.

The results were obtained using the GRS software package AC<sup>2</sup> 2023.





**RUB**

**Thank you for your attention!**

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**Liviusz Lovasz**

GRS

### **Validation of AC2/ATHLET using QUENCH data**

The QUENCH experimental series has been used to validate the severe accident code AC2/ATHLET-CD, which is developed by GRS, for multiple decades. Due to recent strategic decisions, the AC2 subprograms (ATHLET, ATHLET-CD and COCOSYS) have been further unified, particularly the ATHLET thermohydraulic subprogram and the ATHLET-CD severe accident phenomena subprogram. This unified code version of ATHLET and ATHLET-CD offers benefits to users and developers alike. However, to ensure that the refactoring and recent new developments comply with AC2's quality assurance policies, the new unified code version must be extensively validated. The first step towards fully validating the unified code version was to simulate and analyze the QUENCH-L0 experiment in detail, and the results are presented at the 30th QUENCH Workshop. Model specifications and potential future development needs are also discussed.





# Validation of AC2/ATHLET using QUENCH data

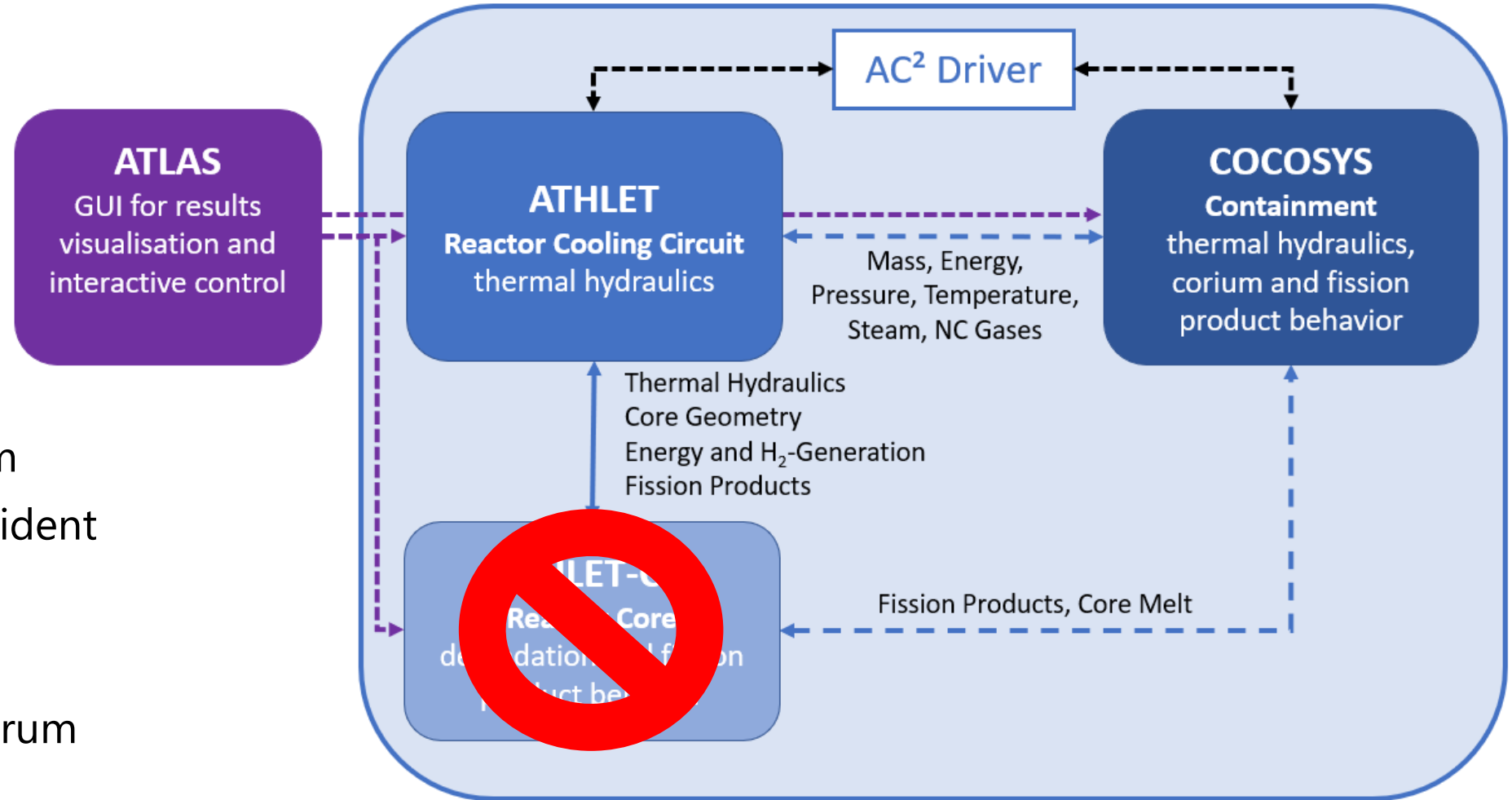
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Liviusz Lovasz, GRS

30<sup>th</sup> International QUENCH Workshop, Karlsruhe, 16-18.12.2025

# What is AC<sup>2</sup>?

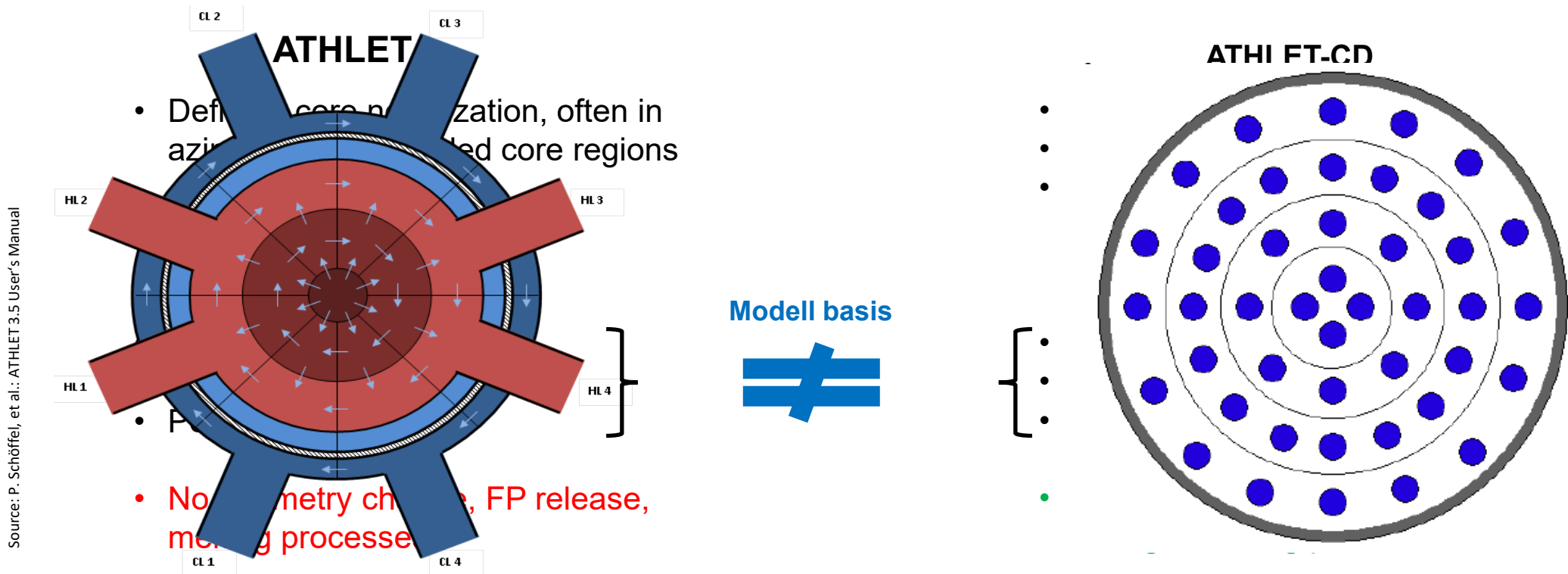
- AC<sup>2</sup>:
  - ATHLET
  - ATHLET-CD
  - COCOSYS
- Deterministic system code system for accident analysis
- Covers a wide spectrum of phenomena



# Using ATHLET-CD (up until now)

- Creating an input deck from scratch for **ATHLET-CD**
- Changing an existing **ATHLET** input deck and adapting it to **ATHLET-CD**

## Simulation of the Core



## Recent development goals

- Review, refactor and transfer or newly develop ATHLET-CD models to ATHLET to cover:
  - Heat generation ✓
  - Heat radiation static ✓ + dynamic ✗
  - Oxidation ✓
  - Fuel deformation ✓
  - Fission product release and transport ✓
  - Structure melting ✓ and relocation ✗

## Overall goals

- Create flexibly usable simulation tool for severe accidents
  - Simple to use for the user
  - Simple to maintain and extend for the developer
- Focus is still on conventional nuclear applications
  - Gen III+ reactors
  - SMR-s
  - Research reactors
  - Spent fuel pools, interim storage

# Validation

- Significantly changed code
  - New models
  - New nodalization
- Validation required
  - QUENCH experiment series (among others) plays a big role
  - Step by step validation
    - DBA phenomena
    - BDBA phenomena

# Validation – QUENCH-L0

- Goal of the experiment
  - Investigate ballooning / bursting and hydriding
- Goal of modelling / validation:
  - Nodalization
  - Basic heat transfer
  - Oxidation
  - Ballooning and bursting

# QUENCH-L0 Experiment

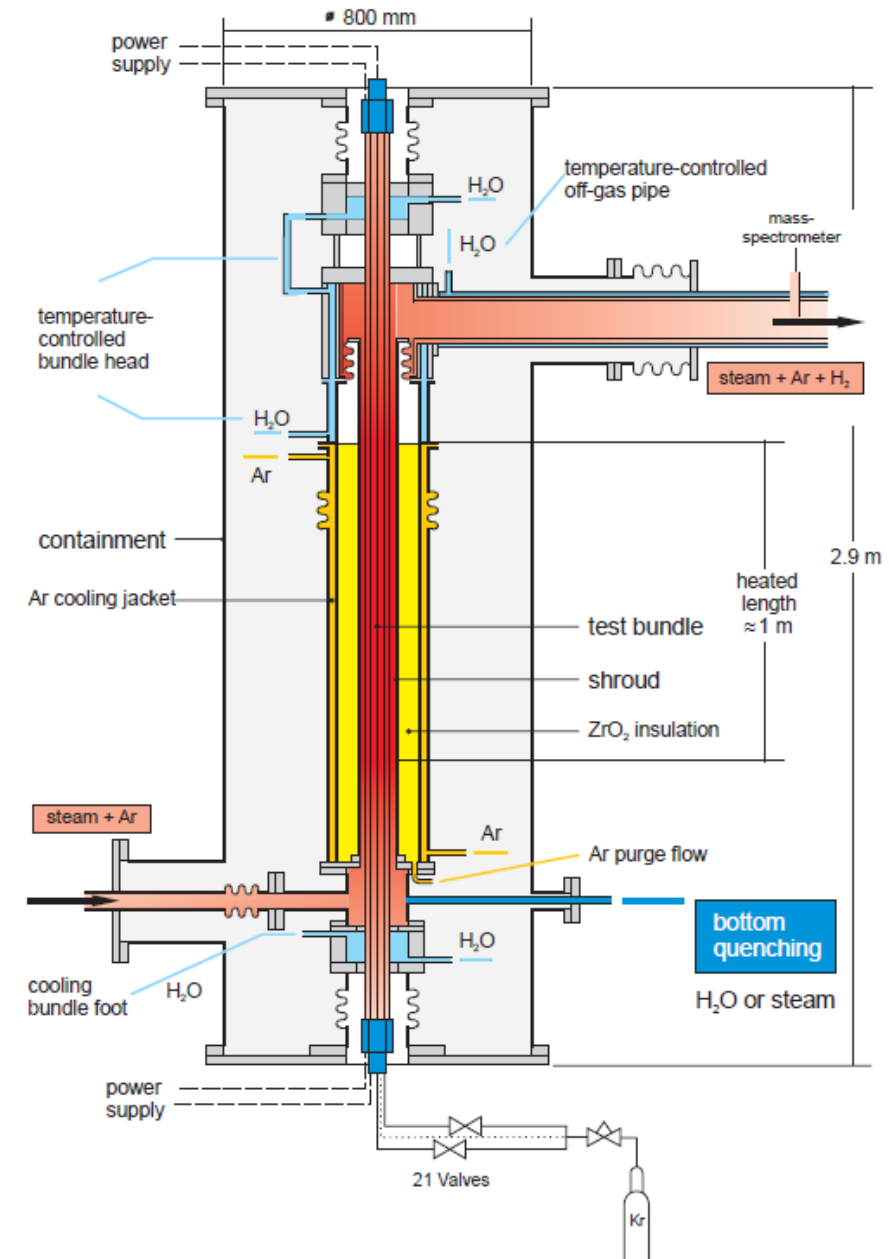
- 21 differently pressurized rod simulators with Zr-4 cladding
- Electrically heated
  - Rapid heating to 1070 °C
  - Bottom quenching



Map of bundle filling

Pressure, bar	Number of rods
<b>3 (system p)</b>	<b>1</b>
35	2
40	4
45	3
50	9
55	2

Source: J. Stuckert, M. Große, C. Rössger, M. Steinbrück, M. Walter, QUENCH - LOCA - REPORTS Nr. 1, Results of the commissioning bundle test QUENCH-L0 performed under LOCA conditions (SR-7571), KIT, 2015

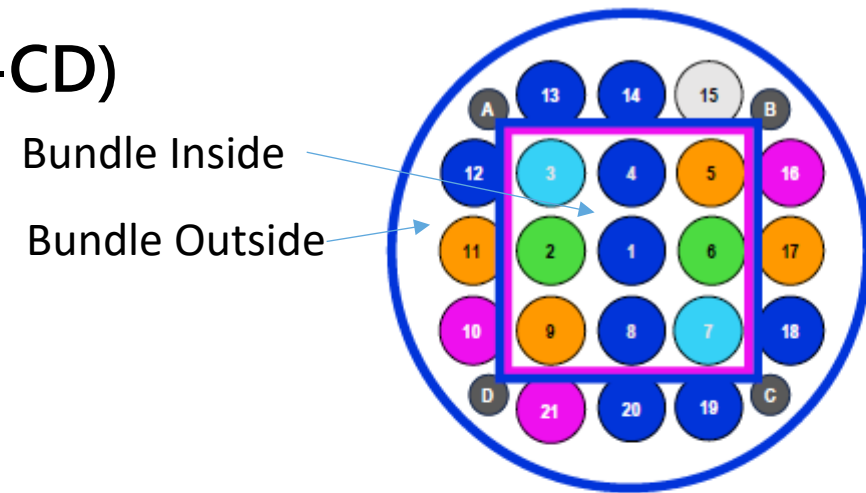


Source: J. Stuckert, M. Große, C. Rössger, M. Steinbrück, M. Walter, QUENCH - LOCA - REPORTS Nr. 1, Results of the commissioning bundle test QUENCH-L0 performed under LOCA conditions (SR-7571), KIT, 2015



# QUENCH-L0 Simulation – old (ATHLET-CD)

- Two thermohydraulic objects horizontally
  - 20 axial subdivision, cross connection
- Rods grouped in 9 segments
  - Based on their initial pressure
  - Pressure evolution not calculated
    - Via user signal implemented
  - Heat radiation incorrect
    - Heat radiation only from I to I-1 / I+1 Object
- Delivers acceptable results
  - Known flaws
  - Limitations



**Table 5. Rod model numbering**

Radial Position	Rod #, model	Rod Press., bar	Rod #, Experiment
Inner Bundle	1	50	1
	2	35	2, 6
	3	40	5, 9
	4	50	4, 8
	5	55	3, 7
Outer Bundle	6	3	15
	7	40	11, 17
	8	45	10, 16, 21
	9	50	12, 13, 14, 18, 19, 20

Source:

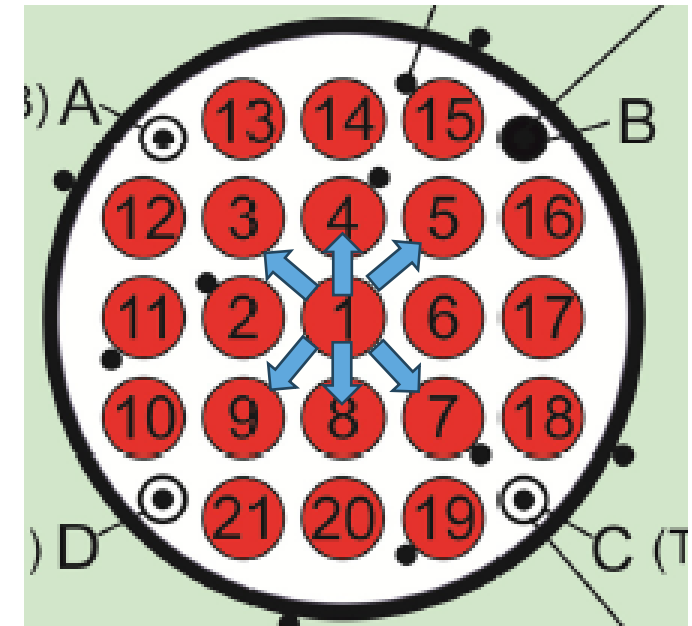
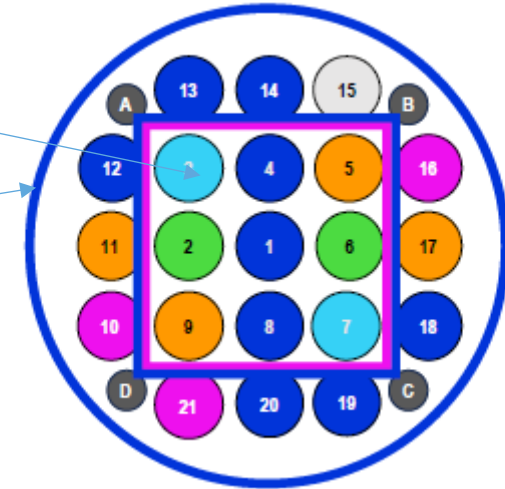
Di Nora, V. A.; Wielenberg, A.; Lovasz, L; Schöffel, P. J., Integration and Validation of Models for Thermal-Mechanical Behaviour of Nuclear Fuel Rods in ATHLET, *Annals of Nuclear Energy* Volume 227, Part A, February 2026, 111915

# QUENCH-L0 Simulation – new (ATHLET+)

- Two thermohydraulic objects horizontally
  - 20 axial subdivision, cross connection
- Each rod modelled individually (21+4)
  - Pressure evolution **IS** calculated
    - Rod deformation, inclusive feedback to TH
    - Gap heat conductance
- Heat radiation between all objects calculated
  - Static, inclusive shroud

Bundle Inside

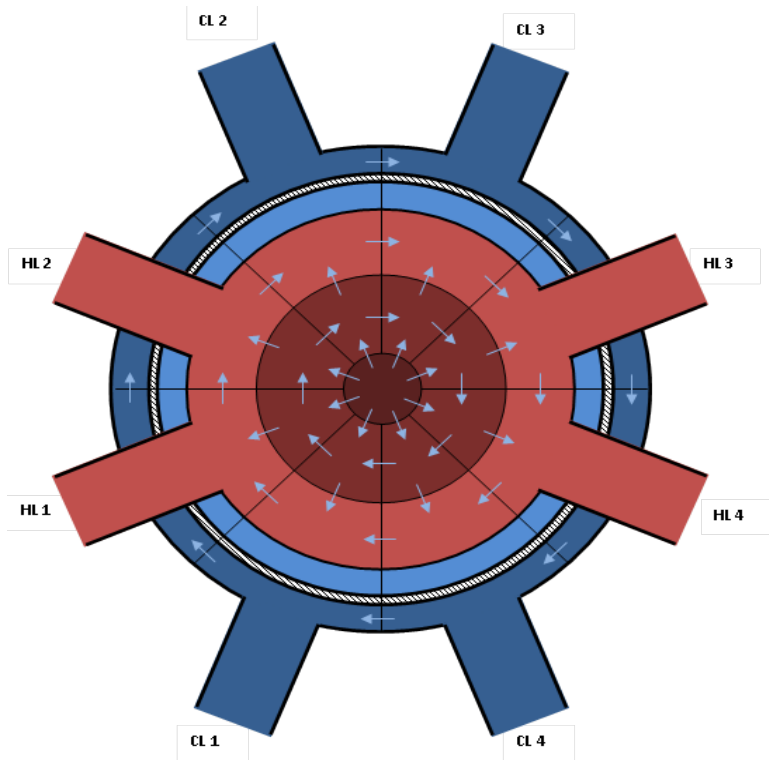
Bundle Outside



Source: J. Stuckert, M. Große, C. Rössger, M. Steinbrück, M. Walter, QUENCH - LOCA - REPORTS Nr. 1, Results of the commissioning bundle test QUENCH-L0 performed under LOCA conditions (SR-7571), KIT, 2015

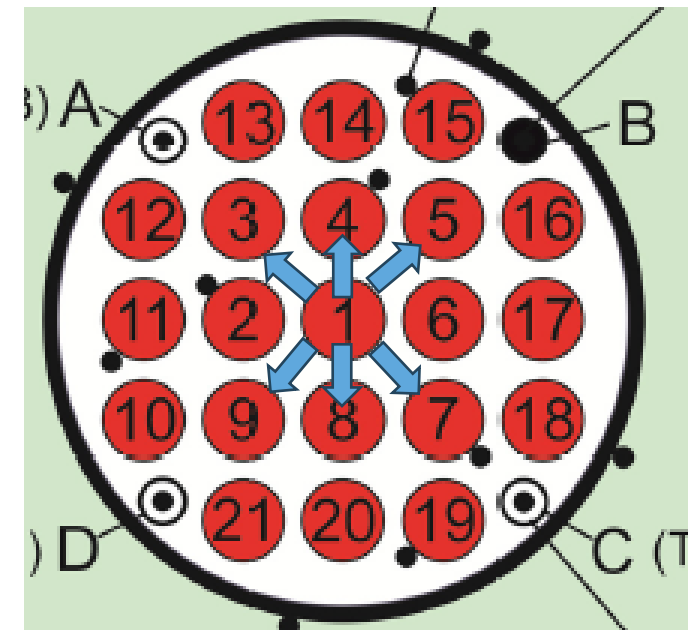
# QUENCH-L0 Simulation – new (ATHLET+)

- Detailed nodalisation too much?
- Standard DBA nodalization for LWR:
  - 2-3 "rings", azimuthal subdivision 4-8 ~ 25



Source: P. Schöffel, et al.: ATHLET 3.5 User's Manual

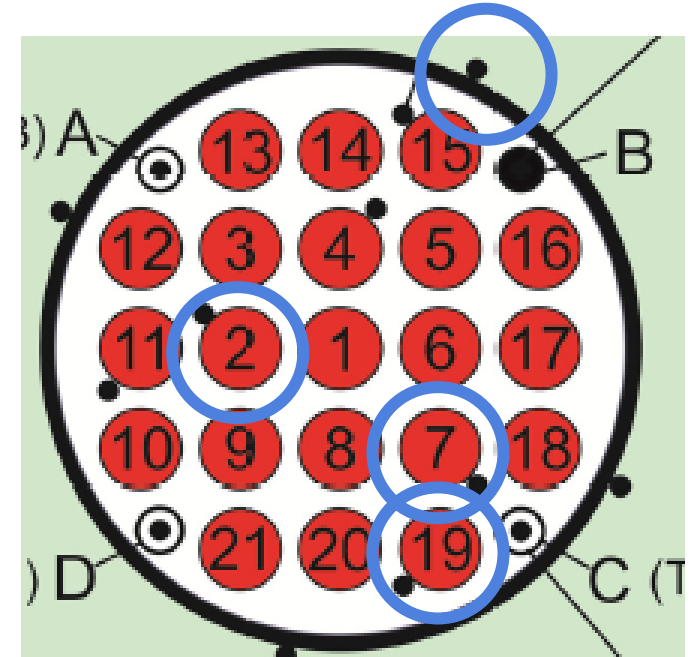
- QUENCH L0 nodalization
- 21+4+1 objects = 26



Source: J. Stuckert, M. Große, C. Rössger, M. Steinbrück, M. Walter, QUENCH - LOCA - REPORTS Nr. 1, Results of the commissioning bundle test QUENCH-L0 performed under LOCA conditions (SR-7571), KIT, 2015

# QUENCH-L0 Simulation – new (ATHLET+)

- Analysed at:
  - Elevation 950 mm for Rod 2, 19 + Shroud
  - Elevation 450 mm for Rod 7
  - Pressure of Rod 2, 19
  - Burst times
  - Strain

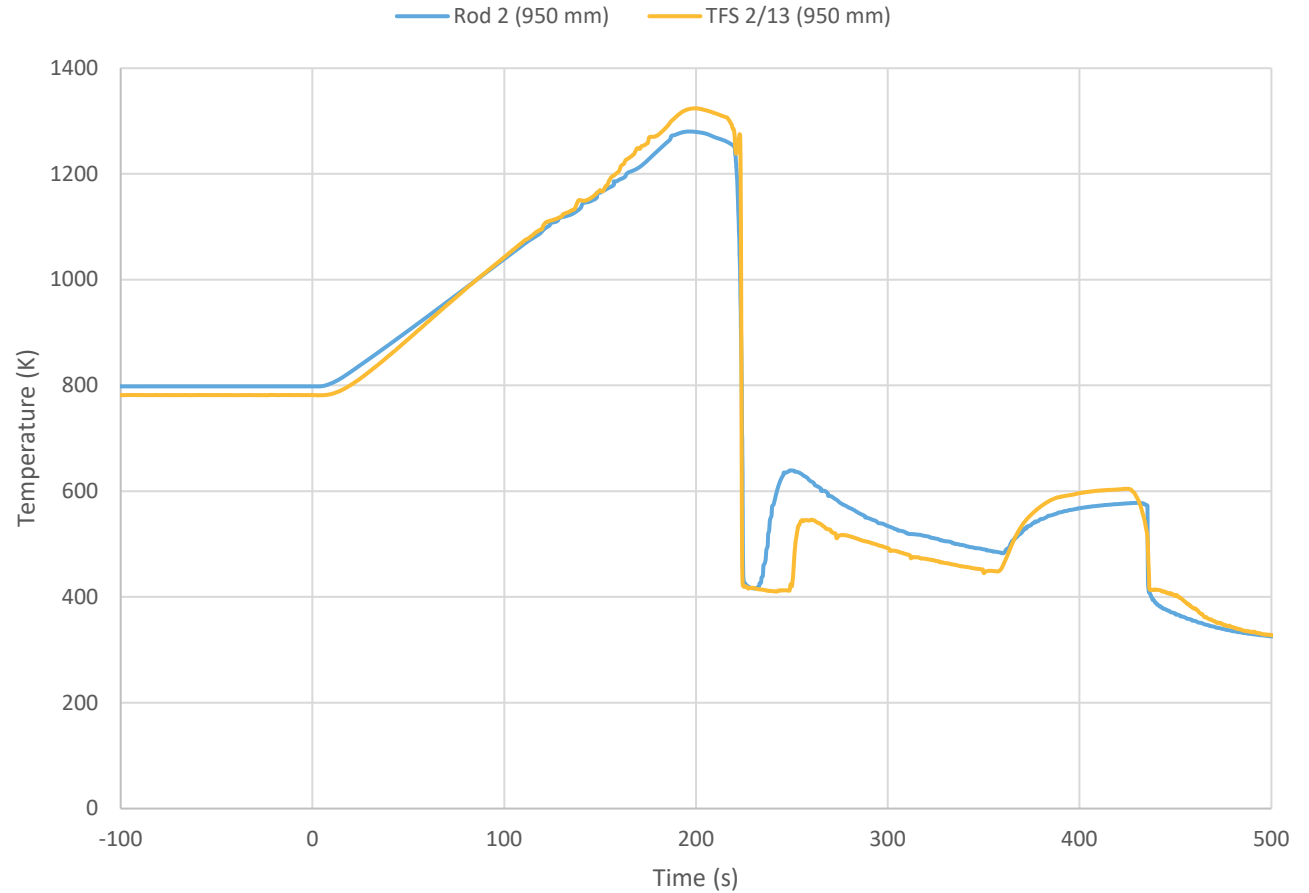
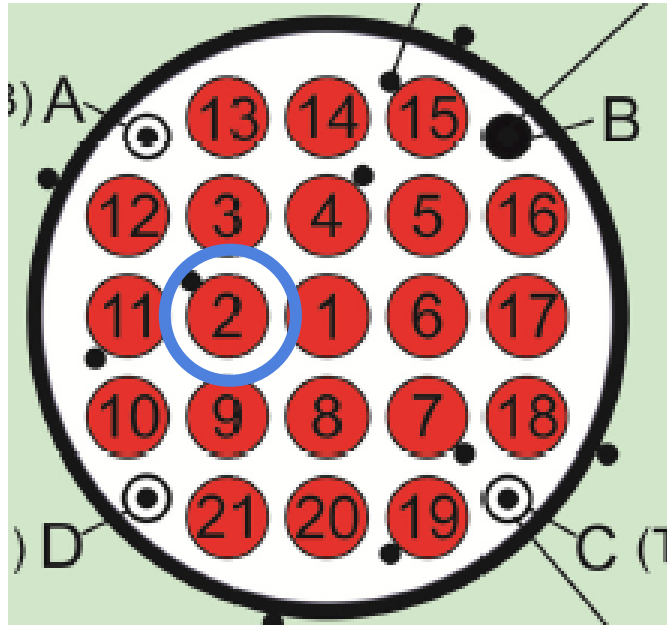


Source: J. Stuckert, M. Große, C. Rössger, M. Steinbrück, M. Walter, QUENCH - LOCA - REPORTS Nr. 1, Results of the commissioning bundle test QUENCH-L0 performed under LOCA conditions (SR-7571), KIT, 2015

# QUENCH-L0 Simulation – new (ATHLET+)

- Rod 2 elevation (950 mm):
  - Good agreement with measurement
  - Slight underestimation before quench
  - Qualitative similarity after quench
    - Faster dryout after quench

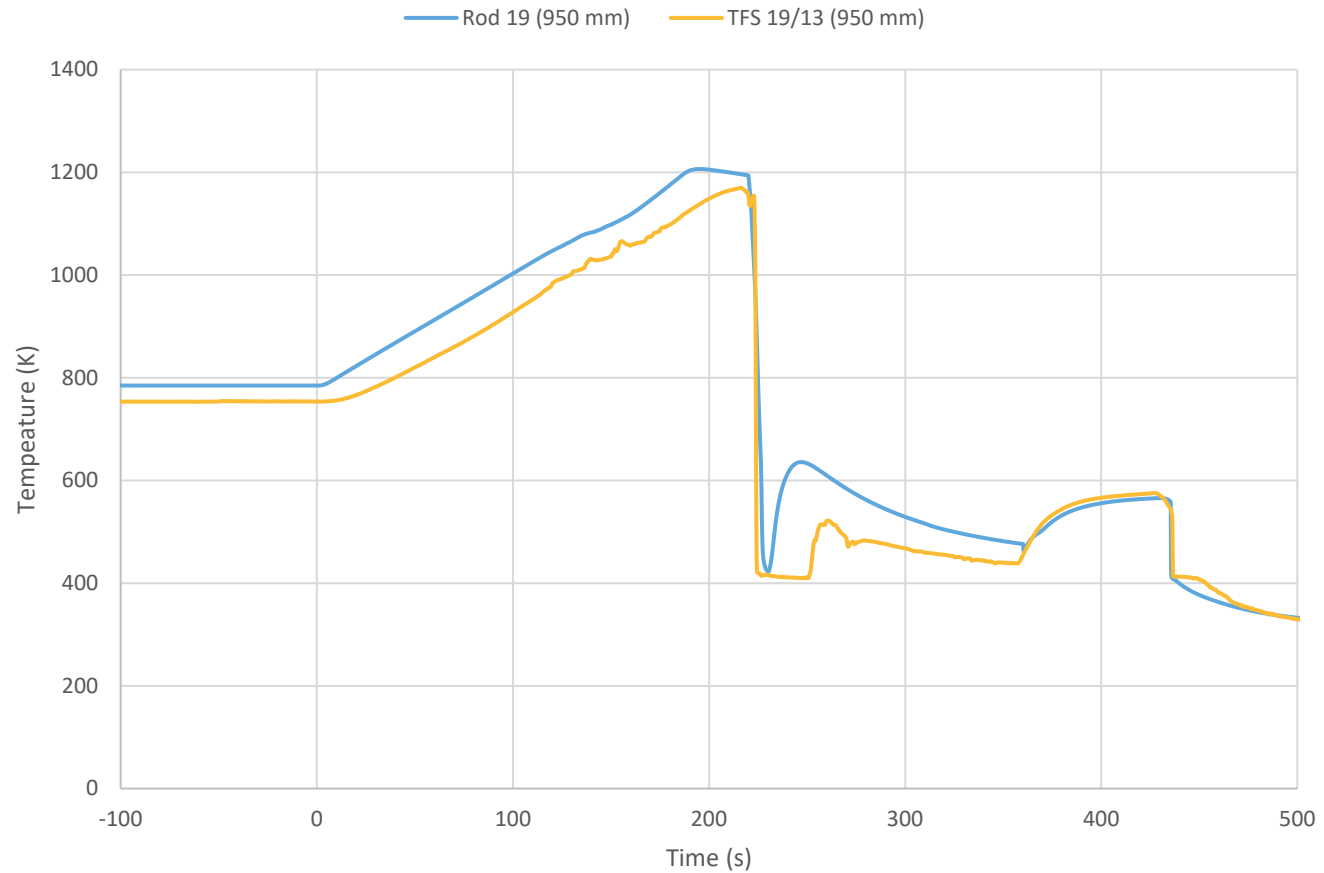
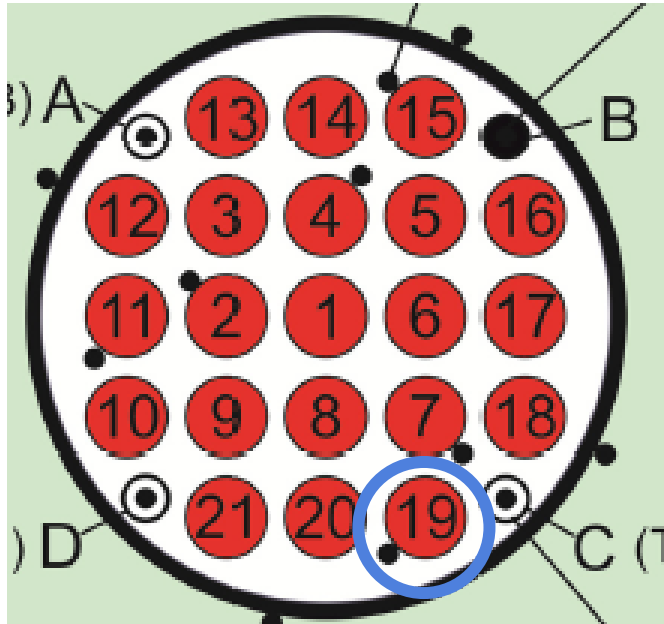
Source: J. Stuckert, M. Große, C. Rössger, M. Steinbrück, M. Walter,  
 QUENCH - LOCA - REPORTS Nr. 1, Results of the commissioning  
 bundle test QUENCH-L0 performed under LOCA conditions (SR-  
 7571), KIT, 2015



# QUENCH-L0 Simulation – new (ATHLET+)

- Rod 19 elevation (950 mm):
  - Similar qualitatively to Rod 2
  - Overestimation of temperatures
    - Location of TC

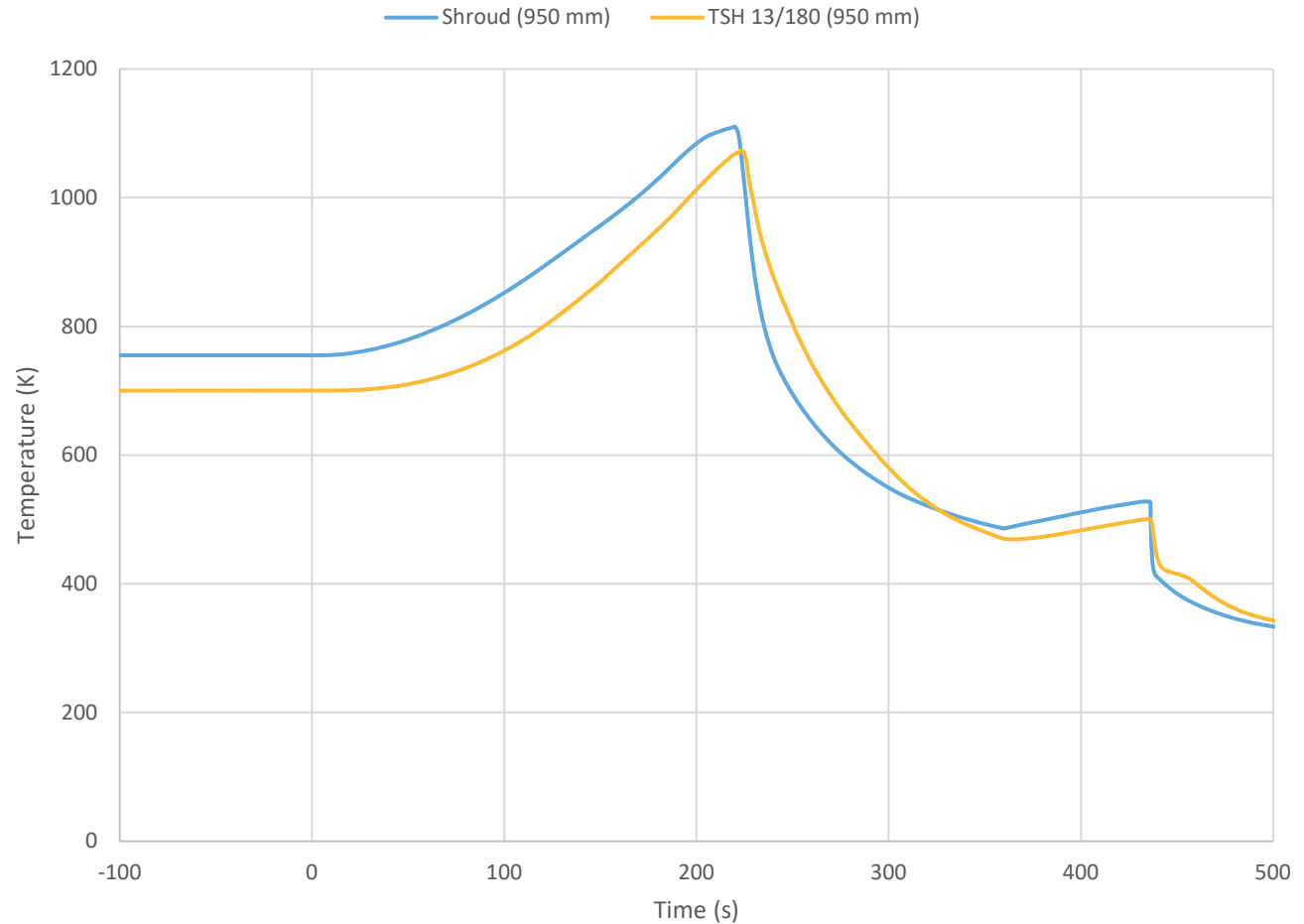
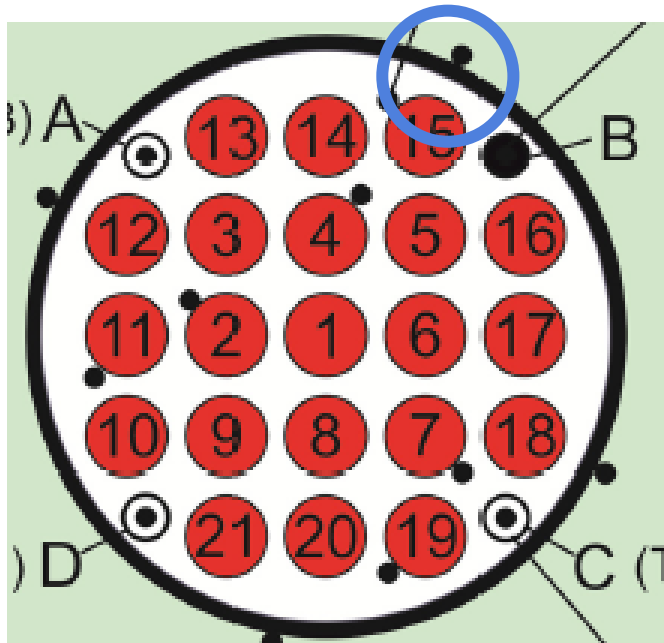
Source: J. Stuckert, M. Große, C. Rössger, M. Steinbrück, M. Walter, QUENCH - LOCA - REPORTS Nr. 1, Results of the commissioning bundle test QUENCH-L0 performed under LOCA conditions (SR-7571), KIT, 2015



# QUENCH-L0 Simulation – new (ATHLET+)

- Shroud elevation (950 mm):
  - Temperature overestimation
  - Cooling process well replicated

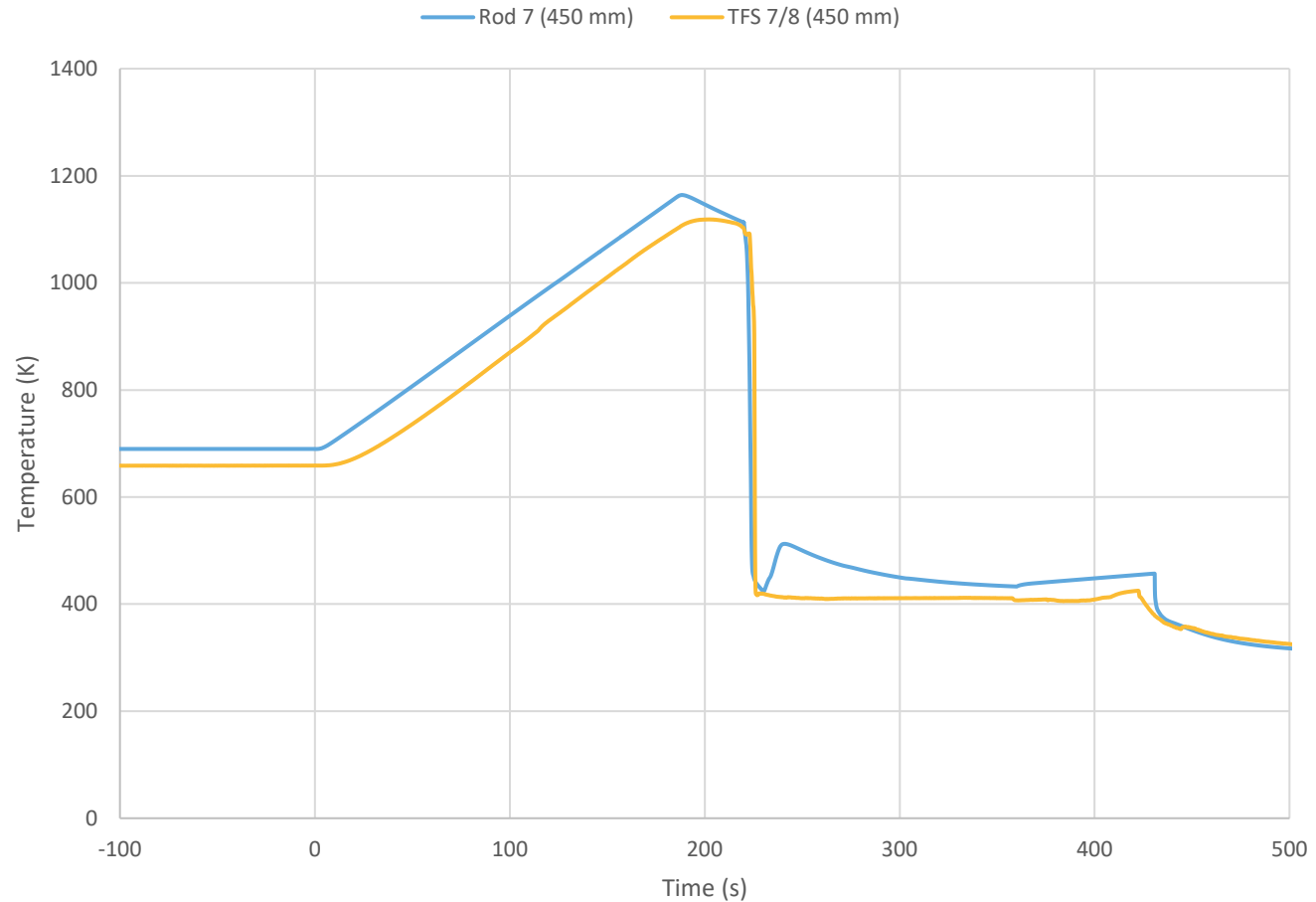
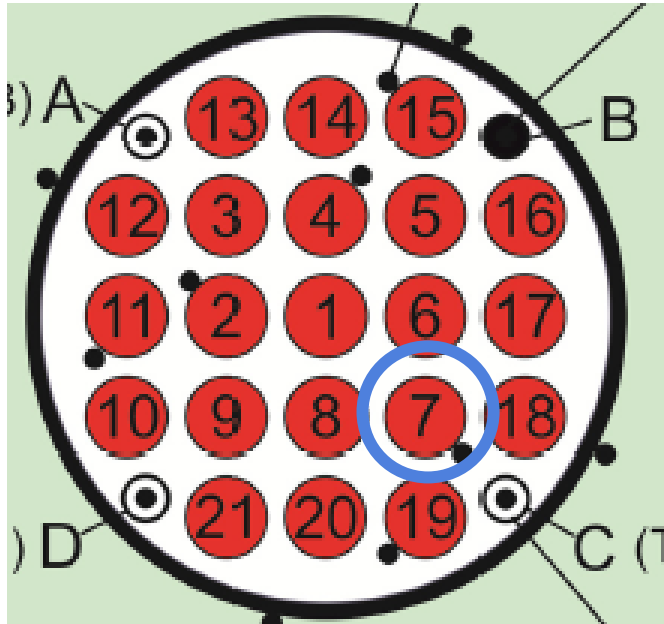
Source: J. Stuckert, M. Große, C. Rössger, M. Steinbrück, M. Walter,  
 QUENCH - LOCA - REPORTS Nr. 1, Results of the commissioning  
 bundle test QUENCH-L0 performed under LOCA conditions (SR-  
 7571), KIT, 2015



# QUENCH-L0 Simulation – new (ATHLET+)

- Rod 7 elevation 450 mm:
  - Overestimation until quenching

Source: J. Stuckert, M. Große, C. Rössger, M. Steinbrück, M. Walter,  
 QUENCH - LOCA - REPORTS Nr. 1, Results of the commissioning  
 bundle test QUENCH-L0 performed under LOCA conditions (SR-  
 7571), KIT, 2015

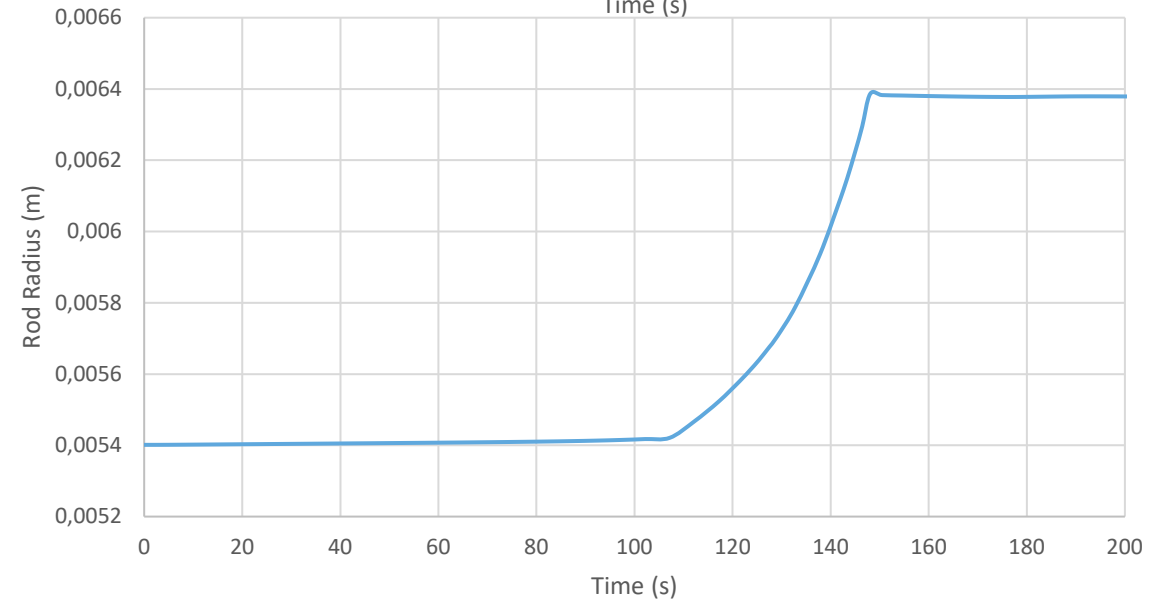
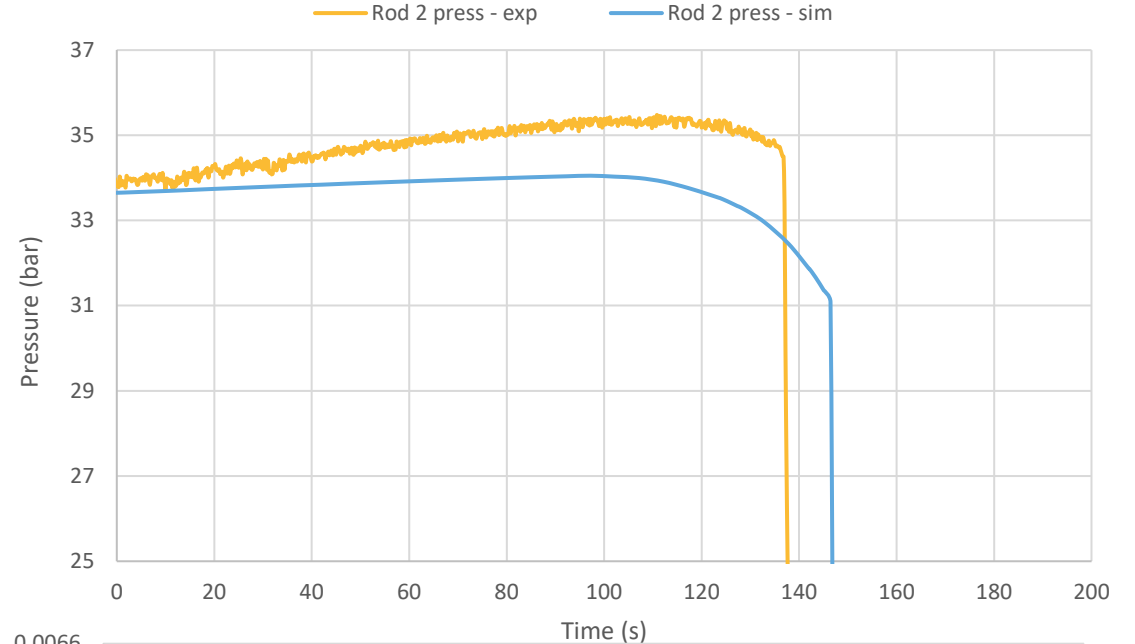
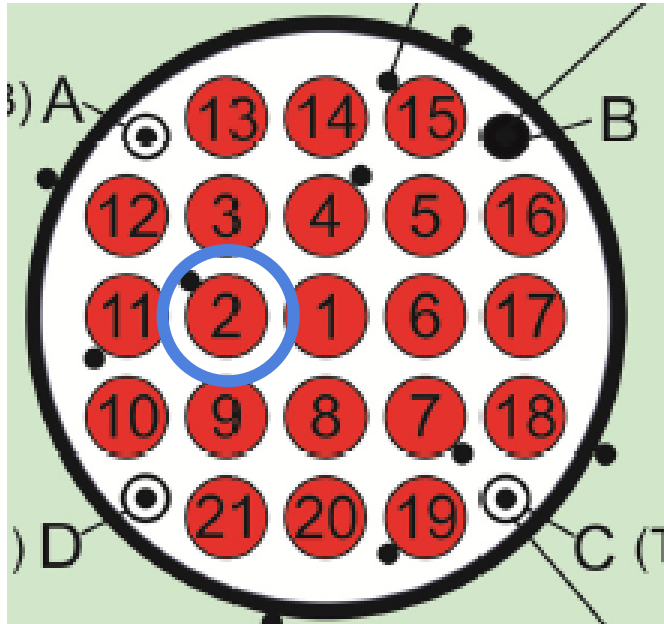




# QUENCH-L0 Simulation – new (ATHLET+)

- Rod 2 pressure:
  - Smaller increase of internal pressure
  - Burst time well predicted
  - Increase of rod diameter

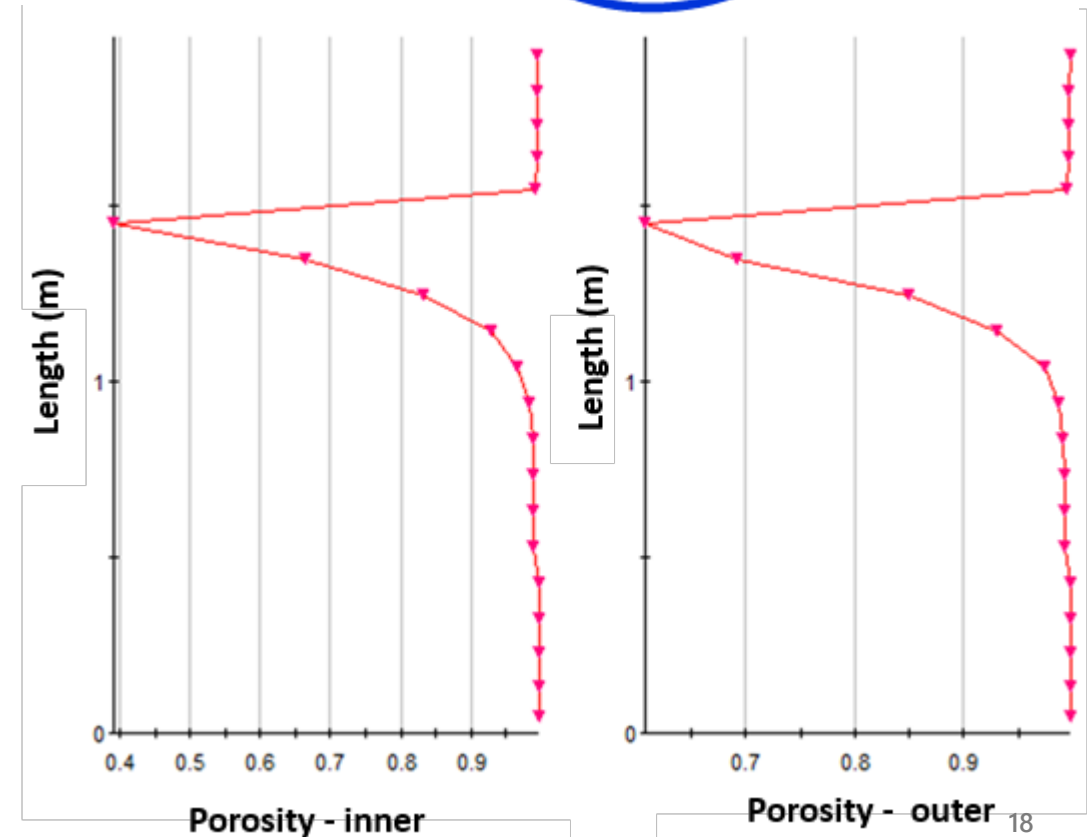
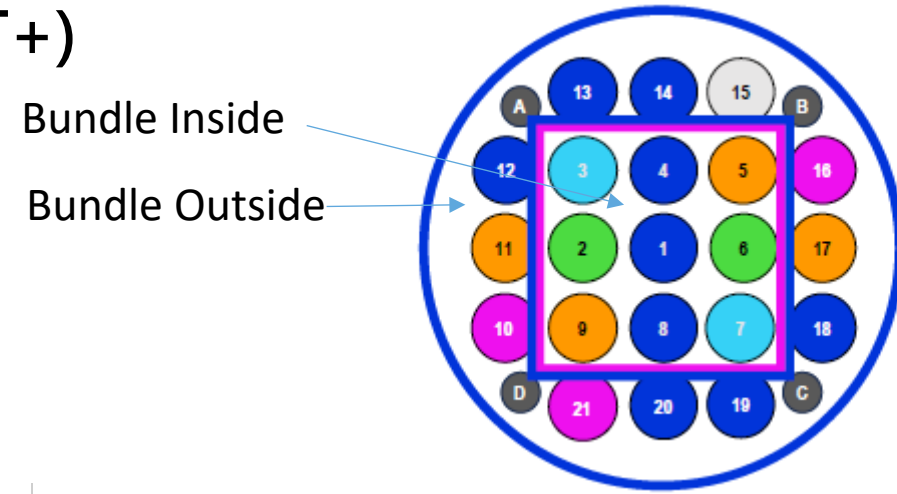
Source: J. Stuckert, M. Große, C. Rössger, M. Steinbrück, M. Walter, QUENCH - LOCA - REPORTS Nr. 1, Results of the commissioning bundle test QUENCH-L0 performed under LOCA conditions (SR-7571), KIT, 2015



# QUENCH-L0 Simulation – new (ATHLET+)

Feedback on the thermohydraulics

- Overall blockage of the channel: 53% (sim.)
- All ballooning at the same elevation (nodalization dependent)
- Experimental data if all ballooning happened at the same elevation: 46% (exp.)



# QUENCH-L0 Simulation – new (ATHLET+)

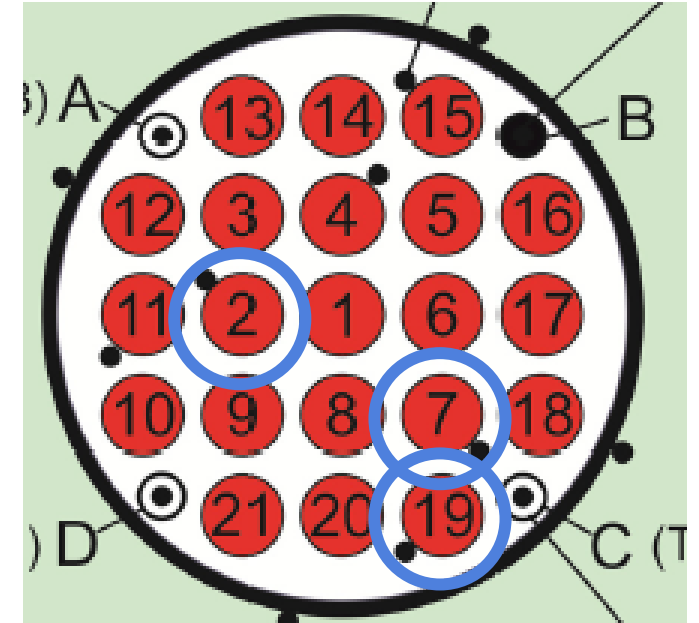
Cause of burst is strain limit: 38%

- Relative good agreement
- Burst times good agreement
- Overall H<sub>2</sub> production underestimated
  - No burst oxidation
  - Temperature at lower elevation underestimated

	Exp. Strain (%)	Sim. Strain (%)
Rod 2	33.8	~38
Rod 19	27.2	~38
Rod 7	40.0	~38

	Exp. Burst Time (s)	Sim. Burst Time (s)
Rod 2	136.8	146
Rod 19	159.6	157
Rod 7	114.2	123

	Exp. Hydrogen gen (g)	Sim. Hydrogen gen (g)
Rod 2	1	0.7



Source: J. Stuckert, M. Große, C. Rössger, M. Steinbrück, M. Walter, QUENCH - LOCA - REPORTS Nr. 1, Results of the commissioning bundle test QUENCH-L0 performed under LOCA conditions (SR-7571), KIT, 2015

## ATHLET+ Validation - Conclusions

- ATHLET+ incorporates and extends ATHLET-CD models
  - Focus of current development
    - DBA phenomena (qualitatively) covered
    - BDBA phenomena under development
- Due to significant modelling changes → Validation needed
- QUENCH LOCA L0 analysed
  - ATHLET input deck created
    - Eliminated old simplifications
  - Phenomena qualitatively covered
- More knowledge with ATHLET+ needed
- Further validation of DBA and BDBA phenomena

# Thank you for your attention!

The development and validation of AC<sup>2</sup>/ATHLET-CD are supported by the German Federal Ministry for the Environment, Climate Action, Nature Conservation and Nuclear Safety.

Supported by:



Federal Ministry  
for the Environment, Climate Action,  
Nature Conservation and Nuclear Safety

based on a decision of  
the German Bundestag



**Tadas Kaliatka**

LEI

## **Modeling of QUENCH-06 and QUENCH-20 tests with RELAP/SCDAPSIM, Focus on Bundle Asymmetry**

Reflooding of an overheated reactor core is a critical severe-accident management strategy, but it can intensify zirconium oxidation and hydrogen production, requiring detailed investigation of the reflood phase. The QUENCH integral tests, performed in Forschungszentrum Karlsruhe, provide valuable experimental data for studying these phenomena. In this work, the QUENCH-06 and QUENCH-20 experiments are simulated using the severe accident code RELAP/SCDAPSIM to evaluate key modeling approaches and benchmark code predictions against measured data.

Although both tests follow similar thermal–hydraulic transient and experimental phases, they differ significantly in bundle configuration. QUENCH-06 employs a symmetric, electrically heated fuel rod bundle, while QUENCH-20 features a strongly asymmetric configuration due to two absorber control blades positioned at two sides of a rectangular bundle. These differences significantly influence phenomenology and physical processes during these experiments. Also, it significantly influences modeling of physical processes. An additional difficulty for the numerical investigation is the fact that all severe accident codes are considering symmetry (bundle or core are modeled from the cylindrical coordination aspects).

To address this, three distinct component-level modeling strategies were developed to approximate the asymmetric QUENCH-20 geometry. The simulations are evaluated against key experimental parameters including bundle temperature evolution (claddings and shroud), oxidation behavior and hydrogen release. The results demonstrate notable differences in local thermal response and oxidation rates depending on the selected modeling approach, with no single method fully reproducing all measured phenomena. However, specific approaches show improved prediction of radial temperature gradients and hydrogen generation trends.

Based on the findings, practical recommendations are proposed for modeling asymmetry in severe accident codes, emphasizing best practices for nodalization, power distribution, and representation of absorber blade regions. The study highlights both the capabilities and limitations of RELAP/SCDAPSIM for asymmetric reflood scenarios and provides guidance for future modeling of complex core geometries.



LITHUANIAN  
ENERGY  
INSTITUTE

# Modeling of QUENCH-06 and QUENCH-20 tests with RELAP/SCDAPSIM, Focus on Bundle Asymmetry

Dr. Tadas Kaliatka, Dr. Noura Elsalamouny  
Lithuanian Energy Institute

30<sup>th</sup> International QUENCH Workshop  
2025-12-17



# Uncertainty and Sensitivity Analysis of QUENCH-03 and QUENCH-06 Experiments

T. Kaliatka, A. Kaliatka, V. Vileiniskis

*20th International QUENCH Workshop*



2017



## Modeling of QUENCH 10 and 16 Experiments on Air Ingress Using RELAP/SCDAPSIM mod 3.5

2016

[Tadas Kaliatka](#)

## Implementation of QUENCH-10 experiment modelling experience for the modelling of severe accidents in spent fuel pools

2017

[Tadas Kaliatka](#)

## Post-test calculation results of QUENCH experiments using different RELAP/SCDAPSIM Mod3.5 code versions

2018

[Tadas Kaliatka](#)

## Evaluation of the processes in the BWR and VVER spent fuel pools during severe accident conditions

2019

T. Kaliatka, A. Kaliatka, V. Vileiniskis

## Implementation of LEI experience on modeling and uncertainty quantification of QUENCH tests for the development of QUENCH-20 numerical model

Noura Elsalamouny, Tadas Kaliatka

2021



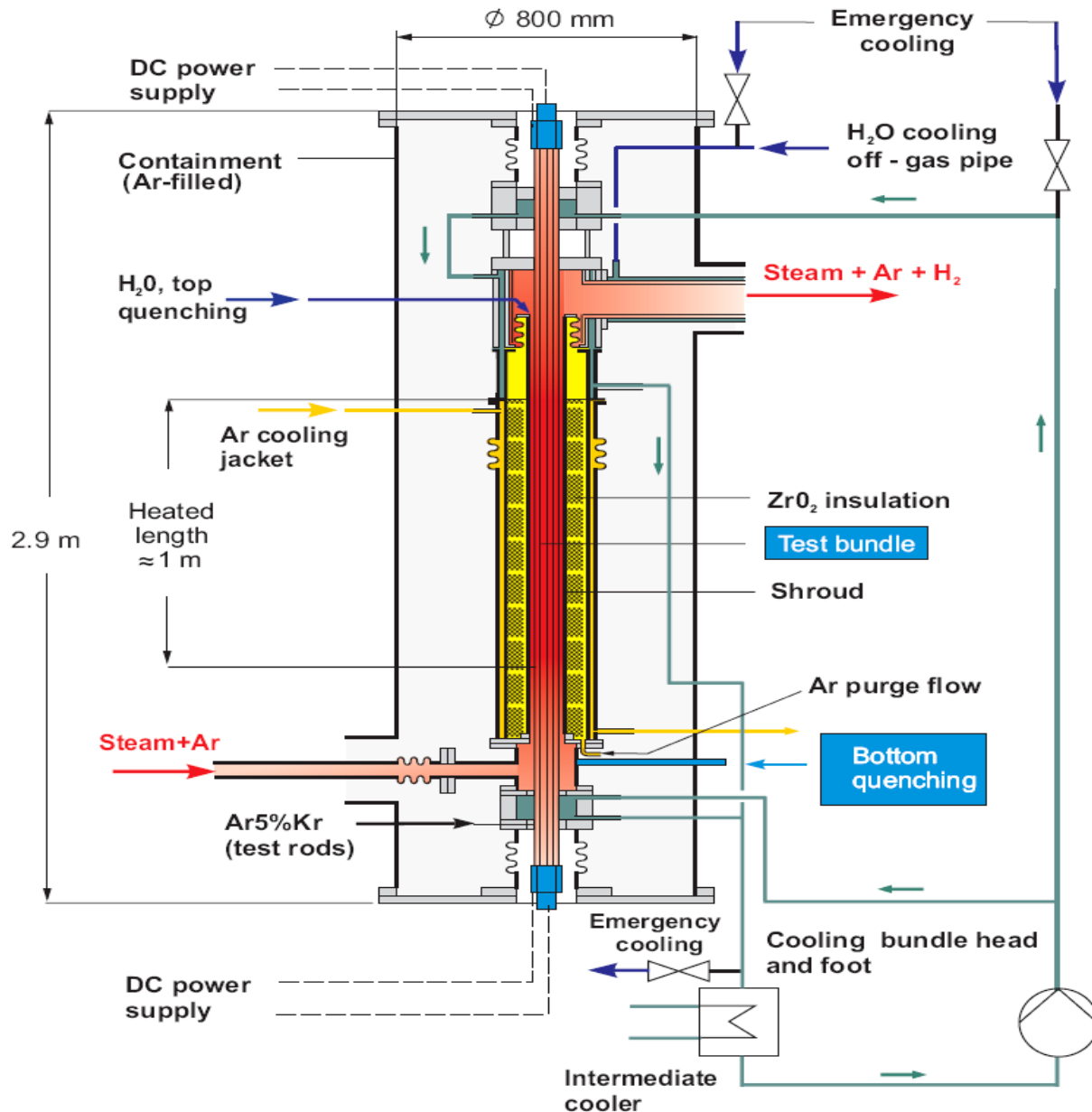
## Preliminary Modelling Results Of QUENCH-20 Test Using RELAP/SCDAPSIM code

[T. Kaliatka](#), [N. Elsalamouny](#) · Lithuanian Energy Institute

2022-09-27, 27th International QUENCH Workshop

2022

# QUENCH test

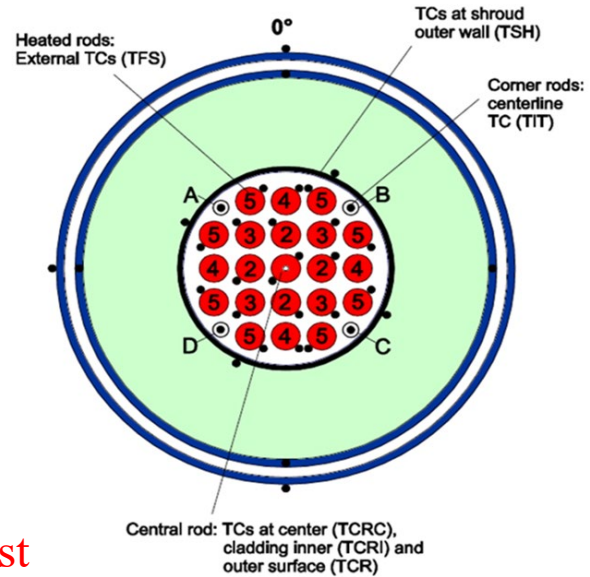


## QUENCH/LICAS facility

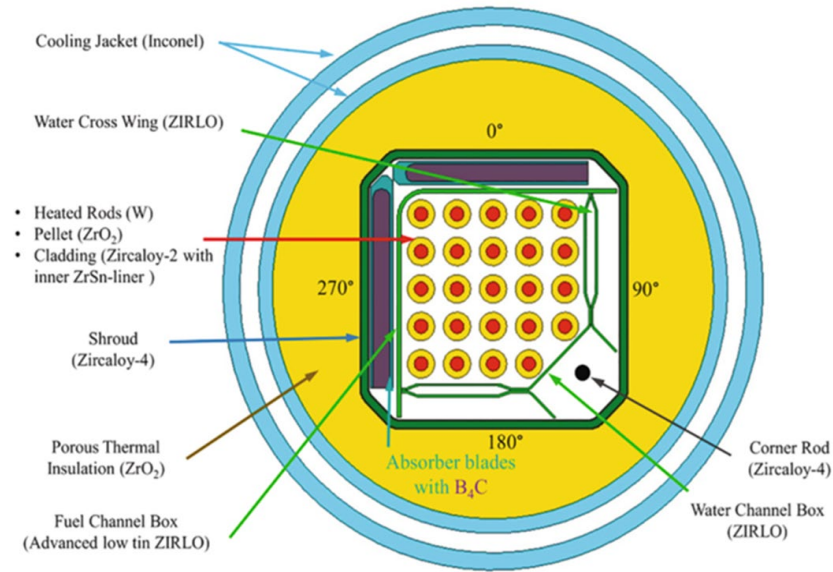
- Unique out-of-pile bundle facility to investigate reflood of an overheated reactor core
- 21-31 electrically heated fuel rod simulators; T up to  $>2000^\circ C$
- Extensive instrumentation for T, p, flow rates, level, etc. + MS
- So far, 20+1 experiments on SA performed (1996-today)
  - Influence of pre-oxidation, initial temperature, flooding rate
  - $B_4C$ , Ag-In-Cd control rods
  - Air ingress; debris formation
  - Advanced cladding alloys & ATF
- 7+1 DBA LOCA experiments with separately pressurized fuel rods

Focus on QUENCH-06 and especially on QUENCH-20

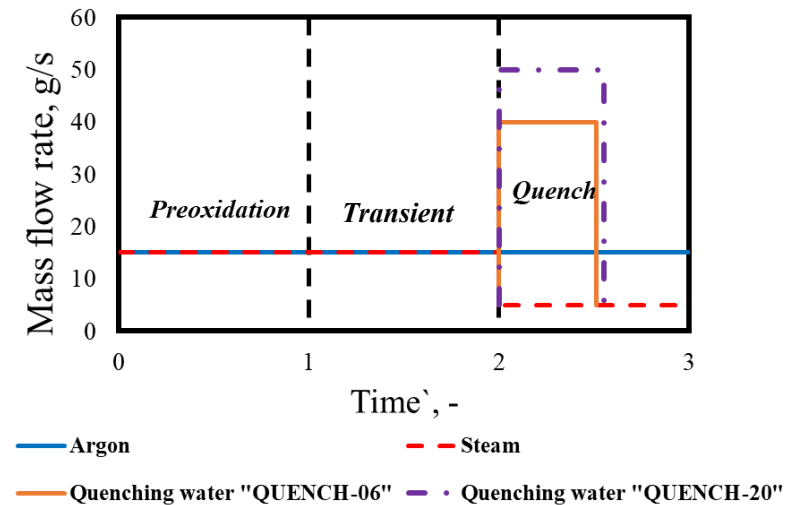
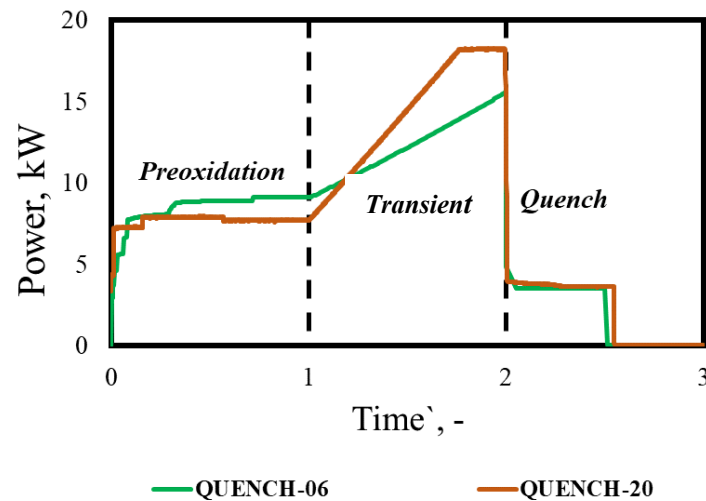
# Similarities and differences between QUENCH-06 and QUENCH-20



QUENCH-06 test



QUENCH-20 test



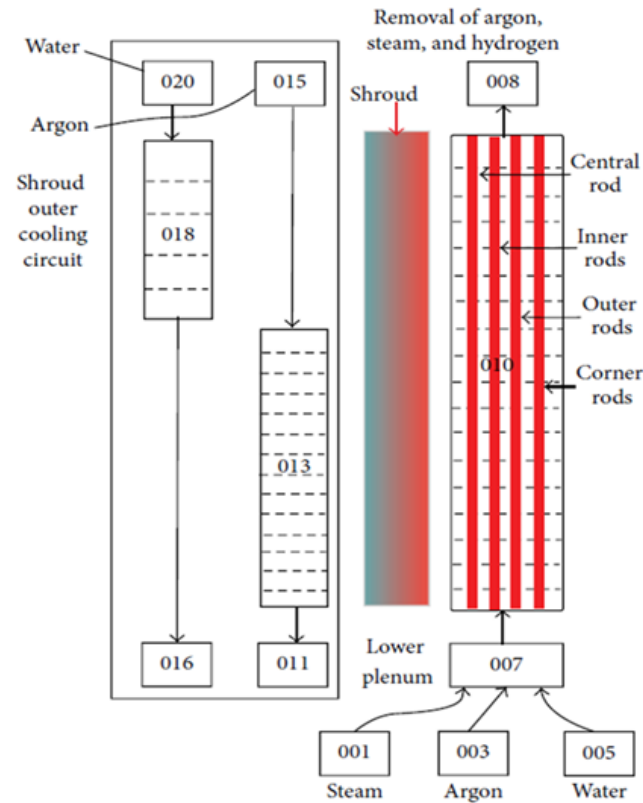
# Model development and Reference calculation

## QUENCH-06

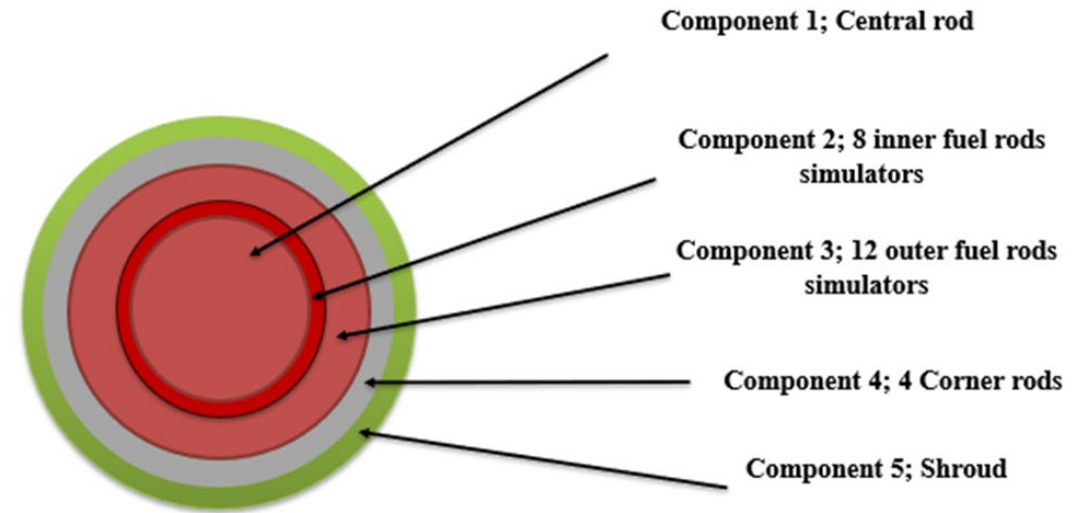


The Figures Of Merit (FOM's) for QUENCH-06

- Total hydrogen generation
- Cladding temperature



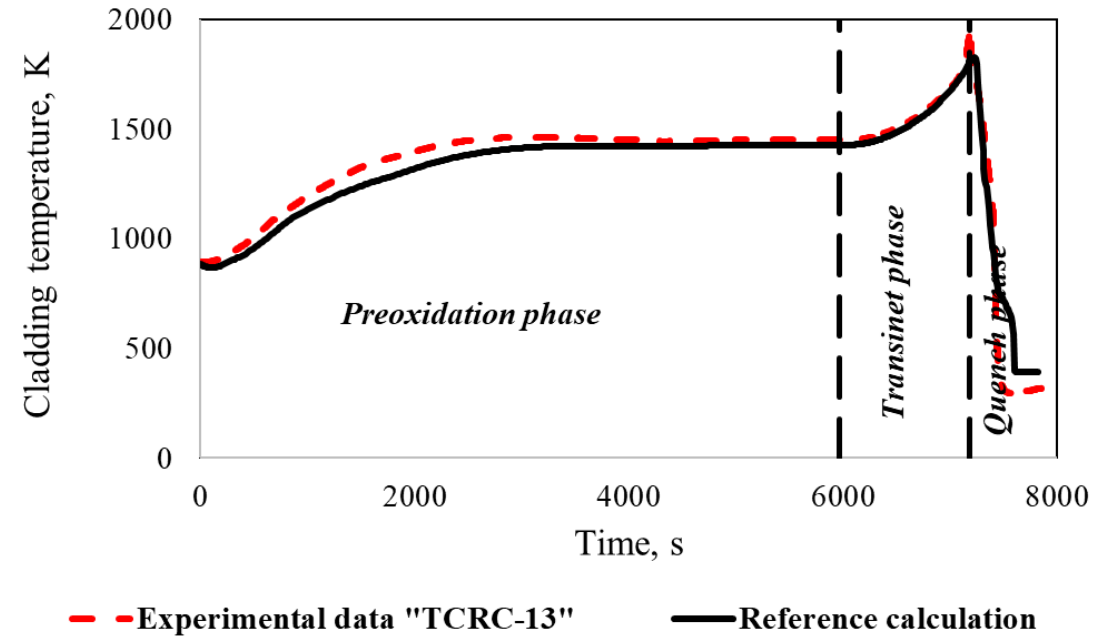
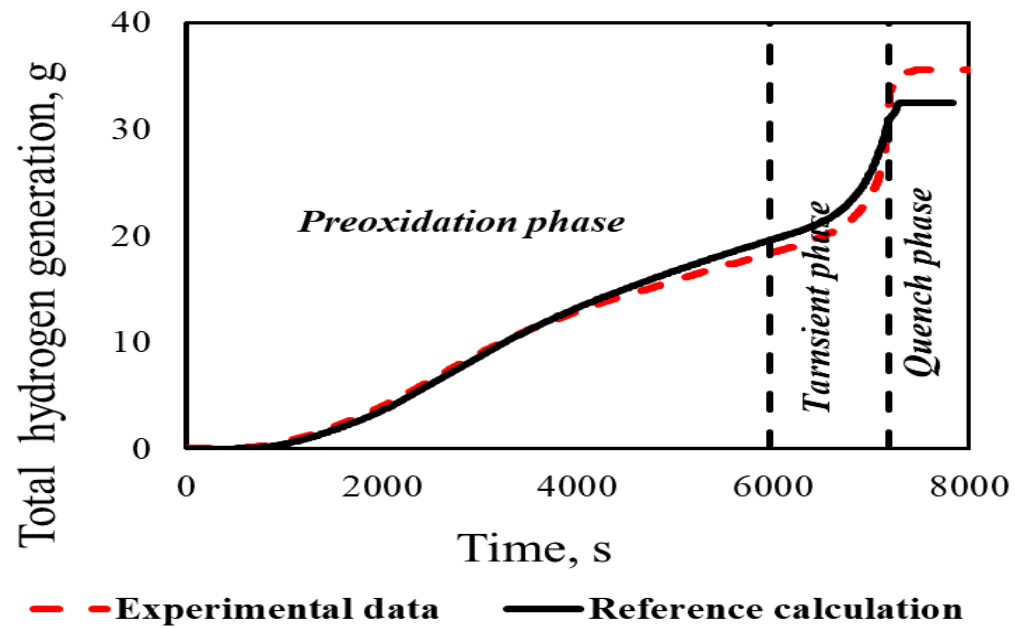
RELAP part



SCDAP part



# Reference calculation



950 mm from the bottom

# Application of BEPU approach

## Approaches

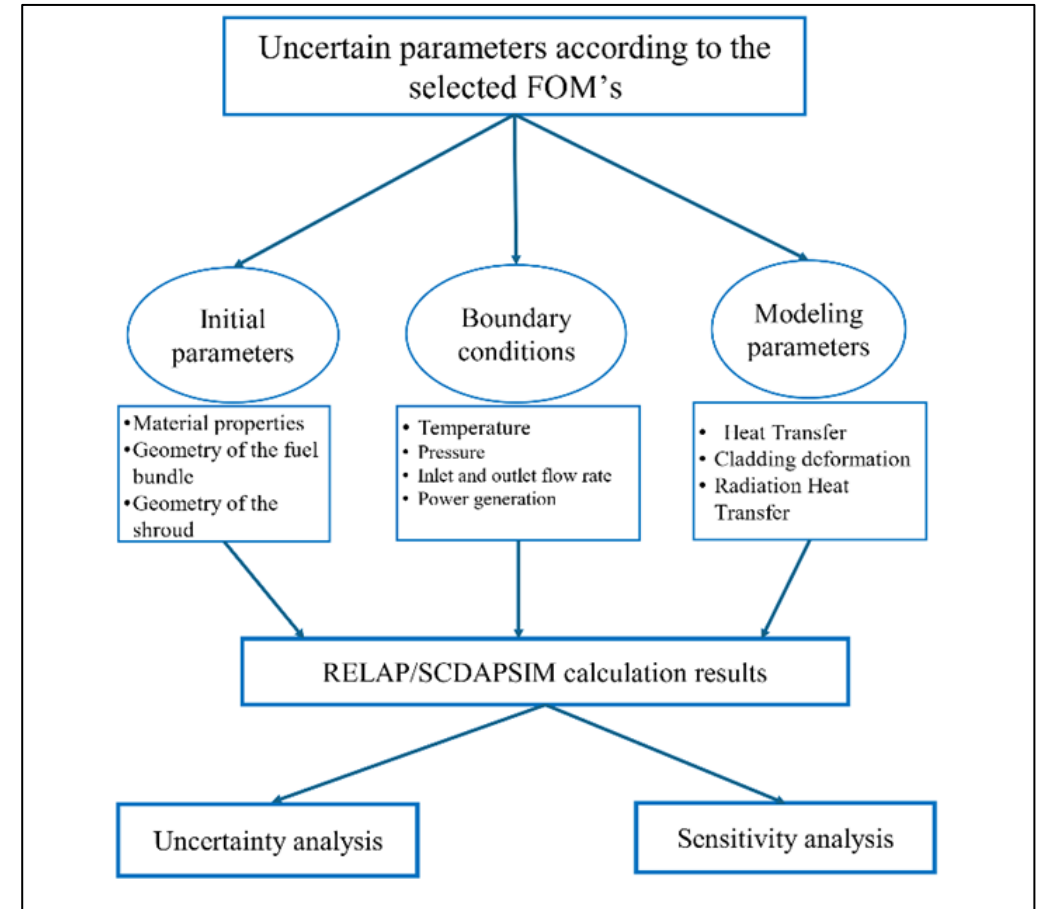
- GRS
- IPSN
- CSAU
- ENUSA
- GSUAM
- BEAU

**GRS**  
Gesellschaft für Anlagen-  
und Reaktorsicherheit  
(German Nuclear Safety  
Organisation)

## Tools

- SUSAS
- SUNSET
- DAKOTA
- RAVEN

**SUSAS**  
(Gesellschaft für  
Anlagen- und  
Reaktorsicherheit)

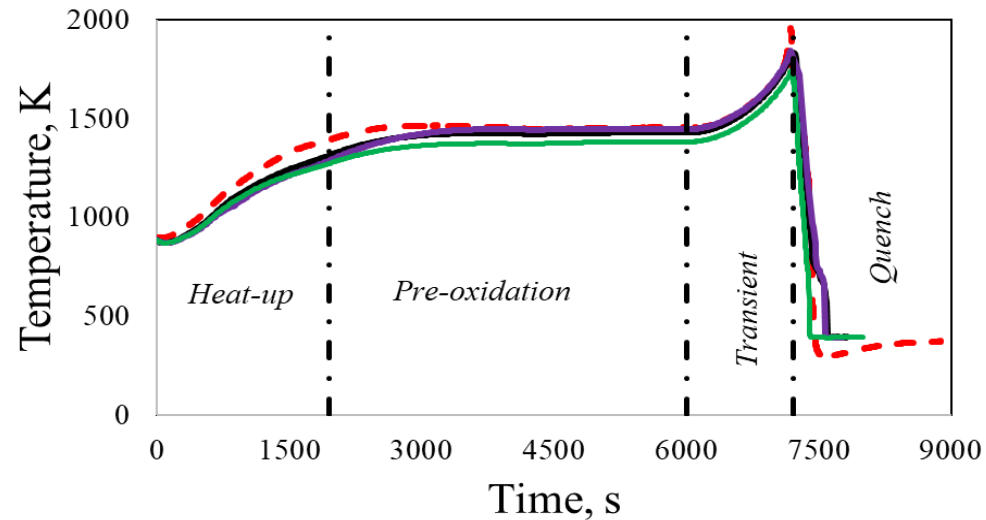


Schematic view of the application of the best estimate approach

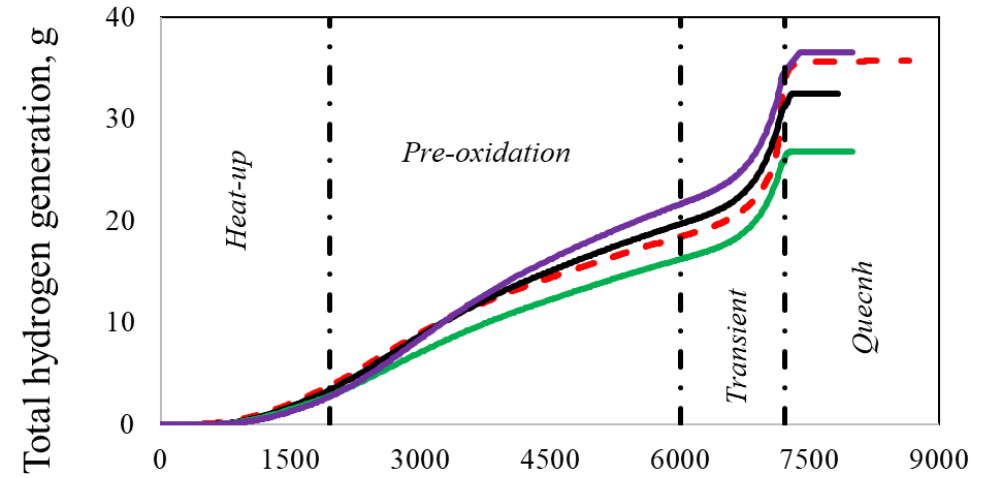
# Uncertainty analysis of QUENCH-06 test

Uncertain parameters:

- Boundary conditions
- Shroud material thermal properties
- Geometry parameters
- Modeling parameters



- - - Exp. TCRC-13
- Reference calculation
- Upper uncertainty limit
- Lower uncertainty limit



- - - Experimental data
- Reference calculation
- Lower uncertainty limit
- Upper uncertainty limit

The uncertainty analysis within BEPU approach allows to evaluate appropriateness of modeling results.

# Results of sensitivity analysis of QUENCH-06 test



Influence of uncertain parameters	Phase			
	Heat up (the 1500s)	Pre-oxidation (5000s)	Transient (6500s)	Quench (7350s)
Total hydrogen generation	Cladding thickness (influence +0.85), Electrical power (influence +0.55), Thickness of the Insulator (influence -0.27).	Electrical power (influence +0.82), Cladding thickness (influence +0.43), Steam mass flow rate at the bundle inlet (influence -0.35).	Electrical power (influence +0.85), Steam mass flow rate at the bundle inlet (influence -0.36), Cladding thickness (influence +0.32).	Electrical power (influence +0.81), Steam mass flow rate at the bundle inlet (influence -0.35), Thickness of the Insulator (influence -0.29).
Temperature of the central rod at 950 mm	Cladding thickness (influence +0.8), Electrical power (influence +0.58).	Electrical power (influence +0.78), Steam mass flow rate at the bundle inlet (influence -0.43).	Electrical power (influence +0.81), Steam mass flow rate at the bundle inlet (influence -0.39).	Quench water injection to the experiment section (influence +0.97).
Oxide layer thickness			Electrical power (influence +0.8), Steam mass flow rate at the bundle inlet (influence -0.4), Cladding thickness (influence +0.35).	Electrical power (influence +0.8), Steam mass flow rate at the bundle inlet (influence -0.4).





# Results of sensitivity analysis of QUENCH-06 test

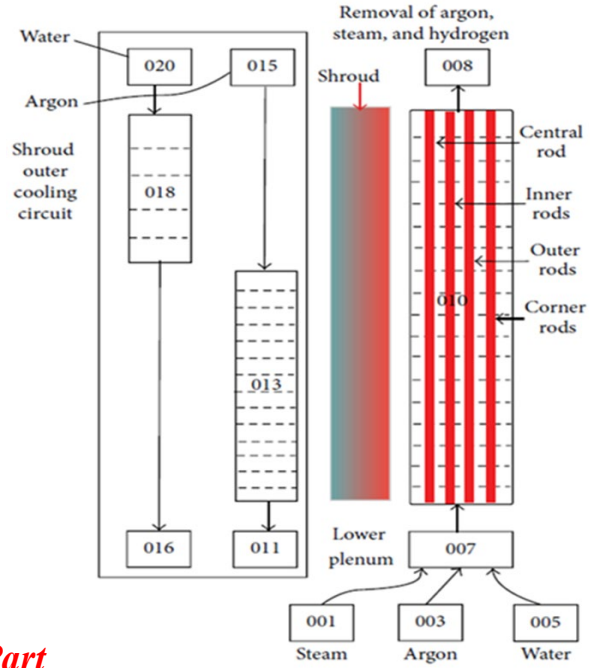
**Material properties** and **thickness of the surrounding structures** for the test facilities as well as **boundary conditions** that describe the heat transfer from the fuel bundle to the surrounding structures have a high impact on calculation results.

For the late bundle degradation phase the influence of **SCDAP parameters and models related to the fuel cladding rupture, oxidation, and bundle degradation** plays a significant role.

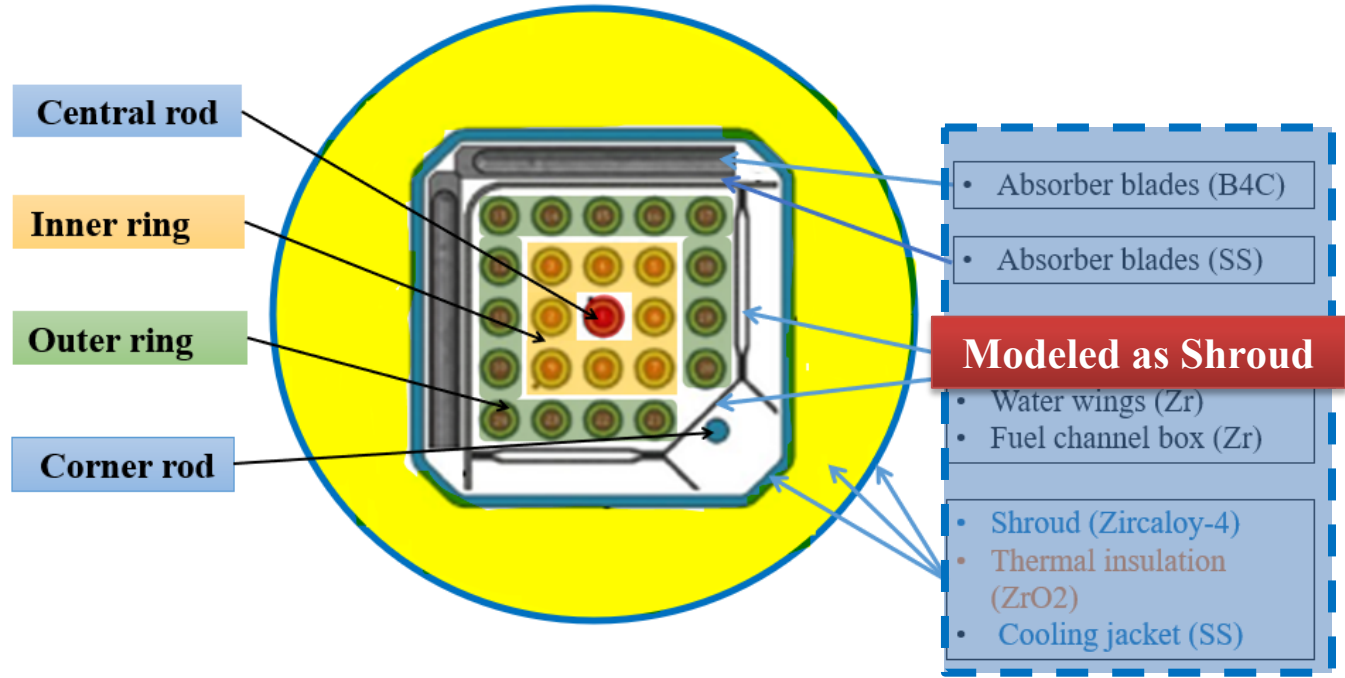
# QUENCH-20, asymmetric geometry



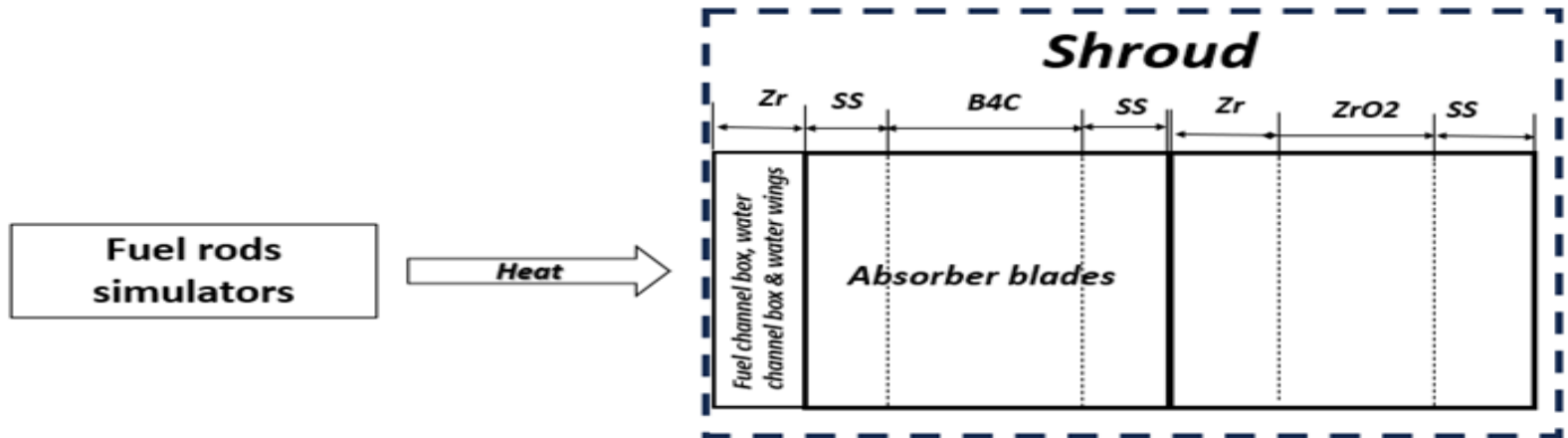
# The QUENCH-20 test developed models: *Pseudo symmetrical model*



RELAP Part

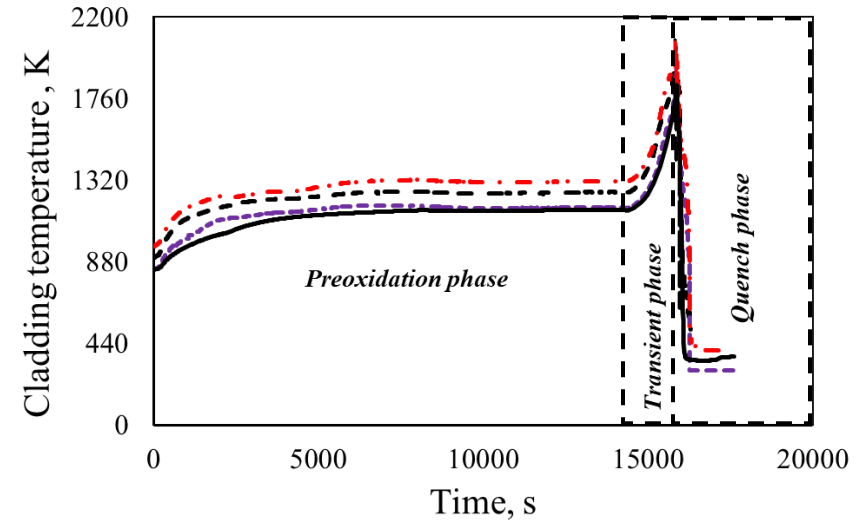
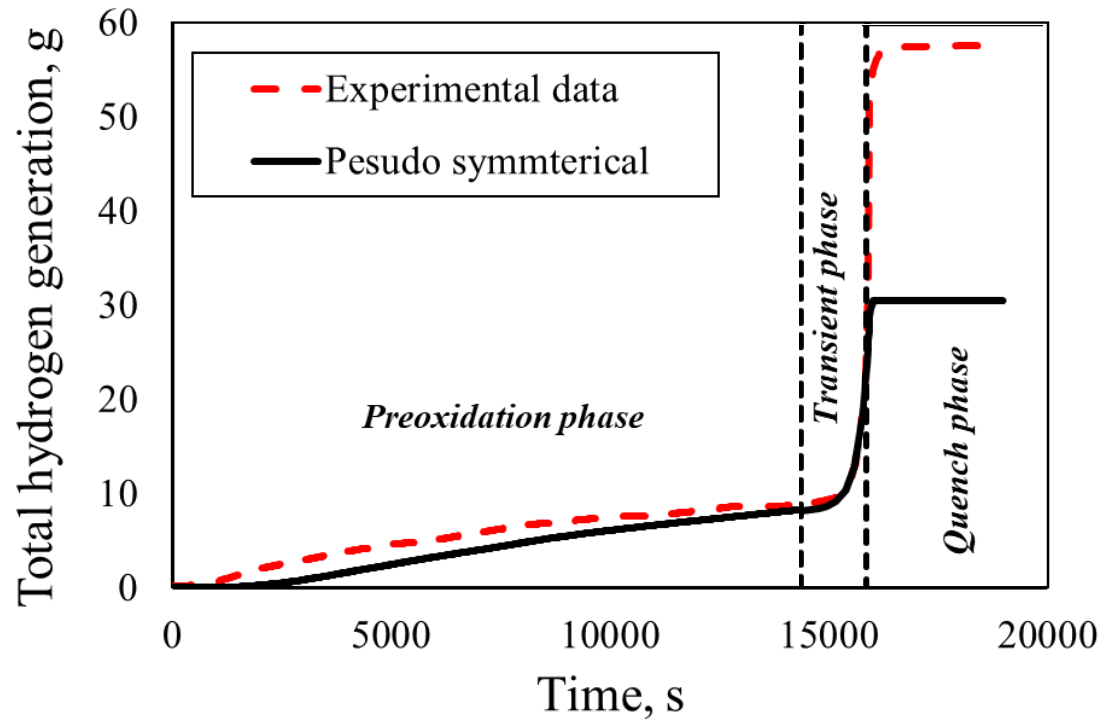


SCDAP part

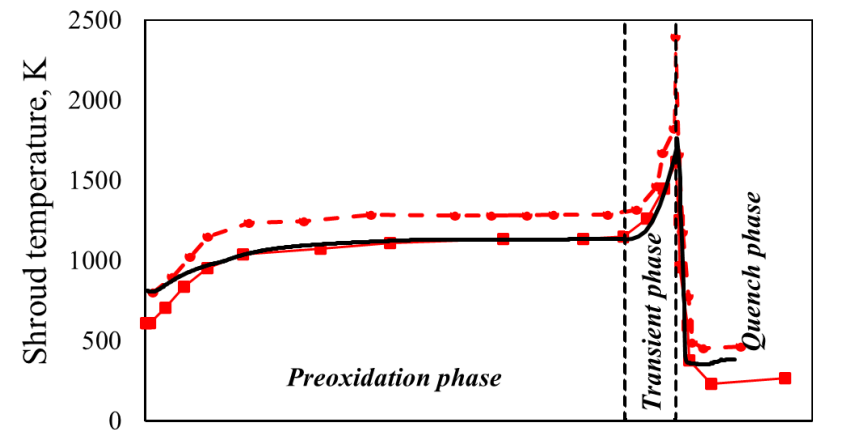




# The QUENCH-20 test developed models: *Pseudo symmetrical model*

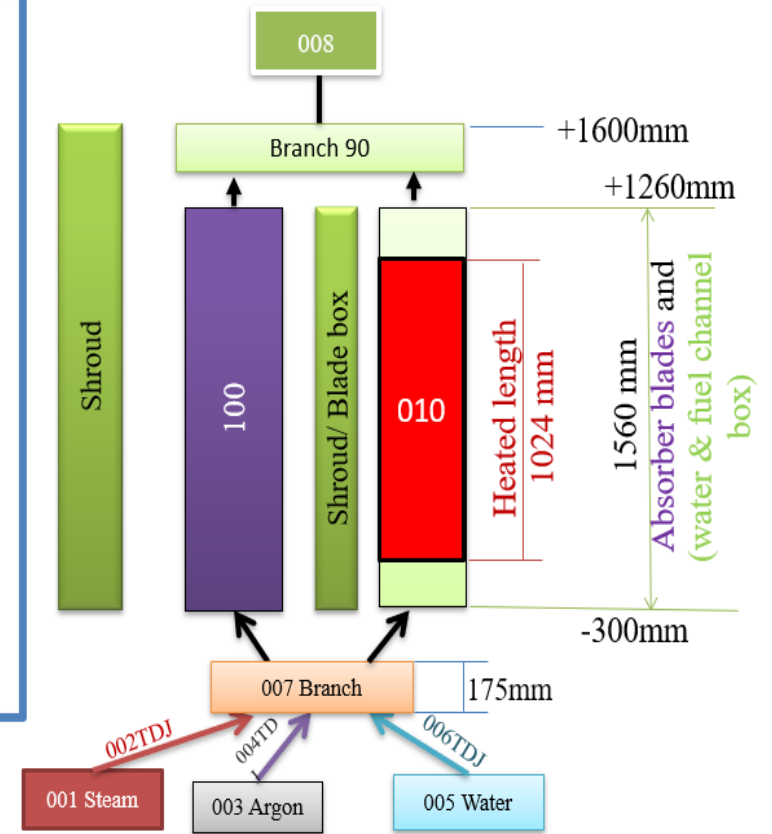
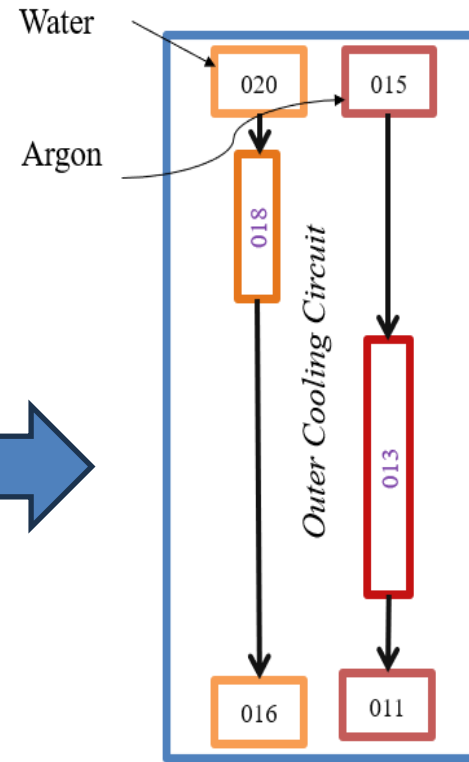
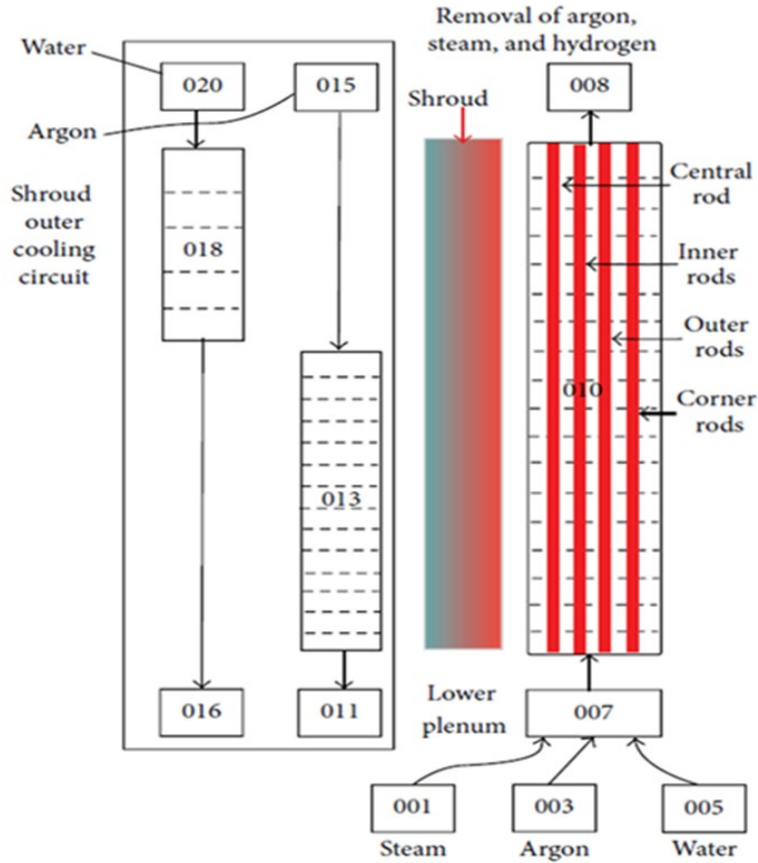


— Experimental data (TFS 1/13)      - - Experimental data (TFS 16/13)  
- · Experimental data (TFS 18/13)      — Pseudo symmetrical



■ Experimental data (TSH 13/180)      ● Experimental data (TSH 13/270)  
— Pseudo symmetrical

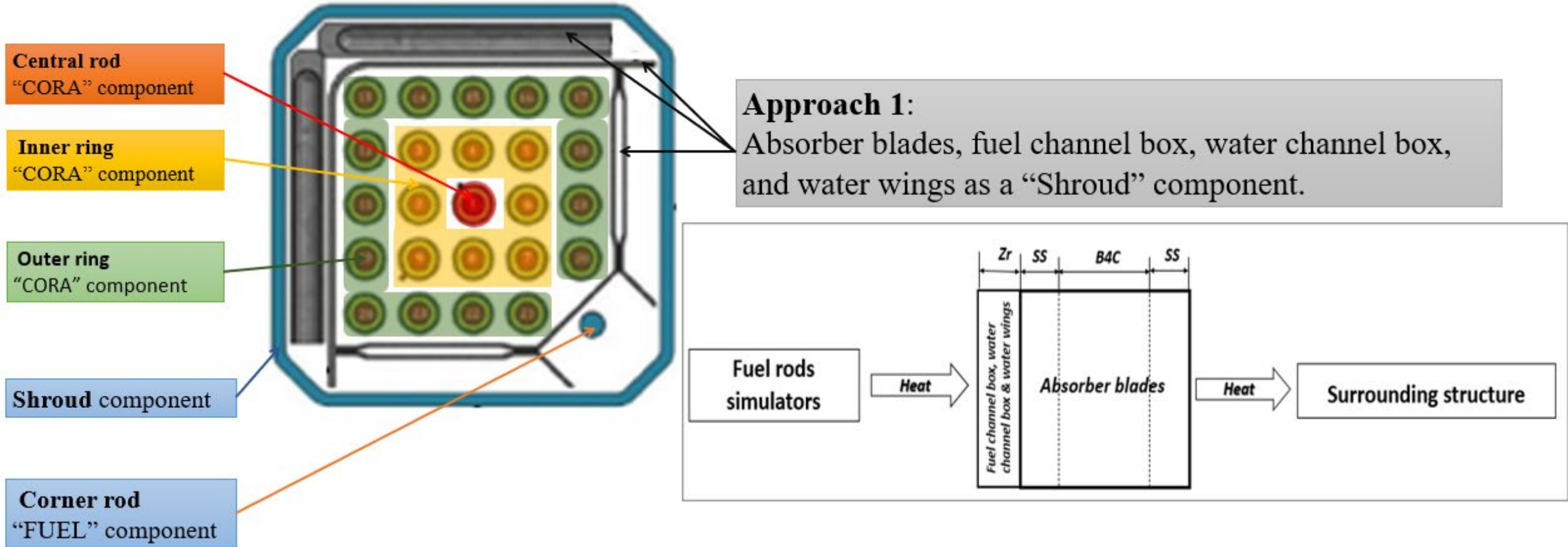
# The QUENCH-20 test developed models: *Component level model*



*RELAP Part*



# The QUENCH-20 test developed models: *Component level model*



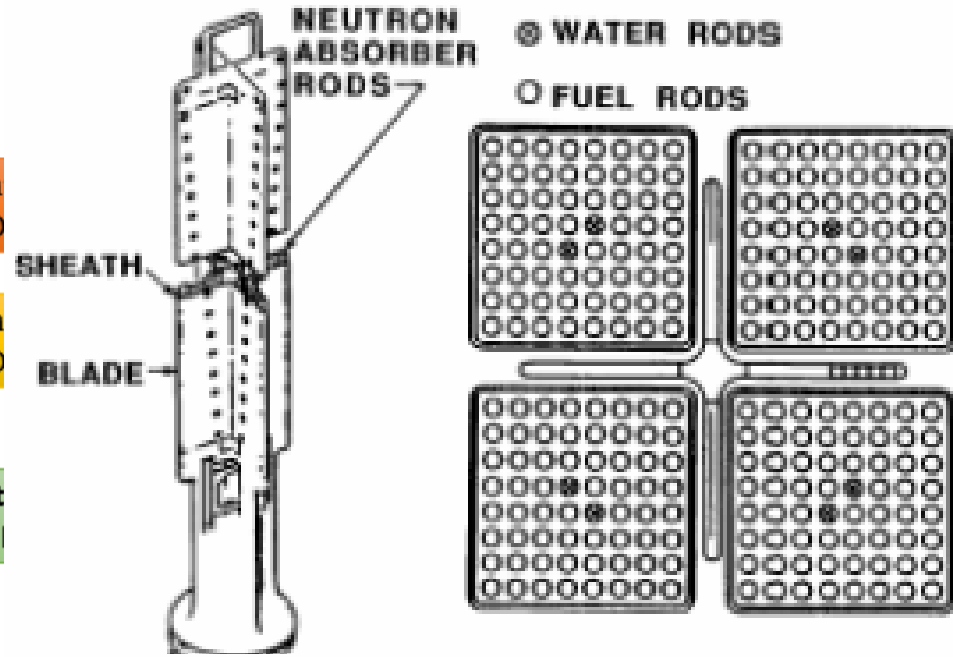
No  $B_4C$  oxidation !

SCDAP part

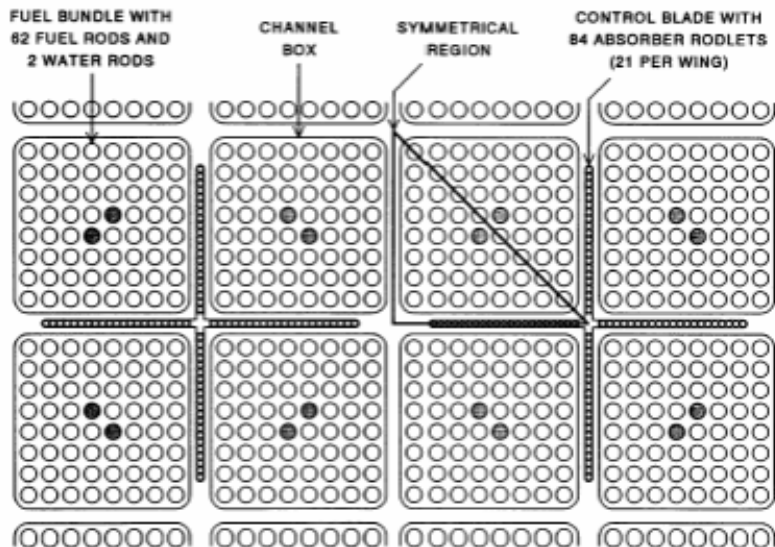
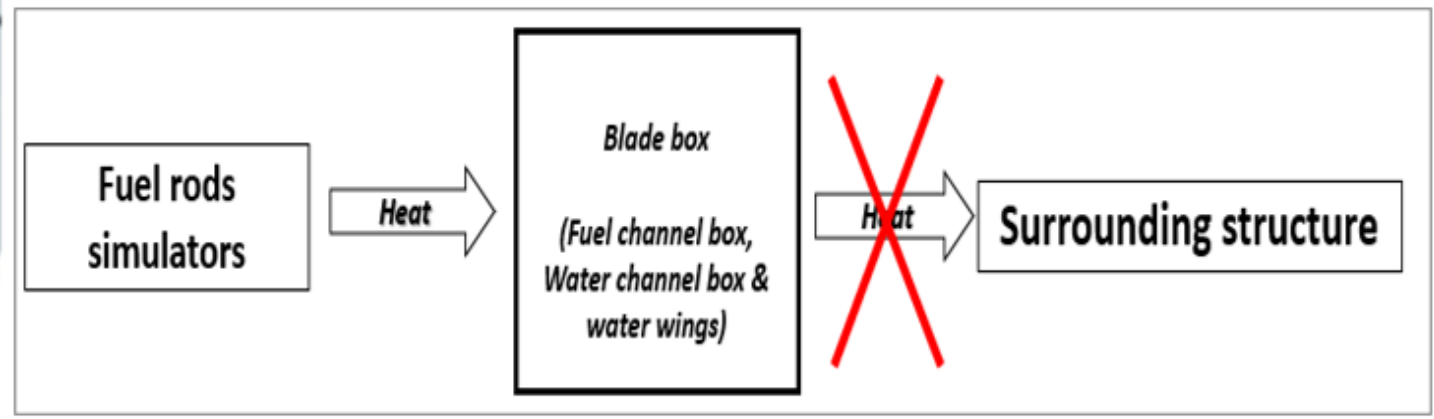


# The QUENCH-20 test developed models: *Component level model*

Cen  
"CO  
Inn  
"CO  
Out  
"CO  
Shr  
Corne  
"FUEL



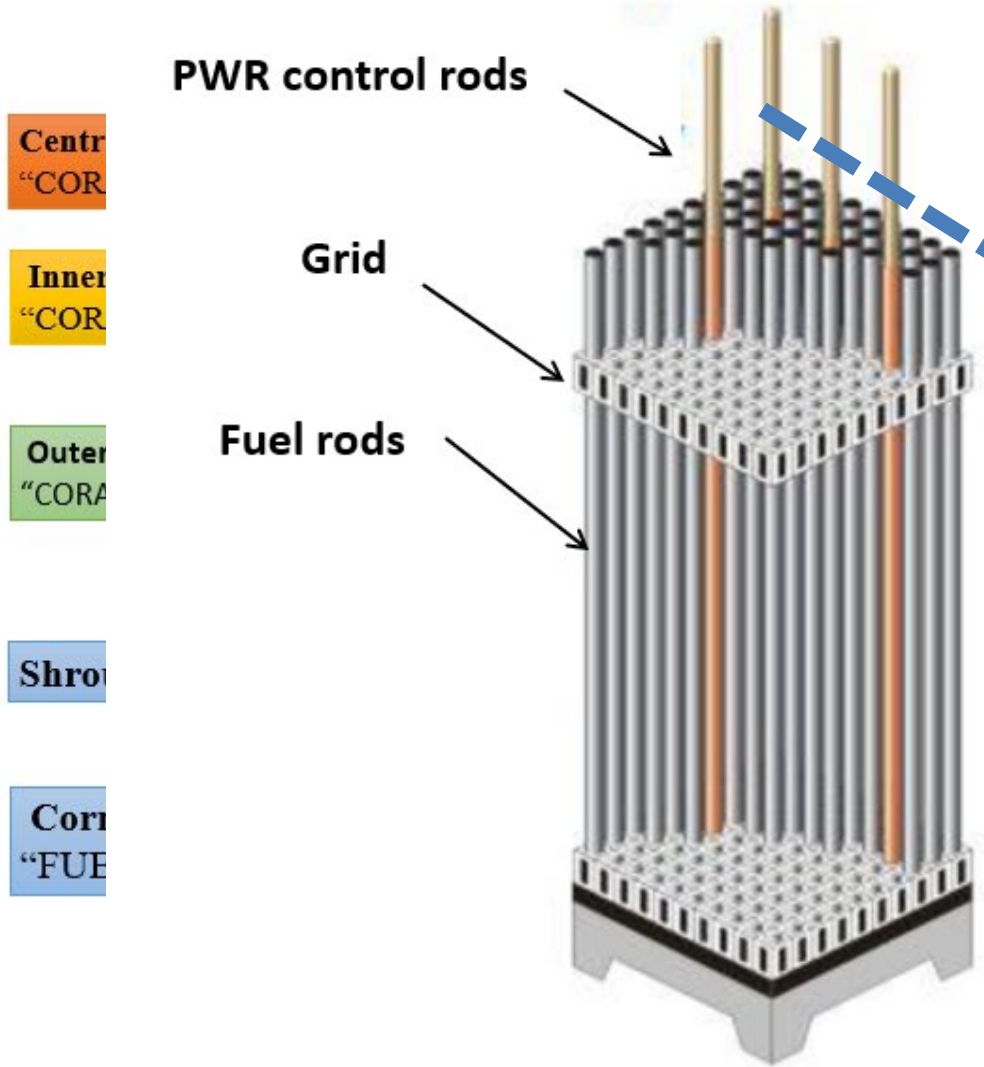
**Approach 2:**  
Absorber blades, fuel channel box, water channel box, and water wings box as "Blade box" component



**B<sub>4</sub>C oxidation was not achieved due to low temp. !**

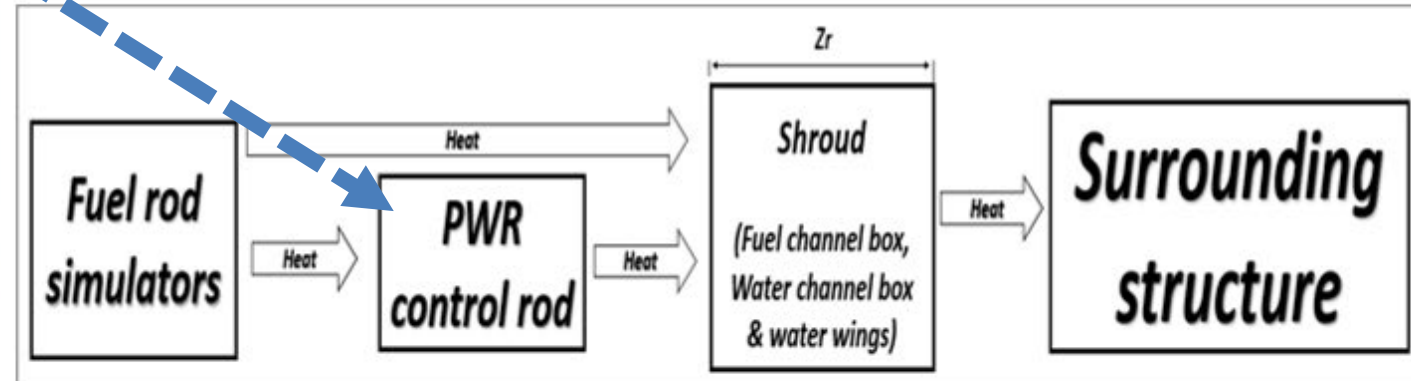


# The QUENCH-20 test developed models: *Component level model*



## Approach 3:

Absorber blades as PWR CR component; fuel channel box, water channel box, and water wings as "Shroud" component

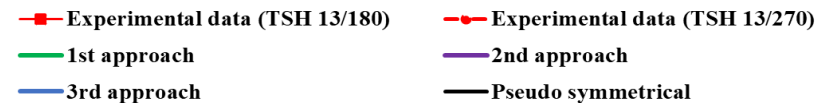
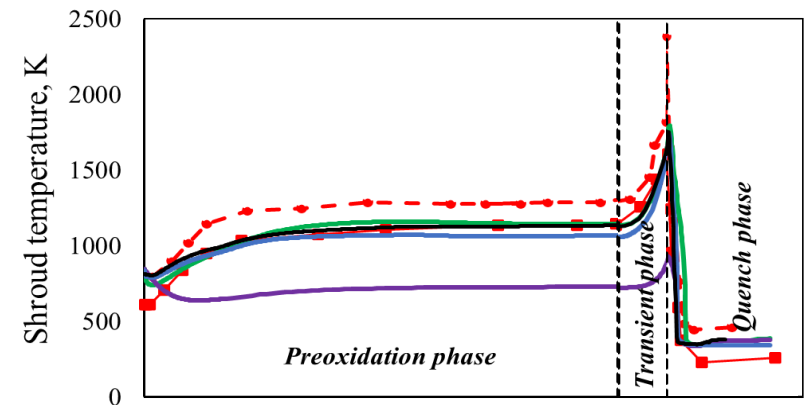
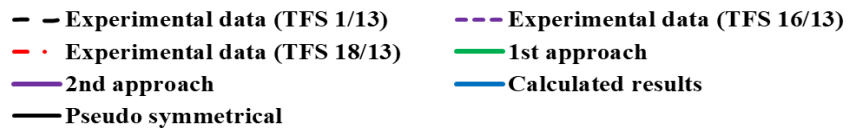
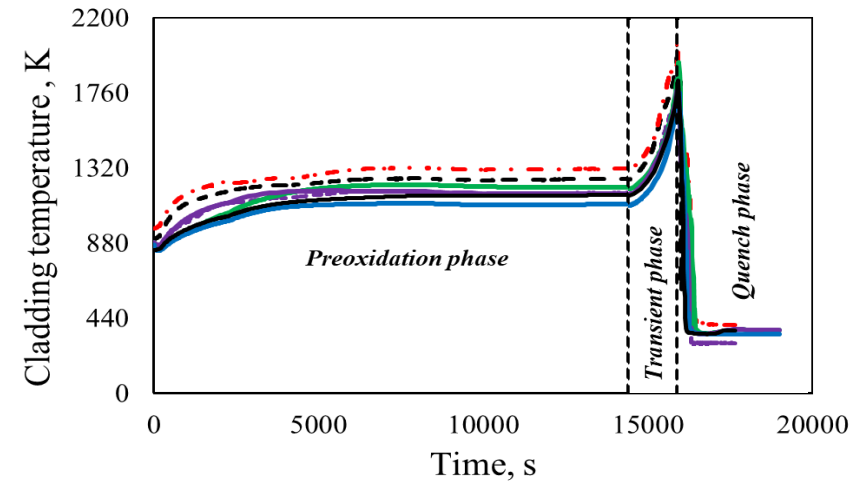
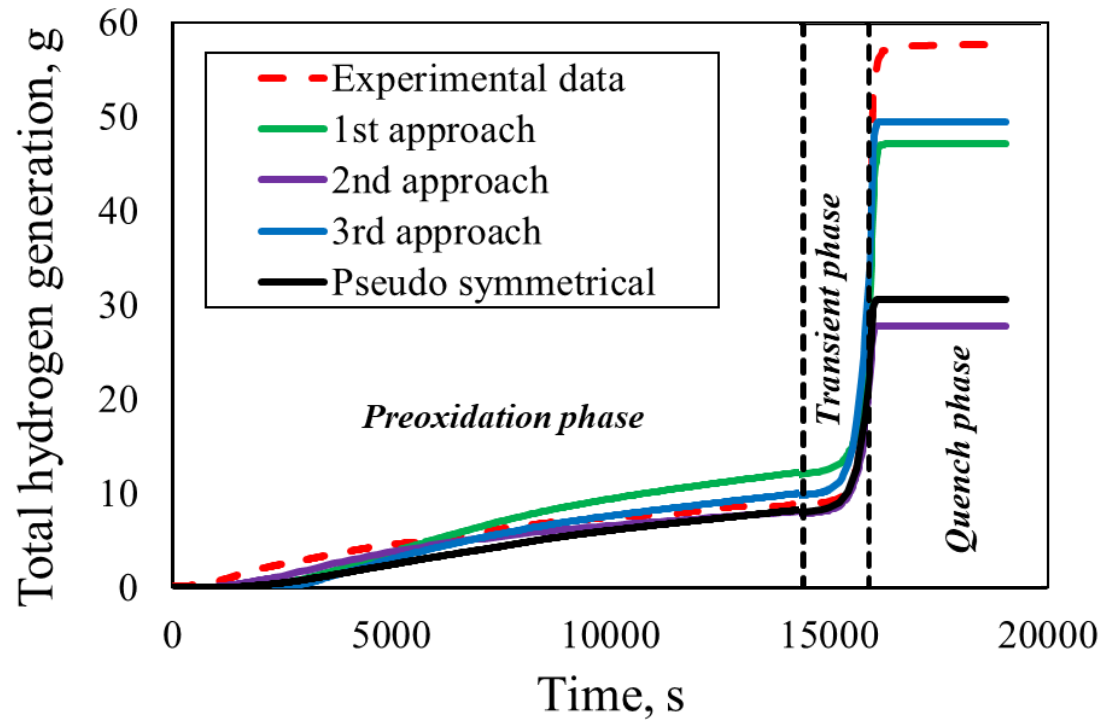


**B<sub>4</sub>C oxidation achieved !**



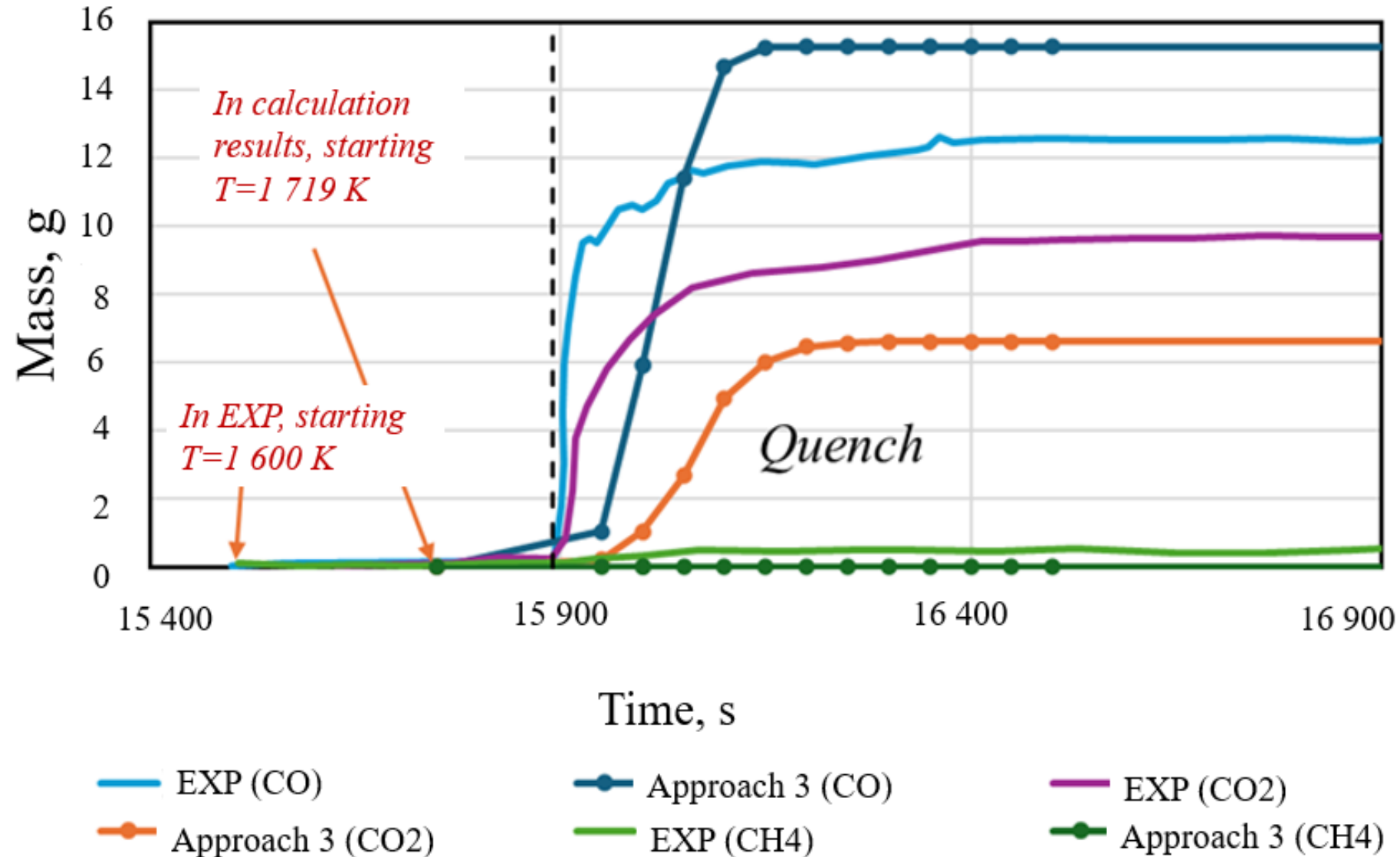


# Results for QUENCH-20 modeling





# Approach 3, gas release from the B<sub>4</sub>C oxidation processes





# CONCLUSIONS AND RECOMMENDATIONS

To develop a methodology for investigating physical processes in nuclear facilities with both symmetric and asymmetric geometries, numerical investigations of severe accident experiments that resulted in partial core melting were conducted. The investigations, performed applying the BEPU approach and severe accident code RELAP/SCDAPSIM together with the SUSA statistical tool, allowed us to summarise the following conclusions:

The BEPU-based uncertainty analysis confirms the reliability of simulation results for the facilities with symmetric geometry; in most analysed cases, the calculated ranges bound experimental data.

Sensitivity analysis highlights:

- Material properties and boundary conditions strongly affect results (Spearman rank correlation coefficient  $>0.78$ ).
- SCDAP parameters related to cladding rupture and oxidation significantly influence late-phase degradation (Spearman rank correlation coefficient  $>0.4$ ).



# CONCLUSIONS AND RECOMMENDATIONS

Building on insights from symmetric geometry experiments, a methodology for the asymmetric geometry was developed and applied. Pseudo-symmetrical and 3 component-level modelling approaches were developed and evaluated for QUENCH-20 experiment:

- Pseudo-symmetrical: this approach allows obtaining accurate pre-quenching results but underestimates hydrogen generation during quenching by ~30%.
- SCDAP Shroud component: using this approach, the obtained results match temperature data well; underestimates hydrogen (~18% or 10g) due to missing B<sub>4</sub>C oxidation modelling.
- SCDAP Blade box component: this approach allows obtaining a good temperature match for cladding; it lacks heat transfer modelling, causing underestimation of oxidation and hydrogen (~50% lower).
- SCDAP PWR control rod + Shroud components: this approach allows the best match with experimental data, calculated hydrogen generation (~12% less); includes B<sub>4</sub>C oxidation effects.



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Happy Holidays and  
a Joyful New Year!

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**Peter Ulrich Bochtler**

BASE

## **Infinite lattice depletion of accident-tolerant fuel pin-cells with OpenMC and cladding inventory analysis with FISPACT-II**

The operation of nuclear power plants with accident-tolerant fuels is foreseeable in the EU. To assess these developments, the BASE in-house research project “ReUnFis” is seeking to assess how such a use would be impacting waste streams and safety aspects than can be derived from the isotopic inventories.

Neutronic impacts due to necessary enrichment offsets reported in (Hall et al. 2021) for FeCrAlC26m and a M5-like alloy with 20  $\mu\text{m}$  Cr (Hall et al. 2021; Reaktor-Sicherheitskommission 2020; Kecek et al. 2016) and changing moderator to fuel ratio are studied through some observables derived from OpenMC (Romano et al. 2015; Romano et al. 2021) infinite lattice depletion simulations of accident-tolerant fuel pin-cells up to 75 MWd/kgHM.

The comparison of the cladding inventory for JEFF-3.3 nuclear data library (Plompen et al. 2020) with FISPACT-II (Sublet et al. 2017) demonstrates how for material activation and transmutation problems both codes can be used in a complementary way.

Various cladding metrics (activity, contact dose rate and elemental build-up) of doped fuel (Arborelius et al. 2006; Hall et al. 2021) with M5-like alloy +20  $\mu\text{m}$  Cr, FeCrAlC26m and SiC filament-wound duplex tube (Koyanagi et al. 2024; Noda et al. 2002) + 10  $\mu\text{m}$  Cr (Quillin et al. 2022; Mouche et al. 2021) are compared in decay space up to 100 y at decay times that may also be relevant to QUENCH experiments. Finally, the presentation highlights the impact of impurity levels (Parga 2018; Yeom et al. 2019; Atlantic Equipment Engineers 2025) and the impact of nuclear data JEFF-4 (NEA 2025) for the case of a M5-like alloy +20  $\mu\text{m}$  Cr.

### **References**

**Arborelius et al. (2006)** Arborelius, J., Backman, K., Hallstadius, L., Limbäck, M., Nilsson, J., Rebensdorff, B., Zhou, G., Kitano, K., Löfström, R. & Rönnerberg, G.: Advanced Doped UO<sub>2</sub> Pellets in LWR Applications. *Journal of Nuclear Science and Technology* 43(9), 967–976, DOI 10.1080/18811248.2006.9711184, 2006.

**Atlantic Equipment Engineers (2025)** Atlantic Equipment Engineers: Datasheet CR-102-105, Chromium Powder, Electrolytic, <https://docs.google.com/document/d/1nOthzZLs93N8a96WYtCCJGtKnPxhrXcD/edit>, abgerufen am 17. Januar 2025

**Hall et al. (2021)** Hall, R., Sweet, R., Belles, R. & Wieselquist, W. A.: Extended Enrichment Accident Tolerant LWR Fuel Isotopic and Lattice Parameter Trends, Oak Ridge National Laboratory (ORNL), ORNL/TM-2021/1961, 2021.

**Kecek et al. (2016)** Kecek, A., Tuček, K., Holmström, S. & van Uffelen, P.: Development of M5 Cladding Material Correlations in the TRANSURANUS Code, ISBN 9279646559, Publications Office of the European Union, 2016.

**Koyanagi et al. (2024)** Koyanagi, T., Hu, X., Petrie, C. M., Singh, G., Ang, C., Deck, C. P., Kim, W.-J., Kim, D., Sauder, C. & Braun, J.: Hermeticity of SiC/SiC composite and monolithic SiC tubes irradiated under radial high-heat flux. *Journal of Nuclear Materials* 588, 154784, 2024.

## 30<sup>th</sup> International QUENCH Workshop

**Mouche et al. (2021)** Mouche, P. A., Koyanagi, T., Patel, D. & Katoh, Y.: Adhesion, structure, and mechanical properties of Cr HiPIMS and cathodic arc deposited coatings on SiC. *Surface and Coatings Technology* 410, 126939, 2021.

**Noda et al. (2002)** Noda, T., Fujita, M., Araki, H. & Kohyama, A.: Effect of nuclear data and impurities on the evaluation of induced activity of CVI SiCf/SiC composites. *Fusion Engineering and Design* 61, 711–716, 2002.

**NEA (2025)** Nuclear Energy Agency (NEA): JEFF-4.0 nuclear data library is now available, [https://www.oecd-nea.org/jcms/pl\\_107619/jeff-4-0-nuclear-data-library-is-now-available](https://www.oecd-nea.org/jcms/pl_107619/jeff-4-0-nuclear-data-library-is-now-available), abgerufen am 27. Oktober 2025, Stand vom 2. Juli 2025.

**Parga (2018)** Parga, C. J.: M5 Alloy Specification for TREAT Conceptual Fuel Cladding Selection, Idaho National Lab.(INL), Idaho Falls, ID (United States), 2018.

**Plompen et al. (2020)** Plompen, A. J. M., Cabellos, O., Saint Jean, C. de, Fleming, M., Algora, A., Abstract for 30th International QUENCH Workshop 10.11.2025

Angelone, M., Archier, P., Bauge, E., Bersillon, O. & Blokhin, A.: The joint evaluated fission and fusion nuclear data library, JEFF-3.3. *The European Physical Journal A* 56(7), 181, 2020.

**Quillin et al. (2022)** Quillin, K., Yeom, H., Dabney, T., Willing, E. & Sridharan, K.: Microstructural and nanomechanical studies of PVD Cr coatings on SiC for LWR fuel cladding applications. *Surface and Coatings Technology* 441, 128577, 2022.

**Reaktor-Sicherheitskommission (2020)** Reaktor-Sicherheitskommission: Ergebnisse und Empfehlungen der 514. Sitzung, [http://www.rskonline.de/sites/default/files/reports/epanlagersk514hp\\_0.pdf](http://www.rskonline.de/sites/default/files/reports/epanlagersk514hp_0.pdf), abgerufen am 5. Januar 2024

**Romano et al. (2015)** Romano, P. K., Horelik, N. E., Herman, B. R., Nelson, A. G., Forget, B. & Smith, K.: OpenMC: A state-of-the-art Monte Carlo code for research and development. *Annals of Nuclear Energy* 82, 90–97, 2015.

**Romano et al. (2021)** Romano, P. K., Josey, C. J., Johnson, A. E. & Liang, J.: Depletion capabilities in the OpenMC Monte Carlo particle transport code. *Annals of Nuclear Energy* 152, 107989, 2021.

**Sublet et al. (2017)** Sublet, J.-C., Eastwood, J. W., Morgan, J. G., Gilbert, Fleming, M. & Arter, W.: FISPACT-II: an advanced simulation system for activation, transmutation and material modelling. *Nuclear Data Sheets* 139, 77–137, 2017.

**Yeom et al. (2019)** Yeom, H., Dabney, T., Johnson, G., Maier, B., Lenling, M. & Sridharan, K.: Improving deposition efficiency in cold spraying chromium coatings by powder annealing. *The International Journal of Advanced Manufacturing Technology* 100, 1373–1382, 2019.



Federal Office  
for the Safety of  
Nuclear Waste Management

# **Infinite lattice depletion of accident-tolerant fuel pin-cells with OpenMC and cladding inventory analysis with FISPACT-II**

**Intermediate results of project 4724B50001**

**Peter Bochtler**

Quench Workshop, Karlsruhe, Germany

16-18.12.2025



# Agenda

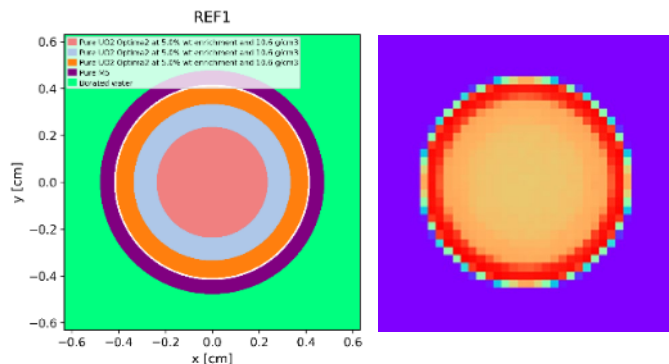
1. OpenMC burn-up simulations of ATF pin-cells
2. Code-to-code comparison of clad inventory: FISPACT-II vs. OpenMC
3. ATF cladding metrics from FP-II

# Motivation for in-house simulations

It is foreseeable that power reactors in Europe will run with accident-tolerant fuels.

In-house research project “ReUnFis” is seeking to answer how the use of such fuels could be impacting waste streams and safety aspects (that can be derived from the isotopic inventories).

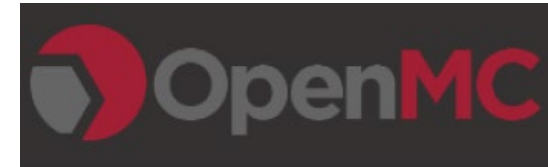
BASE advises and supports the Federal Ministry for the Environment, Climate Action, Nature Conservation and Nuclear regarding issues of disposal of radioactive waste and nuclear safety.



- Period: July 24 to December 26
- Burn-up simulation of pin-cells with **M5+20 $\mu$ mCr**, **FeCrAlC26M**, **SiC/SiC+10 $\mu$ mCr** in OpenMC
- ATF cladding metrics (opt. impurities) with FP-II

# Codes, methods, tools and data

# Codes & Methods



**OpenMC**<sup>[18][19]</sup> originally developed by MIT CRPG (Paul Romano),  
now community-developed Monte Carlo neutron and photon transport simulation code:  
<https://github.com/openmc-dev/openmc>

## Methods

Continuous energy neutron transport “collapse” with track length tallies into reaction rate average determination through many samples (k-eigenvalue method, method of successive generations<sup>[30]</sup>, see [docs.openmc.org](https://docs.openmc.org) and e.g. <sup>[23]</sup>).

→ Solving neutron transport coupled inventory equations with matrix exponentials + IPF  
CRAM48<sup>[30,31,32]</sup> + CE/LI integrator<sup>[34]</sup>

→ Providing tallied neutron spectra for FISPACT-II

# Codes & Methods

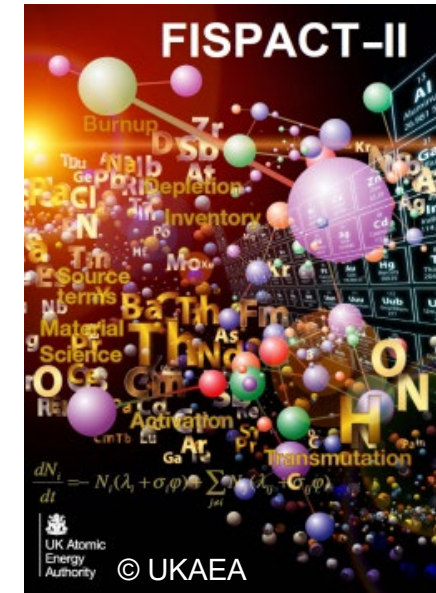
**FISPACT-II**<sup>[20]</sup> code developed by UKAEA, available through OECD-NEA:  
<https://www.oecd-nea.org/tools/abstract/detail/nea-1890/>

## Methods

Point depletion of entire material (here ATF cladding) „lump” with OpenMC tallied neutron spectra in CCFE-709 or UKAEA-1102 group structure<sup>[14]</sup> and flux level (at each BU step).

→ Solving (only) inventory equations with Livermore Solver for Ordinary Differential Equations (LSODE)<sup>[24]</sup> with adaptive time stepping

Additional methods for inventory uncertainty estimation (pathway analysis) and self-shielding correction.



# Tools and Data

Computing on R&D-server with jupyter-notebooks<sup>[25]</sup> (python virtual environments) + complementary calculations on ZUSE HPC-system „Lise“ (test account)

OpenMC **python API** (OpenMP, OpenMPI)

FISPACT **python pseudo API** pypact by Thomas Stainer: <https://github.com/fispact/pypact>

**Neutronics material maker** originally created by Jonathan Shimwell:

[https://github.com/fusion-energy/neutronics\\_material\\_maker](https://github.com/fusion-energy/neutronics_material_maker)

## Nuclear data sources

- [https://git.oecd-nea.org/fispact/nuclear\\_data](https://git.oecd-nea.org/fispact/nuclear_data)
- <https://databank.io.oecd-nea.org/data/jeff>
- <https://openmc.org/data-libraries/>

# .JSON material database for (ATF) materials

## Literature research on

- Composition of 5.0, 5.1 and 5.6 wt% UO<sub>2</sub>, Zr-alloys, FeCrAl and SiC as well as Al<sub>2</sub>O<sub>3</sub>, Cr<sub>2</sub>O<sub>3</sub> and Cr
- Impurity levels in materials see e.g. [16]

## Creation of .JSON material database (neutronics materials maker) for OpenMC and FISPACT-II

- ▣ Pure UO2 Optima2 at 5.0% wt enrichment and 10.6 g/cm3
- ▣ Pure UO2 Optima2 at 5.1% wt enrichment and 10.6 g/cm3
- ▣ Pure UO2 Optima2 at 5.6% wt enrichment and 10.6 g/cm3
- ▣ Impure UO2 Optima2 at 5.0% wt enrichment and 10.6 g/cm3
- ▣ Impure UO2 Optima2 at 5.1% wt enrichment and 10.6 g/cm3
- ▣ Impure UO2 Optima2 at 5.6% wt enrichment and 10.6 g/cm3
- ▣ Doped Pure UO2 Optima2 at 5.0% wt enrichment and 10.68 g/cm3
- ▣ Doped Pure UO2 Optima2 at 5.1% wt enrichment and 10.68 g/cm3
- ▣ Doped Pure UO2 Optima2 at 5.6% wt enrichment and 10.68 g/cm3
- ▣ Doped Impure UO2 Optima2 at 5.0% wt enrichment and 10.68 g/cm3
- ▣ Doped Impure UO2 Optima2 at 5.1% wt enrichment and 10.68 g/cm3
- ▣ Doped Impure UO2 Optima2 at 5.6% wt enrichment and 10.68 g/cm3
- ▣ Pure M5
- ▣ Impure M5
- ▣ Pure Chromium
- ▣ Impure Chromium
- ▣ Pure FeCrAl C26M
- ▣ Impure FeCrAl C26M
- ▣ Pure CVI Hi-Nicalon SiCf/SiC
- ▣ Impure CVI Hi-Nicalon SiCf/SiC
- ▣ Pure filament-wound SiC duplex tube
- ▣ Impure filament-wound SiC duplex tube

Note: Please note that „M5“ is a „M5-like“ Zr-alloy according to the reported references.

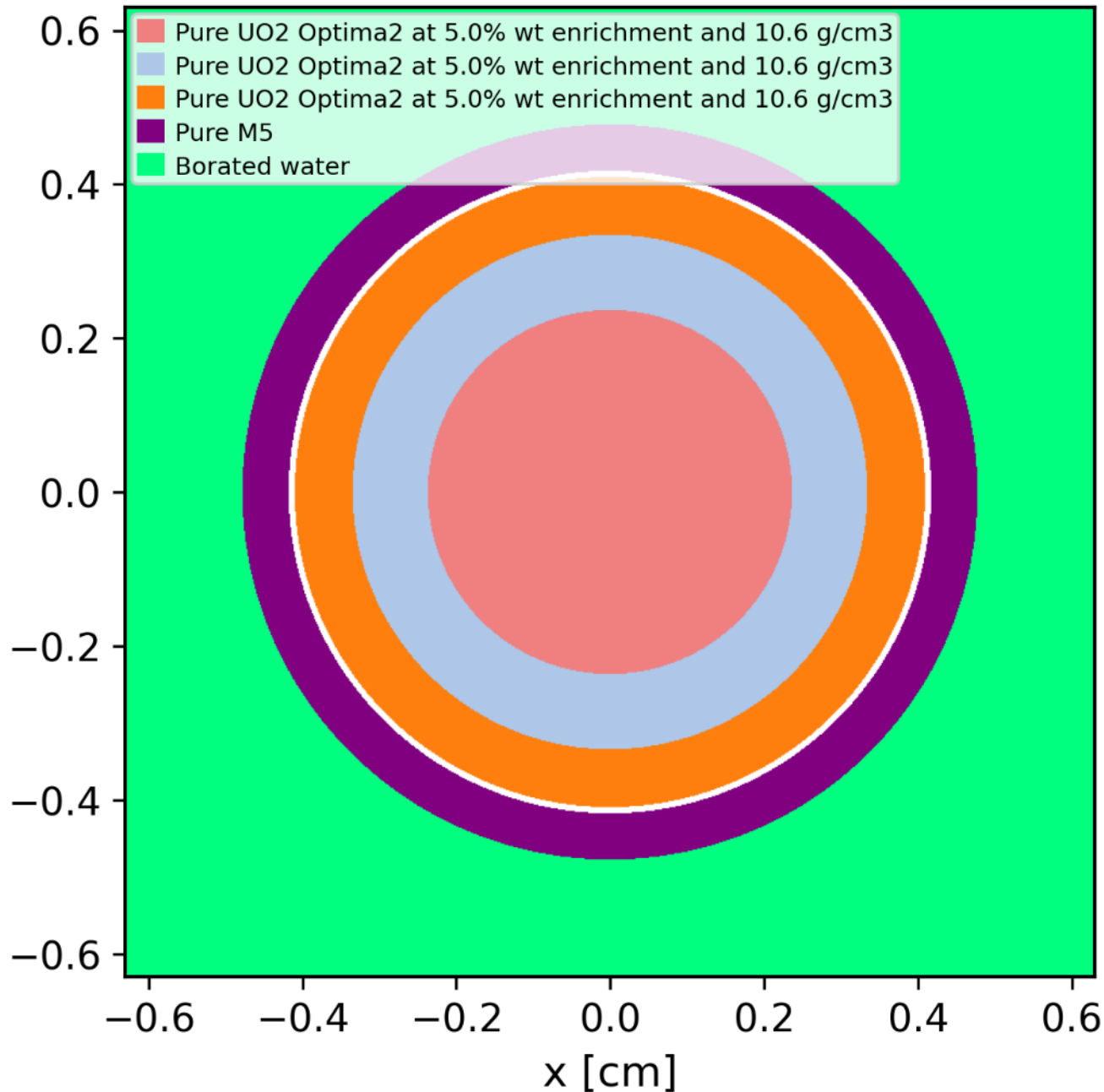
# **Modelling accident-tolerant fuel pin-cells in OpenMC (jeff-3.3)**



# Pin-cell cases overview for „PWR“

	REF1	REF3a	ATF1a	ATF2a	ATF3a
Density [g/cm <sup>3</sup> ]	10.6 <sup>[1]</sup>	10.68 <sup>[1] A)</sup>	10.68 <sup>[1] A)</sup>	10.68 <sup>[1] A)</sup>	10.68 <sup>[1] A)</sup>
Enrichment [wt%]	5.0	5.0	5.1 <sup>[2]</sup>	5.6 <sup>[2]</sup>	5.0
Cladding	M5 <sup>[3]</sup>	M5 <sup>[3]</sup>	M5 <sup>[3]</sup> +20 µm Cr <sup>[2]</sup>	FeCrAl C26m <sup>[2]</sup>	Filament-wound SiC duplex tube <sup>[6]</sup> +10 µm Cr <sup>[7],[8]</sup>
Thickness [mm]	0.601 <sup>[4]</sup>	0.601 <sup>[4]</sup>	0.621	0.385 <sup>[2]</sup>	0.81 <sup>[5]</sup>
HM per model [g/cm]	4.9225	+0.65%	+0.65%	+0.65%	+0.65%

# REF1

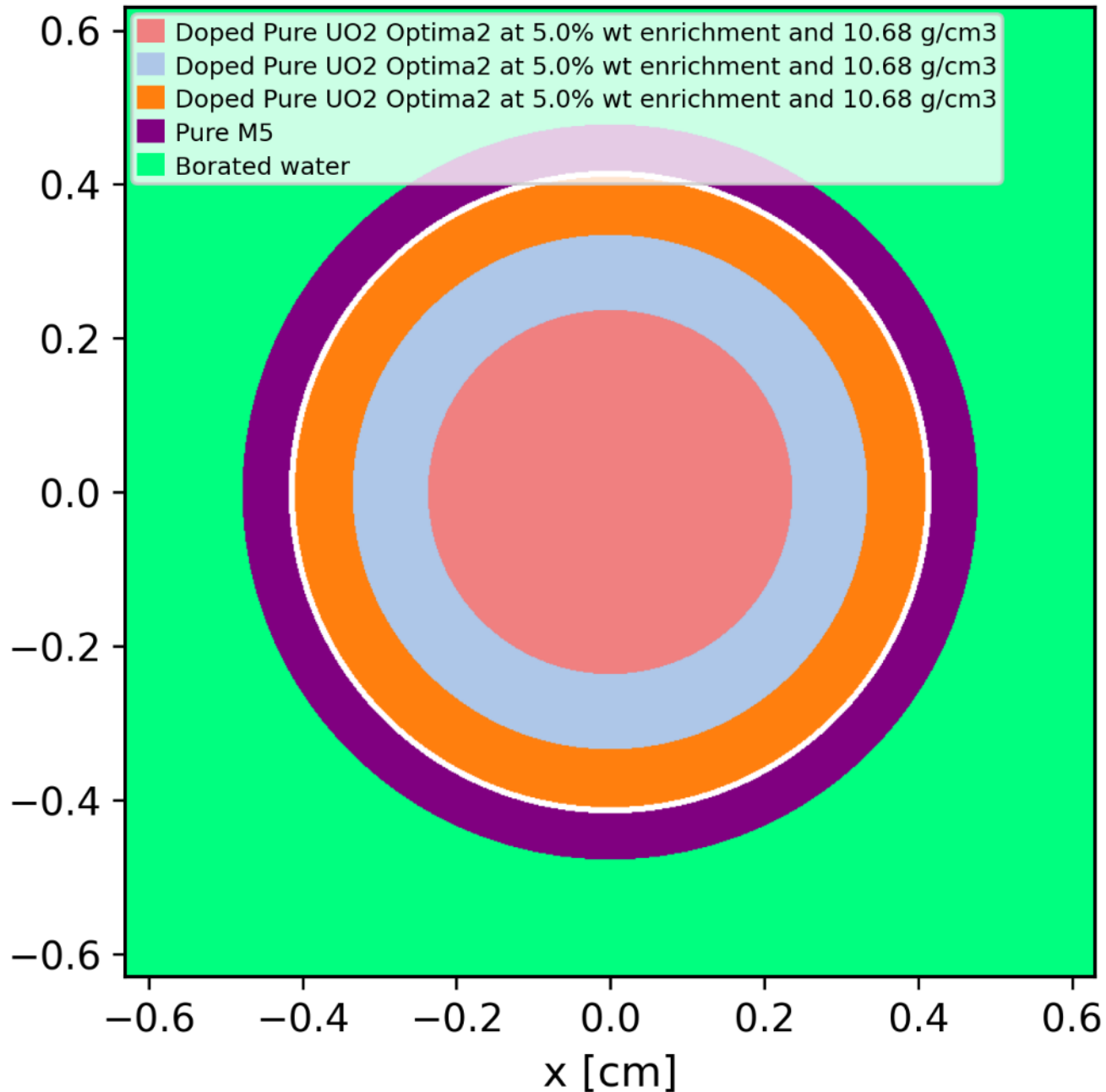


## Infinite 2-D pin-cell depletion

Fuel pin at the core center with constant power over 3 cycles (each 18 months).

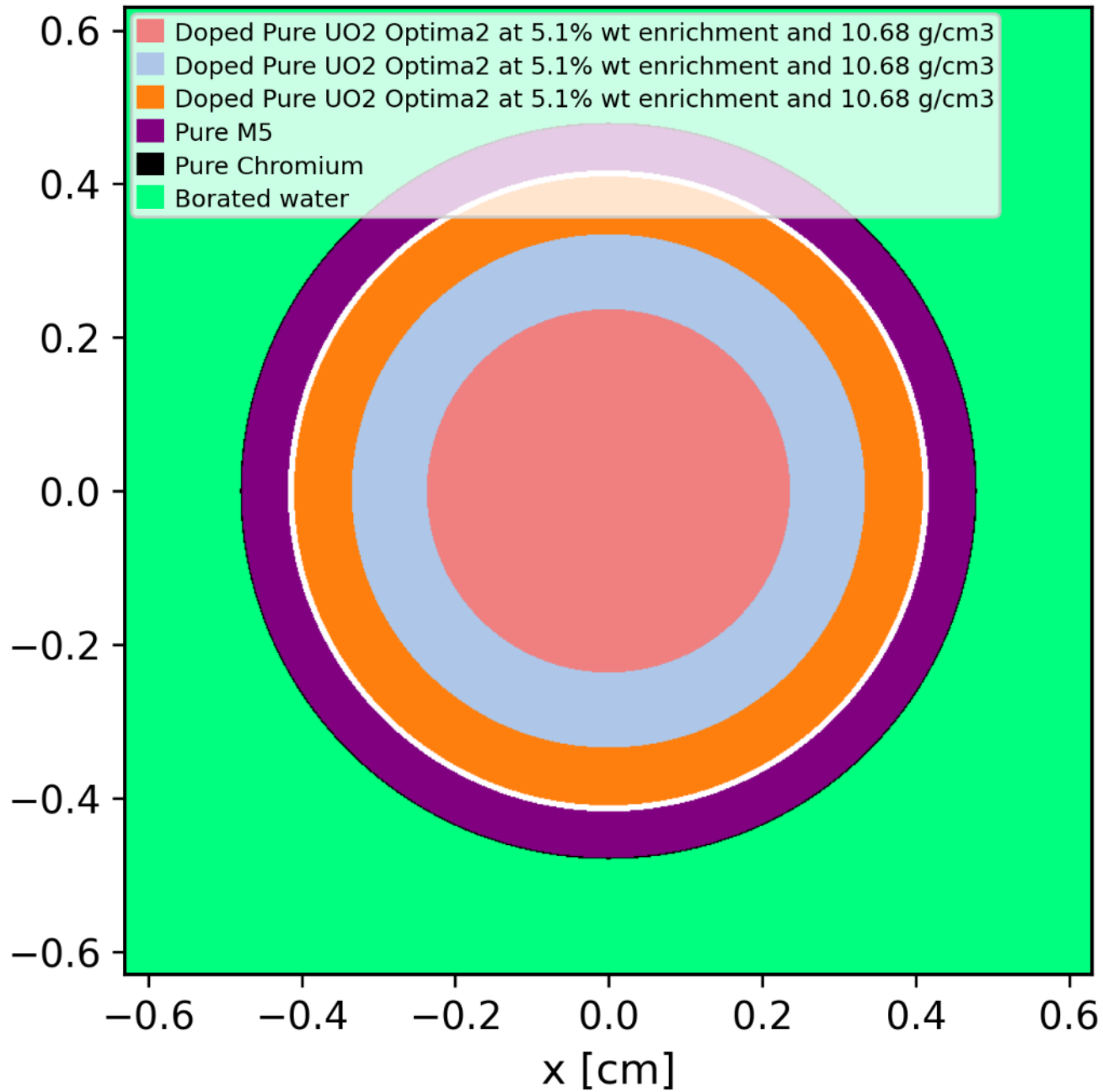
- 45.7 W/gU<sub>i</sub> for 1642.5 days to 75 MWd/kgU<sub>i</sub>
- Pitch = 1.26 cm<sup>[2],[9]</sup>
- 3 fuel depletion zones
- Constant gap = 0.08 mm
- 5.0 wt% at 10.6 g/cm<sup>3</sup>
- Cladding 600 K
- Fuel 900 K
- Moderator 583 K and 15 MPa
- 650 ppm of boron (by weight)<sup>[10]</sup> = constant

# REF3a



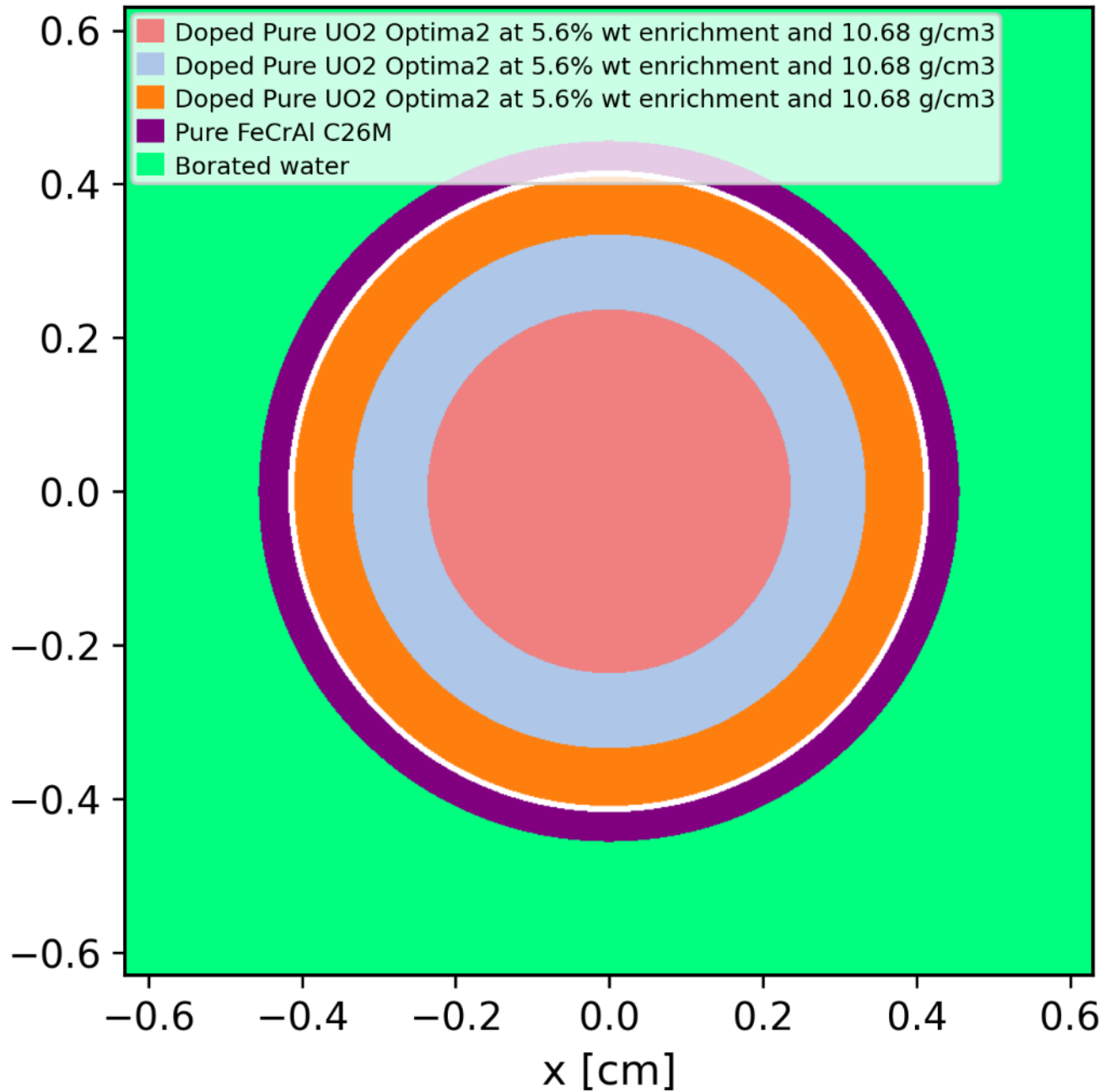
- M5 cladding [3]
- Density increase compared to REF1
- HM +0.65%,  $\rho$  +0.75%<sup>[1]</sup>
- Dopants Cr, Al, O as (n,gamma) absorbers (in 200 ppm Al<sub>2</sub>O<sub>3</sub> and 800 ppm Cr<sub>2</sub>O<sub>3</sub>)<sup>[2]</sup>

# ATF1a



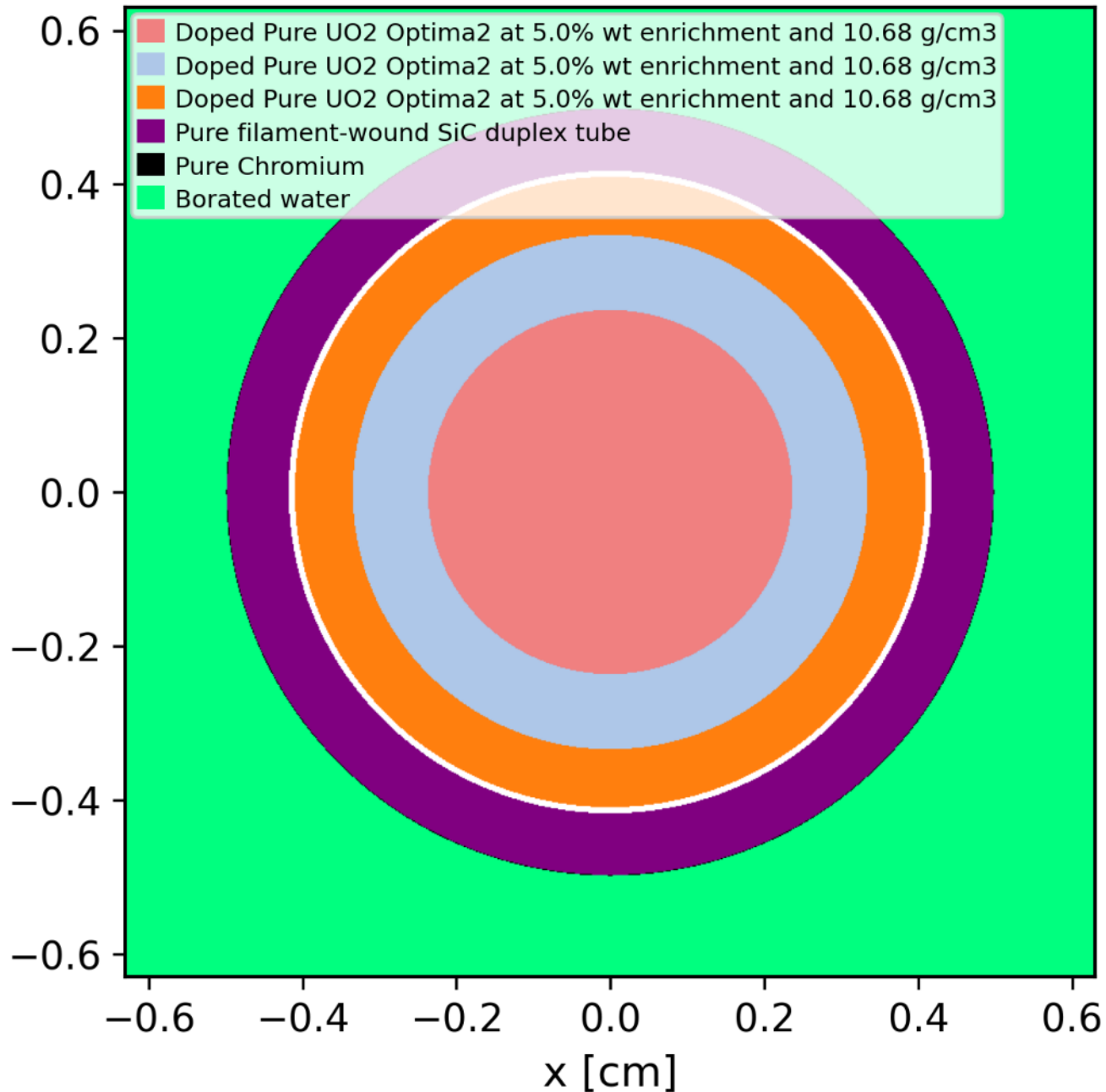
- +20  $\mu\text{m}$  chromium layer [2]
- +0.1 wt% enrichment offset [2]

# ATF2a



- Significant amount of (n, $\gamma$ ) absorbers through FeCrAlC26M [2]
- +0.6 wt% enrichment offset [2]
- Constant pellet + thinner cladding

# ATF3a



- SiC/SiC<sup>[6]</sup>+10 μm chromium layer [7],[8]
- No enrichment offset
- Constant pellet + thicker cladding
- Additional case (ATF3c) with 700 K<sup>[11]</sup> and 1100 K<sup>[12]</sup> for cladding and fuel respectively (lower  $\lambda$ , open gap)<sup>[13]</sup>

# Case comparisons of accident-tolerant fuel pin-cells

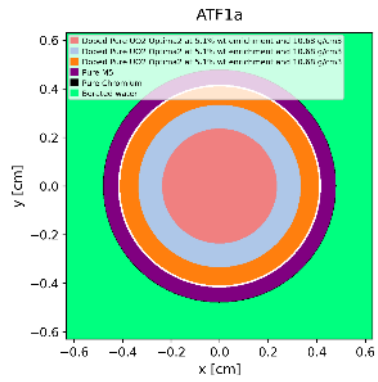
# ATF net impact on $k_{inf}$ and $\Delta\rho$

Reference cell: REF3a doped  $UO_2$  with 5.0% and M5 (0.601 mm)

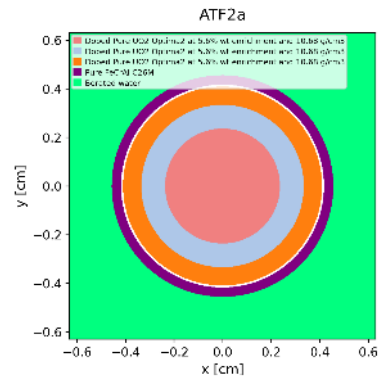
vs.

1. ATF1a doped  $UO_2$  with 5.1% and **M5+20  $\mu\text{m}$  Cr**
2. ATF2a doped  $UO_2$  with 5.6 % and **thinner FeCrAl (0.385 mm)**
3. ATF3a doped  $UO_2$  with 5.0 % and **thicker SiC (0.8 mm) +10  $\mu\text{m}$  Cr**

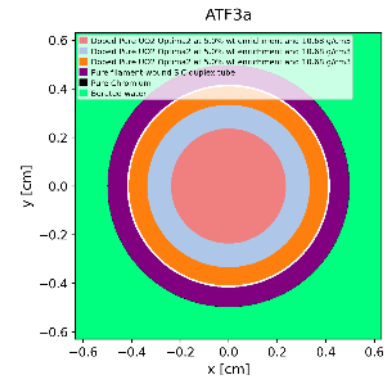




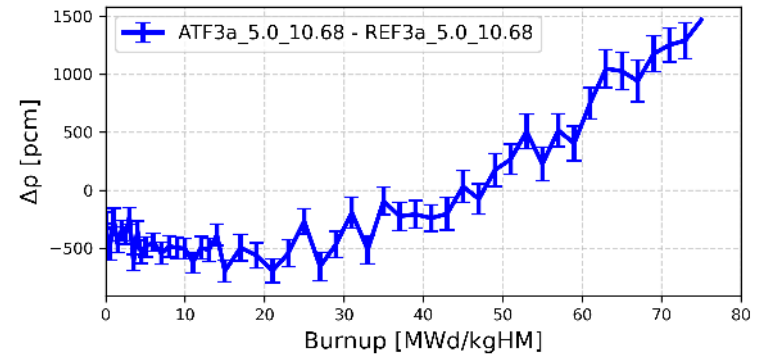
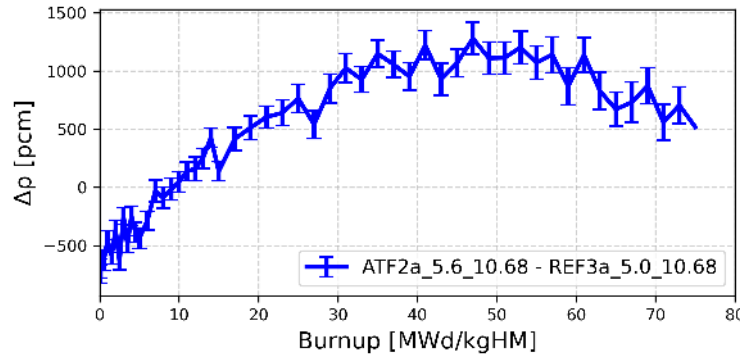
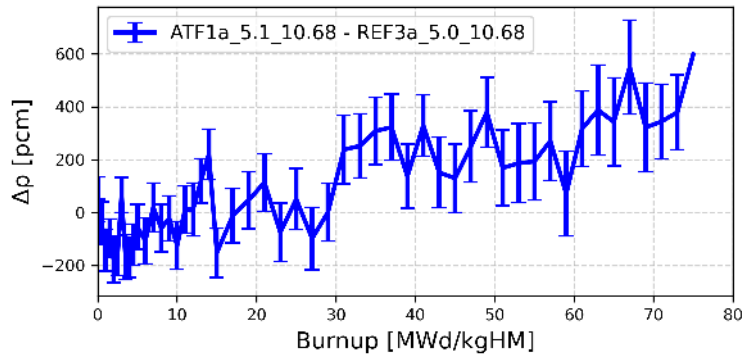
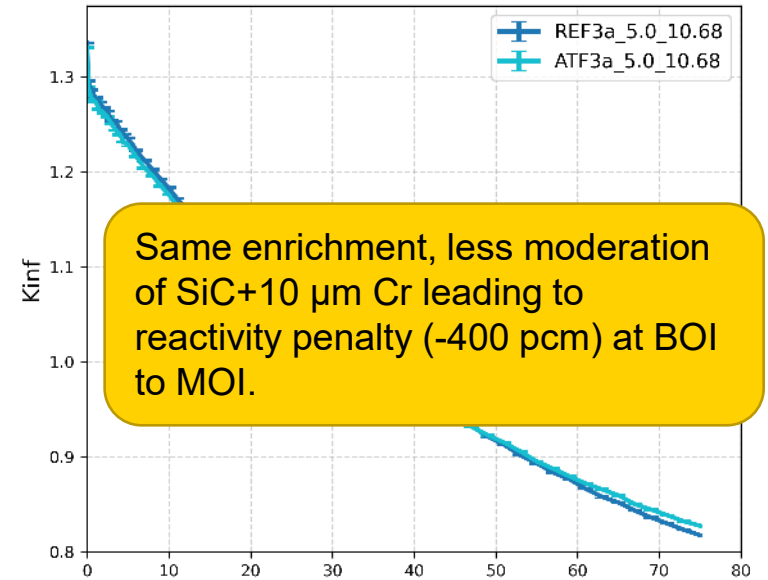
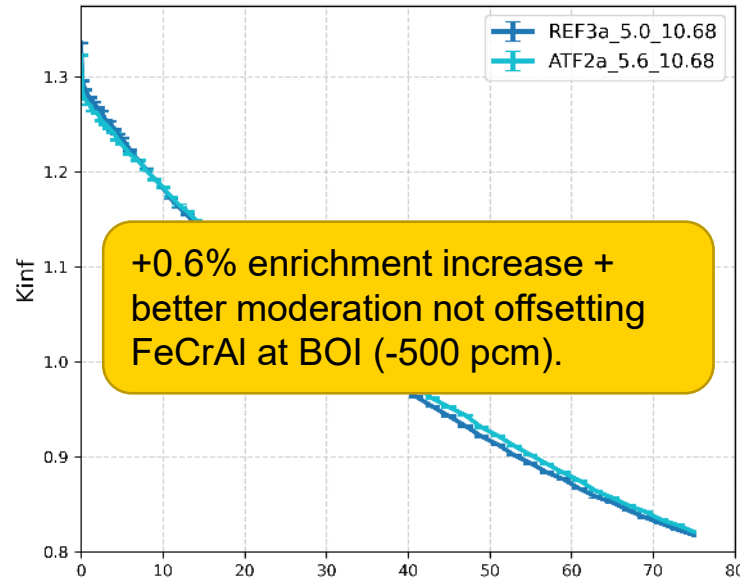
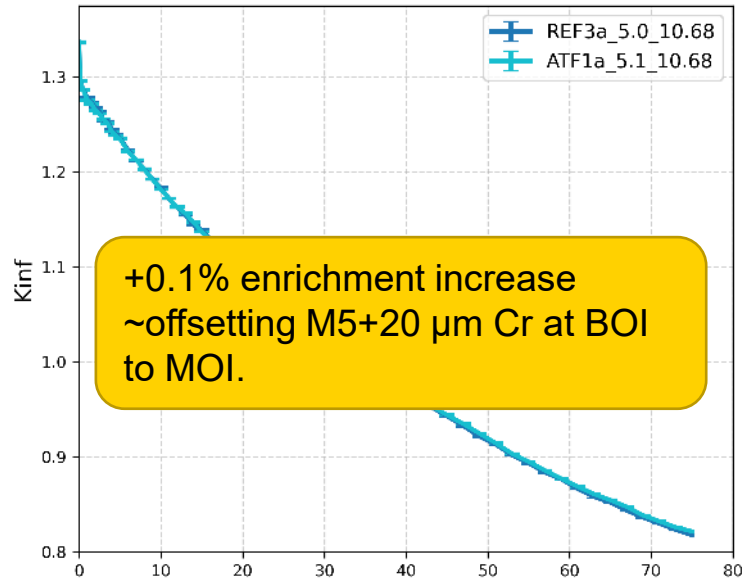
**0.601 mm M5**  
**20  $\mu$ m Cr**  
**5.1%**  
**600 wppm boron**



**0.385 mm FeCrAl**  
**5.6%**  
**600 wppm boron**

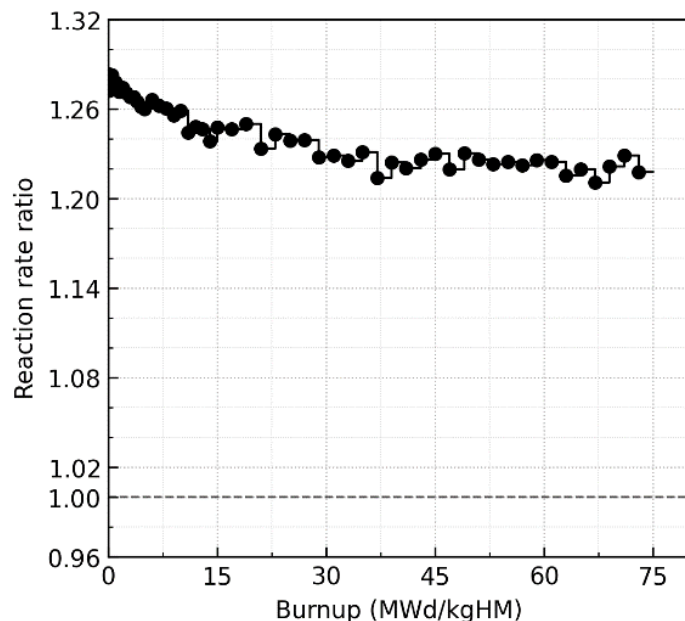


**0.8 mm SiC**  
**10  $\mu$ m Cr**  
**5.0%**  
**600 wppm boron**



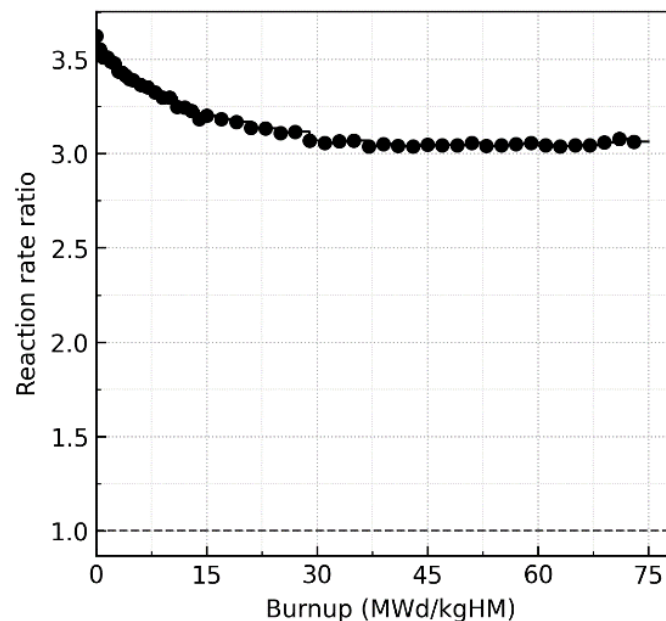
# Clad capture rate ratio comparison

ATF1a/REF3a



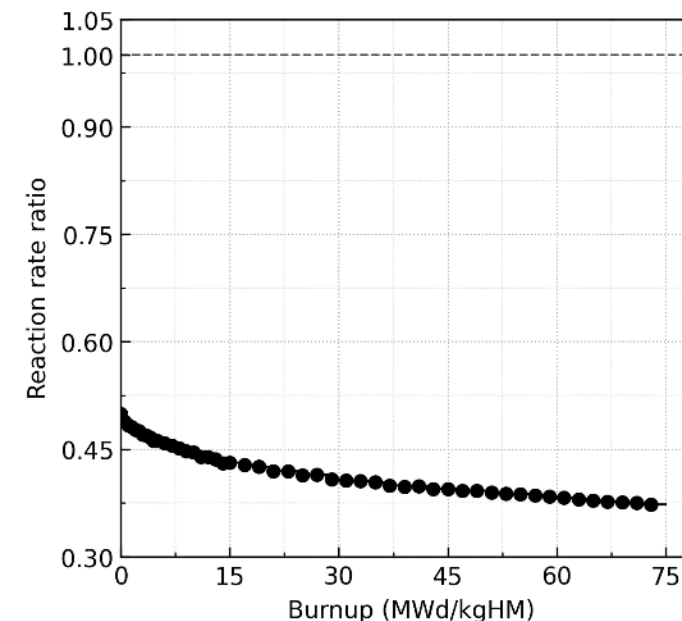
20  $\mu\text{m}$  Cr  $\rightarrow$  ~22% cladding activation rate increase (even at ~same flux level)

ATF2a/REF3a



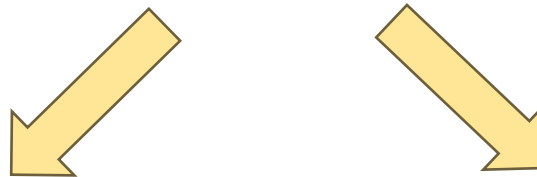
Activation > 3 times higher in thinner FeCrAl (even at lower flux level, minus ~6%).

ATF3a/REF3a



Thicker SiC + 10  $\mu\text{m}$  Cr less than half of M5 activation rate (even at higher flux plus ~+5%)

# Further analysis of $\Delta\rho$ and $k_{inf}$ evolution

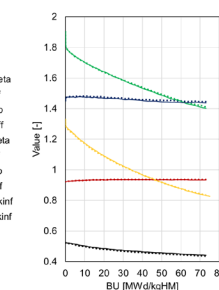
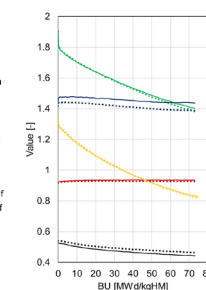
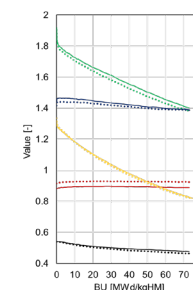
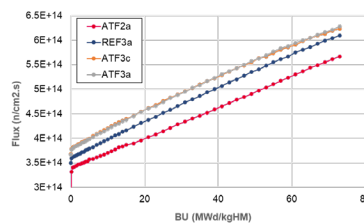
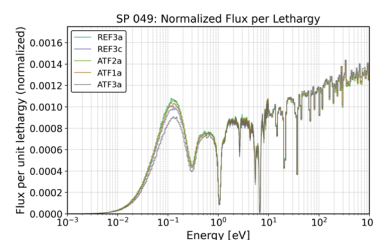
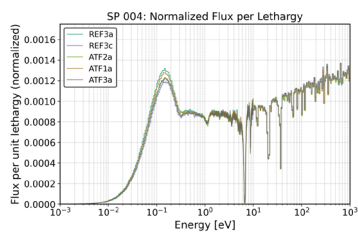


## Analysis of neutron flux shape and neutron flux intensity

Effects of spectral hardening and softening vs. BU different for cases

## Four factor formula evolution with burn-up

- Reproduction  $\eta$
- Thermal utilization  $f$
- Resonance escape probability  $p$
- Fast fission  $\epsilon$



*Deep dive out of scope for this workshop (check my analysis in the annex and discuss with me)!*

# Burn-up conclusions (constant pellet/gap/pitch)

**Enrichment offset is necessary for M5+20 $\mu$ mCr as well as FeCrAlC26m**

→ Safety improvement coming with clad material leads to extra effort for fuel enrichment

**FeCrAlC26M would likely require an adapted boron mngmnt per cycle wrt standard cladding tube**

- Enrichment offset not sufficient at BOI + Reactivity rise-and-fall trend with BU
- Improved moderation ( $p \blacktriangle$ ) for thinner neutron capturing cladding ( $f \blacktriangledown$ ) vs enrichment increase ( $\eta \blacktriangle$ )
- Thicker FeCrAl cladding would impact neutron economy even more significantly.

# Burn-up conclusions (constant pellet/gap/pitch)

## For SiC/SiC (0.8 mm) +10 $\mu$ mCr

- Negative reactivity impact due to moderation reduction (thicker clad at constant pitch)
- Worse moderation ( $p \blacktriangledown \varepsilon \blacktriangle$ ) for thicker neutron-transparent cladding ( $f \blacktriangle$ ).
- Evolution of  $k_{inf}$  very different compared to reference cell ( $\Delta\rho_{BOI}$  -400 pcm, then ever-increasing).
- Additional penalty of ~400 pcm for (more realistic) higher temperature 700K/1100K case at BOI (see ATF3c in annex)
- Need to increase pitch to get back a good H/U ratio, then evaluate enrichment offset necessity (higher pitch  $\blacktriangle \rightarrow$  HM  $\blacktriangledown$  in core volume)  $\rightarrow$  smaller power at same size

# Clad activation comparison: OpenMC vs. FISPACT-II

- JEFF-3.3 library<sup>[21]</sup> for OpenMC<sup>[18],[19]</sup> and FISPACT-II (FP)<sup>[20]</sup>
- Cladding in both codes at 294 K (FP-II ND availability)

# Code benchmark: cladding activation

## Comparing the clad inventory (Bq/cm) in the decay space

- Two type of plots
- 1) **Total activity vs decay time** with dominant nuclides from FP-II as points {half life, activity at  $t_0$ }
  - 2) **Isotopic ratios** of OpenMC/FP vs decay time (nuc > 1% contribution)

**For OpenMC and FISPACT-II users:**

*Check analysis and conclusions in the annex and get in touch!*

Decay time	Description
5min	End of LOCA
10min	LOCA cooling 1
20min	LOCA cooling 2
30min	LOCA cooling 3 (ORNL)
40min	Quench H2 start
115min	Quench H2 end
5d	Core loading (ORNL)
25d	End of outage (ORNL)
100d	Midpoint 1 (ORNL)
500d	Midpoint 2 (ORNL)
5y	Early wet storage end
10y	Late wet storage end
40y	Intermediate storage 1 (ORNL)
100y	Intermediate storage 2

# Accident-tolerant fuel cladding metrics with FP-II



# Clad activity at equal 75 MWd/kgHM<sub>i</sub> (jeff-3.3)

## M5 + 20 μm Cr (6.95e+22 n/cm<sup>2</sup>)

Activity increase up to 100 d (Cr51) ~20% at 5d

## FeCrAlC26m (6.50e+22 n/cm<sup>2</sup>)

0 → 1.15d < M5

- Nb97m, Nb94m, Nb97, Zr97

1.15d → 16y > M5

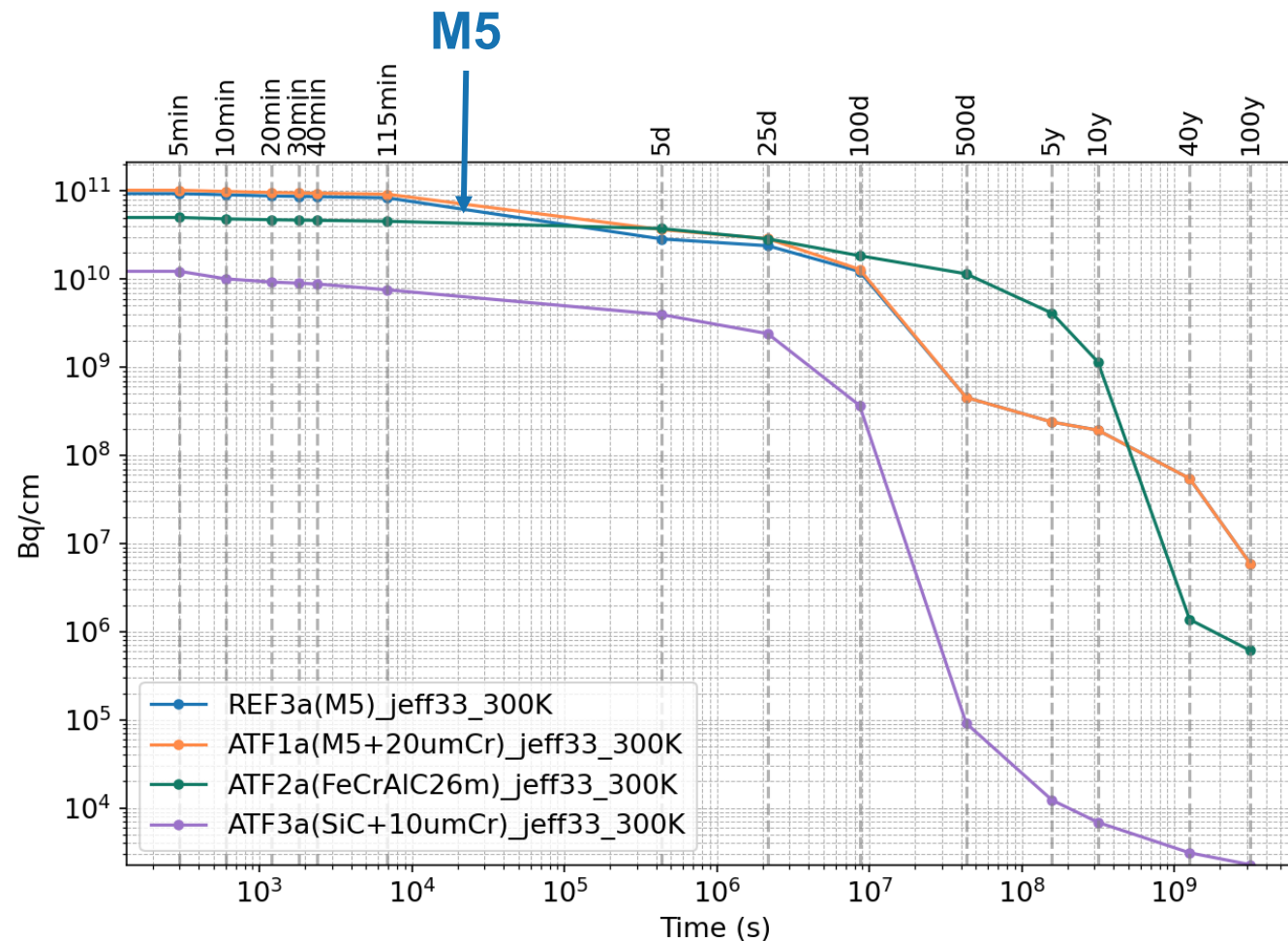
- Cr51, Fe55, Mn54, Co60 vs. Zr95, Nb95

16y → 100y < M5

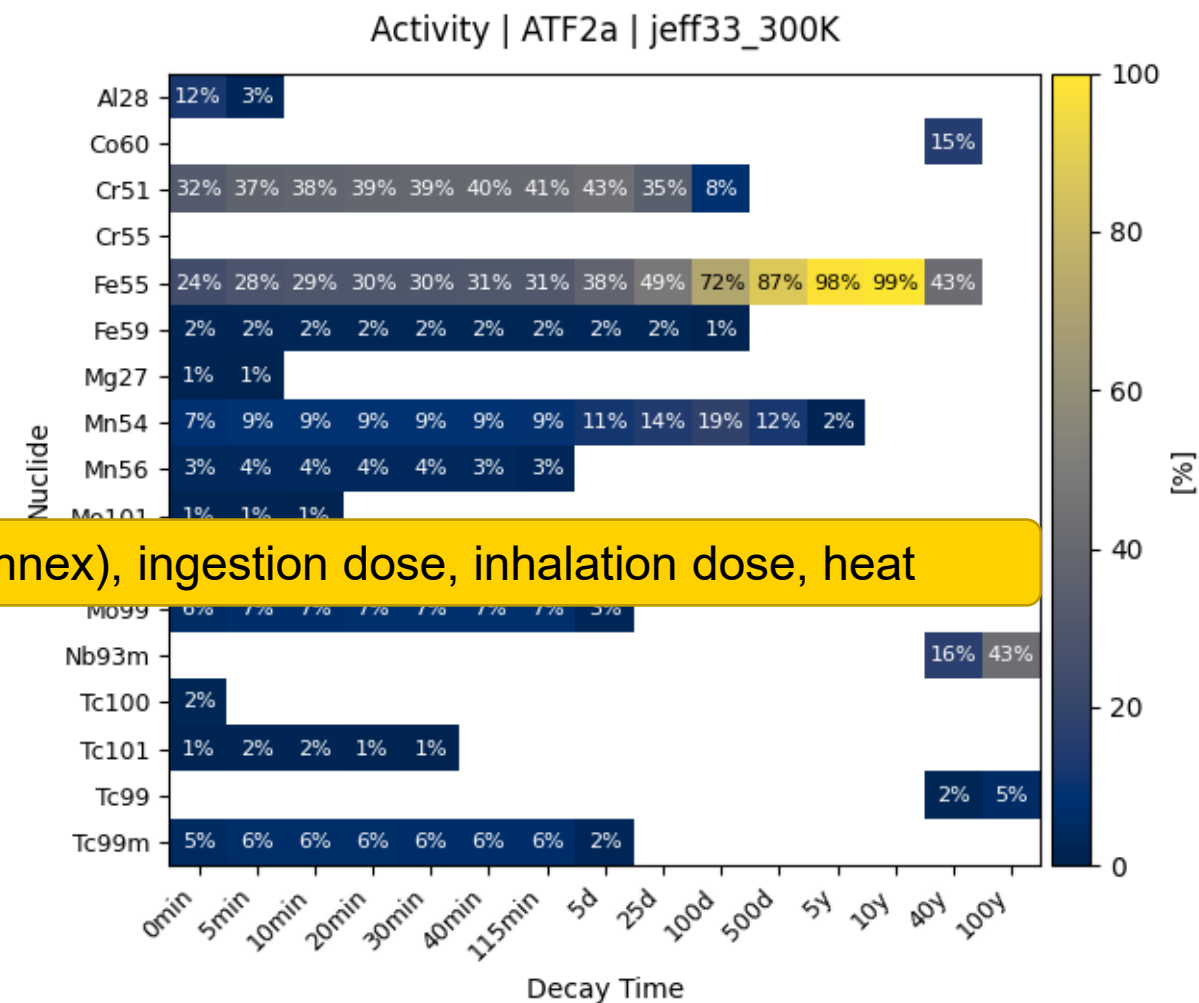
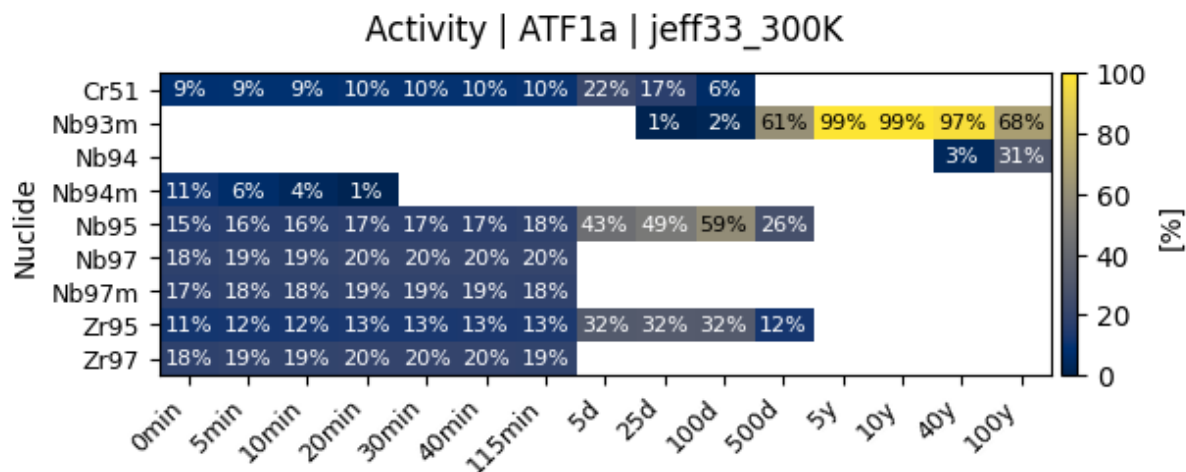
- Mo93 vs. Nb93m, Nb94

## SiC+10 μm Cr (7.25e+22 n/cm<sup>2</sup>)

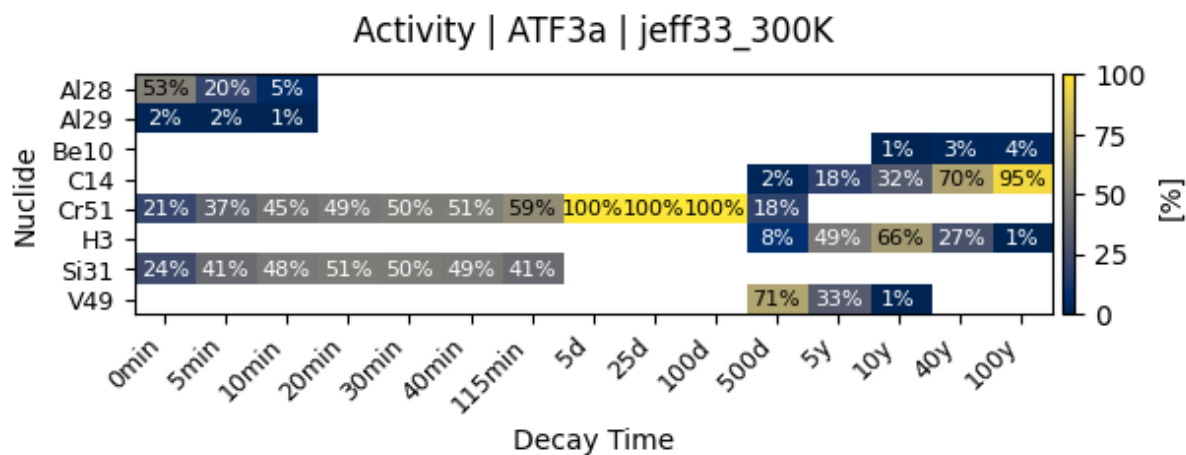
Al28, Si31, V49, H3, C14 + Cr51 < M5



# Activity vector (nuc %) vs decay time



Other possible metrics: contact dose rate (see annex), ingestion dose, inhalation dose, heat



# ATF1a with impurities = ATF1b

Element	wppm
Fe	500
Cr	150
Si	120
C	100
Hf	100
Sn	100
Ta	100
W	100
N	80
Al	75
Ni	70
Cu	50
Mo	50
Ti	50
V	50
Ca	30
Pb	30
H	25
Mg	20
Mn	20
Co	10
U	3.5
B	0.5
Cd	0.5

## Impact of impurities on cladding activity

- M5 at maximum impurities [27]
- Cr powder at maximum impurities [28],[29]

Additional nuclides (>1%): Co60, Fe55, C14, Ni63, Ta182, Ta183

...

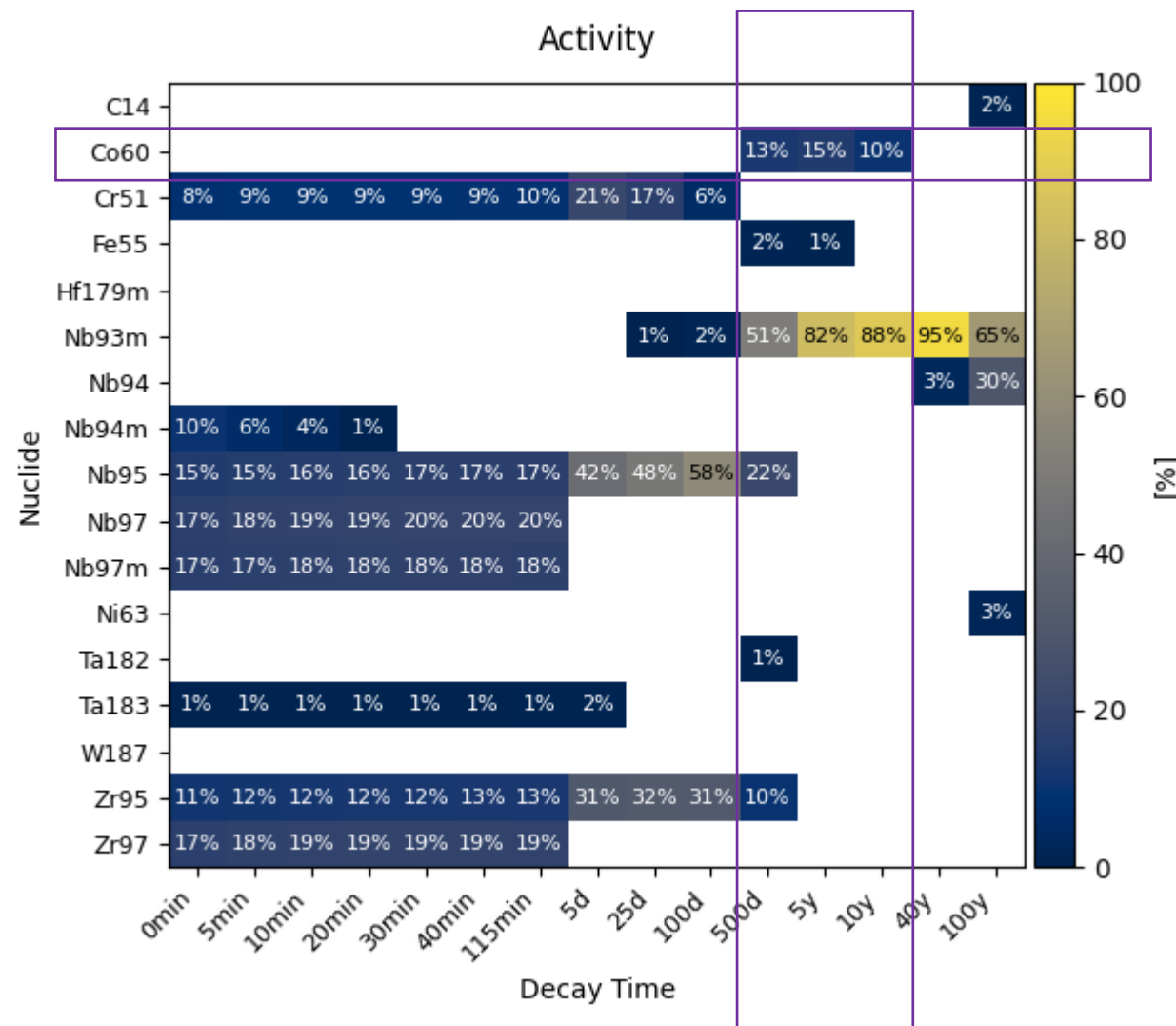
Total activity also increased by ~15% at 5y (Co60) → RP impact

...

100 ppm of Ta (Ta-181)

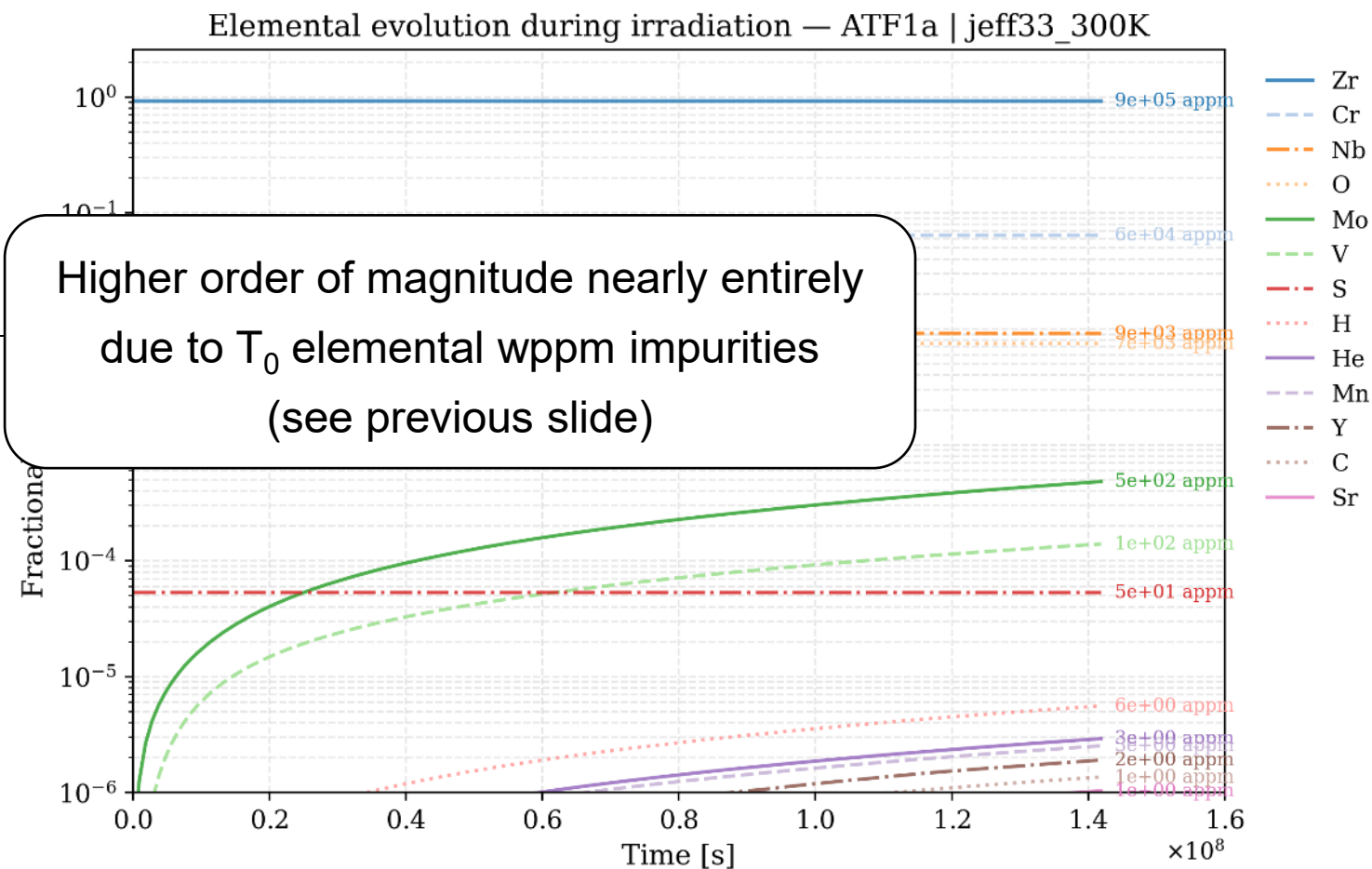
10 ppm Co (Co-59)

70 ppm Ni (Ni-62)



# M5+Cr: Evolution of elemental appm (>1appm)

	ATF1a	ATF1b	
Mo	5e+02	5e+02	
H	6e+00	2e+03	
He	3e+00	5e+00	
Y	2e+00	2e+00	
C	1e+00	7e+02	
V	1e+02	2e+02	
Mn	3e+00	3e+01	
Os		3e+00	Tungsten
Re		5e+00	Tungsten
Sr		1e+00	Uranium



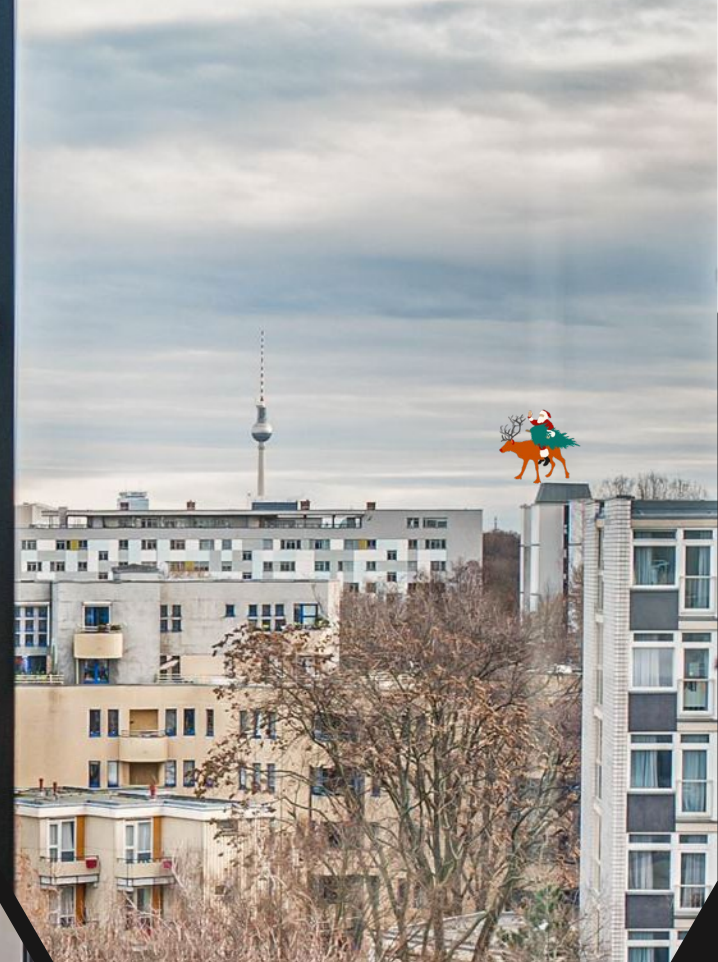
# Outlook and conclusions

# Outlook and conclusions

- More in depth comparison with ORNL report [2] and other publications.
- Simulation of FeCrAl and SiC+Cr with impurities.
- New material developments and fuel (pin cell) designs (impurity levels, nuclear data) can be analyzed with the complementary use of OpenMC and FISPACT-II.
- BASE-F4 is open to support related research projects with the presented simulation tools.



Thank you very much for your attention —  
it is greatly appreciated!



# References (1)

- 1 Arborelius, Jakob; Backman, Karin; Hallstadius, Lars; Limbäck, Magnus; Nilsson, Jimmy; Rebensdorff, Björn et al. (2006): Advanced Doped UO<sub>2</sub> Pellets in LWR Applications. In: Journal of Nuclear Science and Technology 43 (9), S. 967–976. DOI: 10.1080/18811248.2006.9711184.
- 2 Hall, Robert; Sweet, Ryan; Belles, Randy; Wieselquist, William A. (2021): Extended Enrichment Accident Tolerant LWR Fuel Isotopic and Lattice Parameter Trends. Oak Ridge National Laboratory (ORNL) (ORNL/TM-2021/1961).
- 3 M5 composition  
Reaktor-Sicherheitskommission (RSK) (2020): Ergebnisse und Empfehlungen der 514. Sitzung. Online verfügbar unter [http://www.rskonline.de/sites/default/files/reports/epanlagersk514hp\\_0.pdf](http://www.rskonline.de/sites/default/files/reports/epanlagersk514hp_0.pdf), zuletzt geprüft am 05.01.2024.
- 3 M5 density  
Kecek, Adam; Tuček, Kamil; Holmström, Stefan; van Uffelen, Paul (2016): Development of M5 Cladding Material Correlations in the TRANSURANUS Code: Publications Office of the European Union.
- 4 Mitchell, D.; Dunn, B.: Evaluation of Advanced Cladding and Structural Material (M5) in PWR Reactor Fuel. Non Proprietary Version. Framatome Cogema Fuels. 3315 Old Forest Road, Lynchburg, Virginia 24506-0935 (Topical Report BAW-10227-A).
- 5 Haynes, T. A.; Shepherd, D.; Wenman, M. R. (2020): Preliminary modelling of crack nucleation and propagation in SiC/SiC accident-tolerant fuel during routine operational transients using peridynamics. In: J. Nucl. Mater. 540, S. 152369. DOI: 10.1016/j.jnucmat.2020.152369.
- 6 SiC/SiC duplex tube architecture (60 v% SiC composite + 40 v% CVD SiC)  
SiC composite architecture (20 v% Hi-Nicalon Type S fiber + 80 v% CVI SiC)  
Density of duplex tube, monolithic CVD and CVI SiC  
Koyanagi, Takaaki; Hu, Xunxiang; Petrie, Christian M.; Singh, Gyanender; Ang, Caen; Deck, Christian P. et al. (2024): Hermeticity of SiC/SiC composite and monolithic SiC tubes irradiated under radial high-heat flux. In: J. Nucl. Mater. 588, S. 154784.
- 6 Density of Hi-Nicalon Type S fiber  
Noda, Tetsuji; Fujita, Mitsutane; Araki, Hiroshi; Kohyama, Akira (2002): Effect of nuclear data and impurities on the evaluation of induced activity of CVI SiCf/SiC composites. In: Fusion Engineering and Design 61, S. 711–716.
- 7 Quillin, Kyle; Yeom, Hwasung; Dabney, Tyler; Willing, Evan; Sridharan, Kumar (2022): Microstructural and nanomechanical studies of PVD Cr coatings on SiC for LWR fuel cladding applications. In: Surface and Coatings Technology 441, S. 128577.
- 8 Mouche, Peter A.; Koyanagi, Takaaki; Patel, Deep; Katoh, Yutai (2021): Adhesion, structure, and mechanical properties of Cr HiPIMS and cathodic arc deposited coatings on SiC. In: Surface and Coatings Technology 410, S. 126939.
- 9 McCarthy, Kathryn A.; Dixon, B.; Choi, Yong-Joon; Boucher, L.; Ono, Kiyoshi; Alvarez-Velarde, Francisco et al. (2012): Benchmark Study on Nuclear Fuel Cycle Transition Scenarios - Analysis Codes. Organisation for Economic Co-Operation and Development, Nuclear Energy Agency - OECD/NEA. Le Seine Saint-Germain, 12 boulevard des Iles, F-92130 Issy-les-Moulineaux (France) (NEA/NSC/WPFC/DOC(2012)16). Online verfügbar unter <https://inis.iaea.org/records/0txzt-4km86/files/44089401.pdf?download=1>, zuletzt geprüft am 06.10.2025.
- 10 Papukchiev, Angel (2008): Methoden zur Optimierung der Kernauelegung von Druckwasserreaktoren mit reduziertem Borsäureeinsatz. Dissertation. Technische Universität München. Fakultät für Elektrotechnik und Informationstechnik. Online verfügbar unter <https://mediatum.ub.tum.de/625419>, zuletzt geprüft am 06.10.2025.



## References (2)

- 11 Increased by 100 K in comparison to M5 for 225 W/cm and conductivities of 15 and 5 W/m.K for M5 and SiC respectively assuming that SiC conductivity range in [6] for 155 W/cm is applicable.  
M5 conductivity  
Geelhood, K.; Luscher, W.; Porter, I.; Kyriazidis, L.; Goodson, C.; Torres, E. (2020): MatLib-1.0: Nuclear Material Properties Library. In: PNNL-29728.
- 12 George, Nathan Michael; Terrani, Kurt; Powers, Jeff; Worrall, Andrew; Maldonado, Ivan (2015): Neutronic analysis of candidate accident-tolerant cladding concepts in pressurized water reactors. In: Annals of Nuclear Energy 75, S. 703–712.
- 13 Ben-Belgacem, M.; Richet, Victor; Terrani, Kurt A.; Kato, Yutai; Snead, Lance Lewis (2014): Thermo-mechanical analysis of LWR SiC/SiC composite cladding. In: J. Nucl. Mater. 447 (1-3), S. 125–142.
- 14 Sublet, Jean-Christophe; Fleming, Michael; Gilbert, Mark R. (2017): From cutting-edge pointwise cross-section to groupwise reaction rate: A primer. In: EPJ Web Conf 146, S. 2003. DOI: 10.1051/epjconf/201714602003.  
UKAEA-1102: [https://fispact.ukaea.uk/wiki/UKAEA-1102\\_group\\_structure](https://fispact.ukaea.uk/wiki/UKAEA-1102_group_structure)  
CCFE-709: [https://fispact.ukaea.uk/wiki/CCFE-709\\_group\\_structure](https://fispact.ukaea.uk/wiki/CCFE-709_group_structure)
- 15 Žerovnik, Gašper (2024): Characterisation of spent LWR fuel with SMR-relevant initial compositions and operational conditions. Federal Office for the Safety of Nuclear Waste Management (BASE). IAEA. Vienna, 21.10.2024. Online verfügbar unter <https://conferences.iaea.org/event/374/contributions/31353/>, zuletzt geprüft am 07.10.2025.
- 16 Häkkinen, Silja (2020): Impurities in LWR fuel and structural materials. VTT Technical Research Centre of Finland (VTT Research Report No. VTT-R-00184-20). Online verfügbar unter <https://cris.vtt.fi/en/publications/impurities-in-lwr-fuel-and-structural-materials>, zuletzt geprüft am 06.10.2025.
- 17 Terrani, Kurt A. (2018): Accident tolerant fuel cladding development: Promise, status, and challenges. In: J. Nucl. Mater. 501, S. 13–30.
- 18 Romano, Paul K.; Horelik, Nicholas E.; Herman, Bryan R.; Nelson, Adam G.; Forget, Benoit; Smith, Kord (2015): OpenMC: A state-of-the-art Monte Carlo code for research and development. In: Annals of Nuclear Energy 82, S. 90–97.
- 19 Romano, Paul K.; Josey, Colin J.; Johnson, Andrew E.; Liang, Jingang (2021): Depletion capabilities in the OpenMC Monte Carlo particle transport code. In: Annals of Nuclear Energy 152, S. 107989.
- 20 Sublet, J-Ch; Eastwood, J. W.; Morgan, J. G.; Gilbert, Fleming, M.; Arter, W. (2017): FISPACT-II: an advanced simulation system for activation, transmutation and material modelling. In: Nuclear Data Sheets 139, S. 77–137.
- 21 Plompen, Arjan J. M.; Cabellos, O.; Saint Jean, Cyrille de; Fleming, Michael; Algora, A.; Angelone, Maurizio et al. (2020): The joint evaluated fission and fusion nuclear data library, JEFF-3.3. In: The European Physical Journal A 56 (7), S. 181.
- 22 Koning, A. J.; Rochman, D.; Sublet, J-Ch; Dzysiuk, N.; Fleming, M.; van der Marck, S. (2019): TENDL: complete nuclear data library for innovative nuclear science and technology. In: Nuclear Data Sheets 155, S. 1–55.
- 23 Mickus, Ignas (2021): Towards Efficient Monte Carlo Calculations in Reactor Physics: Criticality, Kinetics and Burnup Problems. KTH Royal Institute of Technology.
- 24 Radhakrishnan, Krishnan; Hindmarsh, Alan C. (1993): Description and use of LSODE, the Livermore solver for ordinary differential equations.
- 25 Kluyver, Thomas; Ragan-Kelley, Benjamin; Pérez, Fernando; Granger, Brian E.; Bussonnier, Matthias; Frederic, Jonathan et al. (2016): Jupyter Notebooks—a publishing format for reproducible computational workflows. In: Elpub 2016, S. 87–90.
- 26 Thomas, Fred; Fleming, Michael (2018): Optimised energy group structures for fusion activation calculations. In: Fusion Engineering and Design 136, S. 1479–1483.

# References (3)

- 27 Parga, Clemente J. (2018): M5 Alloy Specification for TREAT Conceptual Fuel Cladding Selection. Idaho National Lab.(INL), Idaho Falls, ID (United States). Online verfügbar unter <https://www.osti.gov/biblio/1484704>, zuletzt geprüft am 15.10.2025.
- 28 99.8 % powder purity reported  
Yeom, Hwasung; Dabney, Tyler; Johnson, Greg; Maier, Benjamin; Lenling, Mia; Sridharan, Kumar (2019): Improving deposition efficiency in cold spraying chromium coatings by powder annealing. In: The International Journal of Advanced Manufacturing Technology 100, S. 1373–1382.
- 29 Atlantic Equipment Engineers (2025): Datasheet CR-102-105, Chromium Powder, Electrolytic. Online verfügbar unter <https://docs.google.com/document/d/1nOtHzZLs93N8a96WYtCCJGtKnPxhrXcD/edit>, zuletzt geprüft am 17.01.2025.
- 30 J. Lieberoth, "A Monte Carlo Technique to Solve the Static Eigenvalue Problem of the Boltzmann Transport Equation," Nukleonik, 11, 213-219 (1968).
- 31 Pusa, M., & Leppänen, J. (2010). Computing the Matrix Exponential in Burnup Calculations. Nuclear Science and Engineering, 164(2), 140–150. <https://doi.org/10.13182/NSE09-14>
- 32 Pusa, M. (2011). Rational Approximations to the Matrix Exponential in Burnup Calculations. Nuclear Science and Engineering, 169(2), 155–167. <https://doi.org/10.13182/NSE10-81>
- 33 Maria, P. (2016). Higher-Order Chebyshev Rational Approximation Method and Application to Burnup Equations. Nuclear Science and Engineering, 182(3), 297–318. <https://doi.org/10.13182/NSE15-26>
- 34 Thalhammer, M. (2006). A fourth-order commutator-free exponential integrator for nonautonomous differential equations. SIAM journal on numerical analysis, 44(2), 851-864.

# Annex

# **BASE missions and tasks**

# BASE – Mission and Tasks

- **Regulation:** Disposal, storage and transport of HLW.



- **Supervision:** Deep geological disposals for LAW and MAW.



- **Site selection:** Repository site process and public participation.



- **Expertise:** Advisory role to the federal ministry.



- **Research:** Conducting and financing task-related research



# Research at BASE

BASE initiates **in-house research projects** and awards **research contracts to companies and institutes** also in the field of nuclear safety (SMR, P&T, ATF)...

## Funding of BASE research

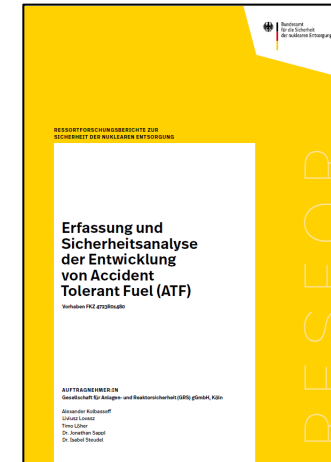
- **Own research budget** (~3.2 M€/a)
- **Personnel expenses** (desk/scientific officers)
- **PhD program** (1 finished, 2 ongoing)
- **Departmental research plan** of the Federal Ministry for the Environment, Climate Action, Nature Conservation and Nuclear Safety (BMUKN)



# Research regarding accident-tolerant fuels

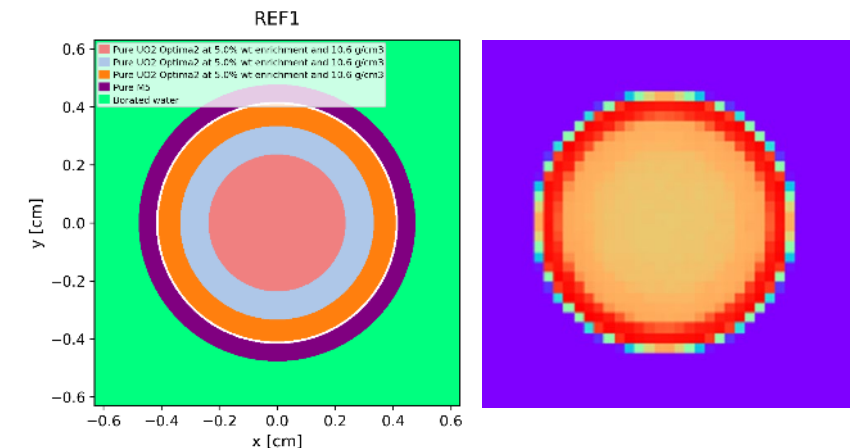
## Recently finished research project conducted by GRS

- Up-to-date summary of developments
- Simulation of accident scenarios (TMI-2 und Fukushima Daiichi) with FeCrAl cladding with AC2
- [https://www.base.bund.de/de/forschung/themenfelder/nukleare-sicherheit/documents/atf\\_sicherheitsanalyse.html](https://www.base.bund.de/de/forschung/themenfelder/nukleare-sicherheit/documents/atf_sicherheitsanalyse.html)



## Ongoing in-house research project “ReUnFis”

- Period: July 24 to December 26
- Burn-up simulation of pin-cells with M5+20 $\mu$ mCr, FeCrAlC26M, SiC/SiC+10 $\mu$ mCr in OpenMC
- ATF cladding metrics (opt. impurities) with FP-II



# **Constant pellet/gap and pitch impacts**



# Constant pellet impact

## Modelling choice

Constant pellet and gap dimensions & change of cladding outer diameter (at constant pitch)

→  $HM_i \approx \text{constant}$

→ Fair comparison on BU scale (MWd per kgHM<sub>i</sub>)

## Main impacts in ATF cells

1. Reactivity change due to change in cladding thickness (H/U atom ratio change)
2. Reactivity penalty due to cladding neutron capture (FeCrAl, Cr)
3. Reactivity change due to necessary enrichment offset (counterbalance Nr. 2)
4. Differently evolving reactivity impact due to fuel neutron capture (FPs, trans-U, NT-coupled inventory change)

**OpenMC  $k_{inf}$**

# Definition of $k_{inf}$ (in OpenMC)

$$K_{inf} = A / (B-C)$$

A: Fission neutrons produced per src

B: Neutrons absorbed per src

C: Neutrons prod. by (n,xn) per src

**A = Fission rate [fiss/s] \* v [neutrons/fiss]**

All models with same power and energy deposition (heating-local tally)

→ Flux level adjustment to total nuclear heating (eV from reactions)

→ Thermal flux level main driver of heating (fission)

→ Fission rate driven by flux level

→ BU leads to shift in flux level (FPs) and v (U35→Pu39)

**B = Neutron absorption in model (fuel +moderator +clad)**

Main source of evolving neutron poison: neutron capture rate in fuel

+ neutron capture in the cladding

→ For interpretation of  $k_{inf}$  difference

**C: (skipped)**

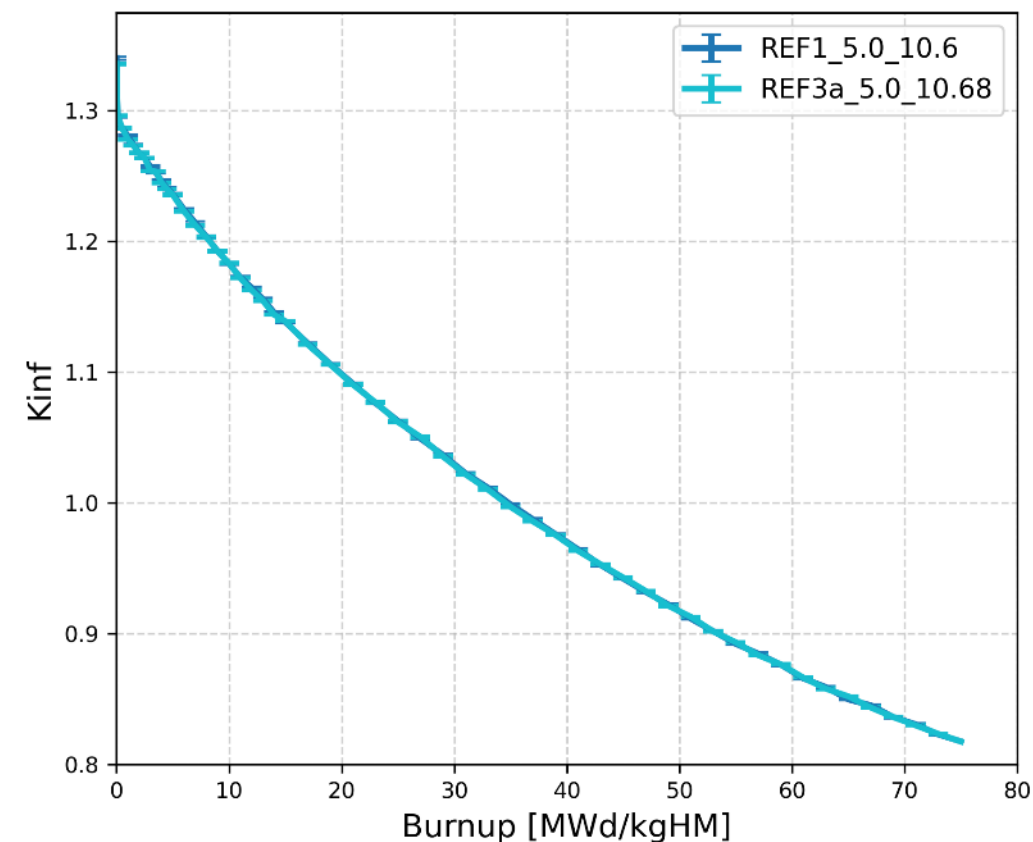
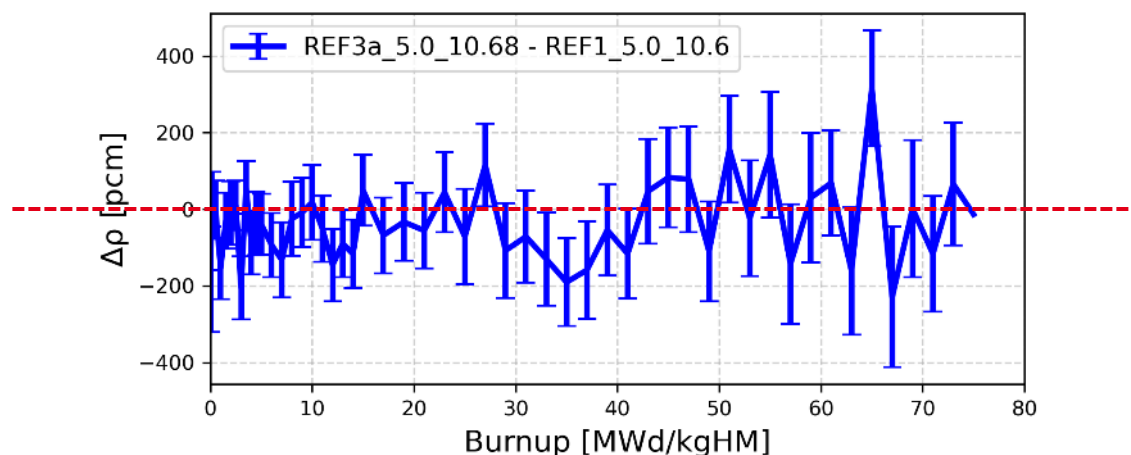
# **OpenMC: Effect of pure dopants**

**Homogenous dilution**

# Impact of doping with $\text{Cr}_2\text{O}_3$ and $\text{Al}_2\text{O}_3$

800 ppm of pure  $\text{Cr}_2\text{O}_3$  and pure 200 ppm  $\text{Al}_2\text{O}_3$   
HM +0.65%, density increase +0.75%

**Reactivity difference around 0.**  
**Negligible impact on reactivity for pure dopants.**

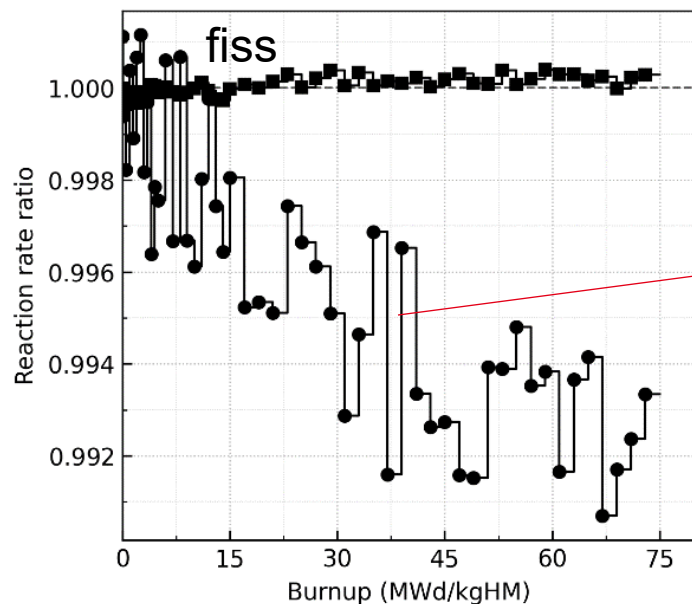


# **Fuel fission and capture rate ratio vs. BU**

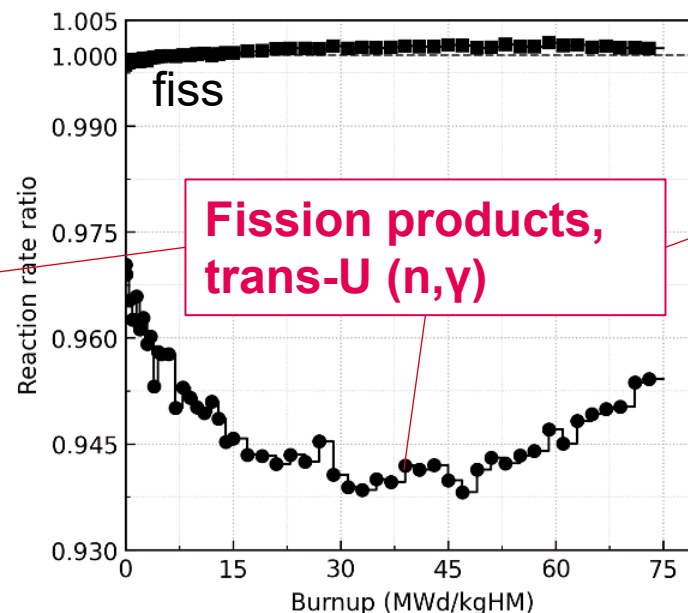
**ATF1a, ATF2a, ATF3a vs REF3a**

# Fuel fission and fuel capture rate case ratios

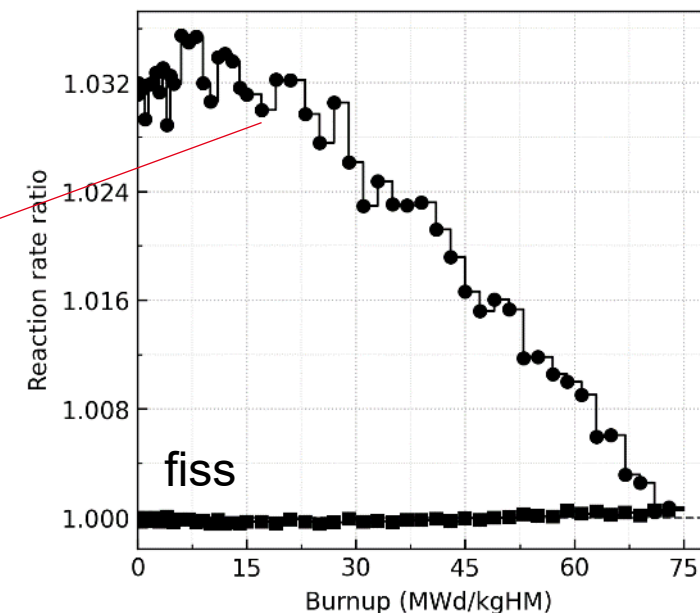
ATF1a/REF3a



ATF2a/REF3a



ATF3a/REF3a



- Decreasing fuel capture rate in ATF1a (wrt REF3a)
- Higher reactivity of ATF1a at later BU

- Lower fuel capture in ATF2a (wrt REF3a).
- Higher clad capture outweighs lower fuel capture at BOI (net reactivity penalty).
- Capture evolution consistent with  $\Delta\rho$  evolution

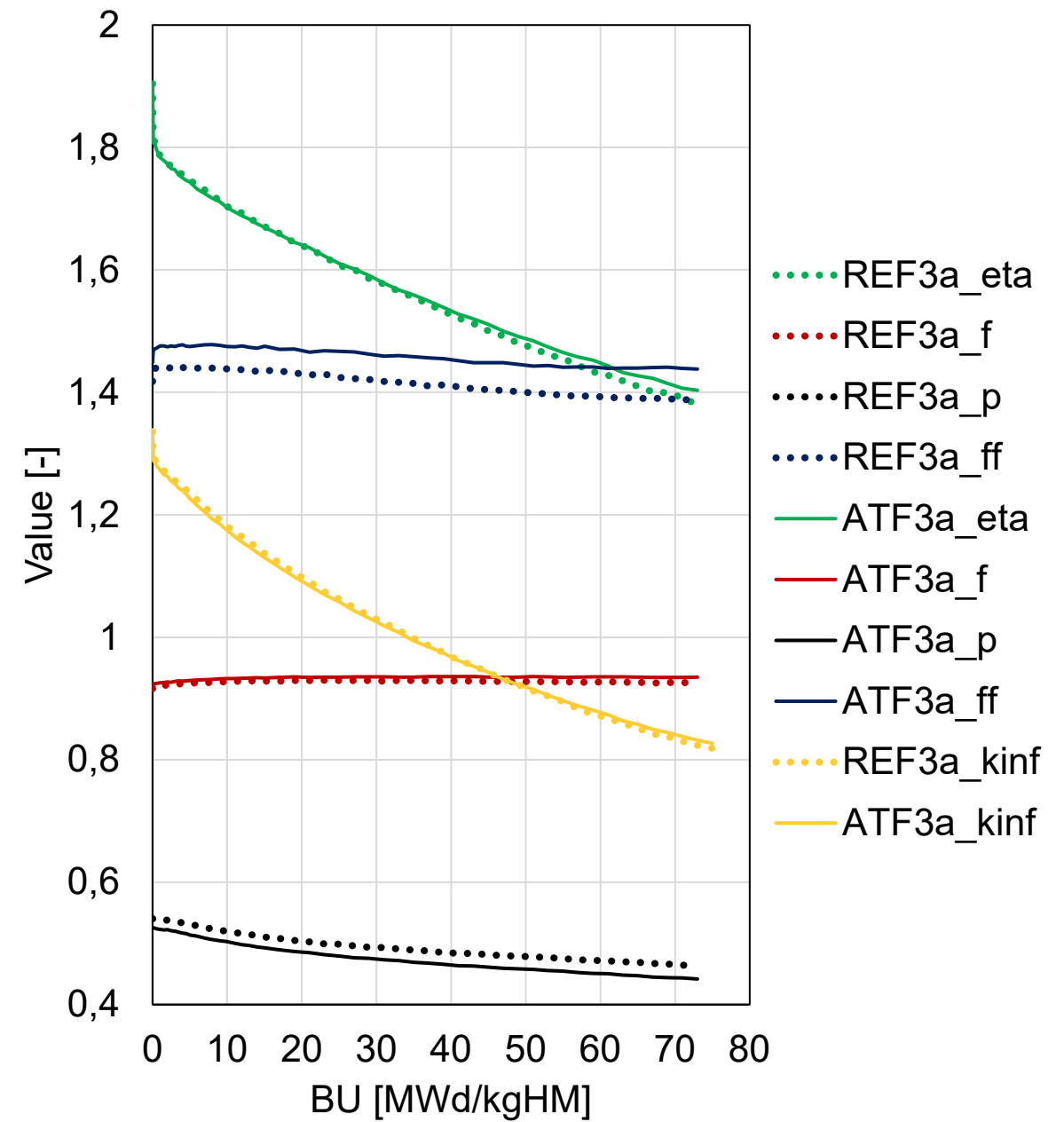
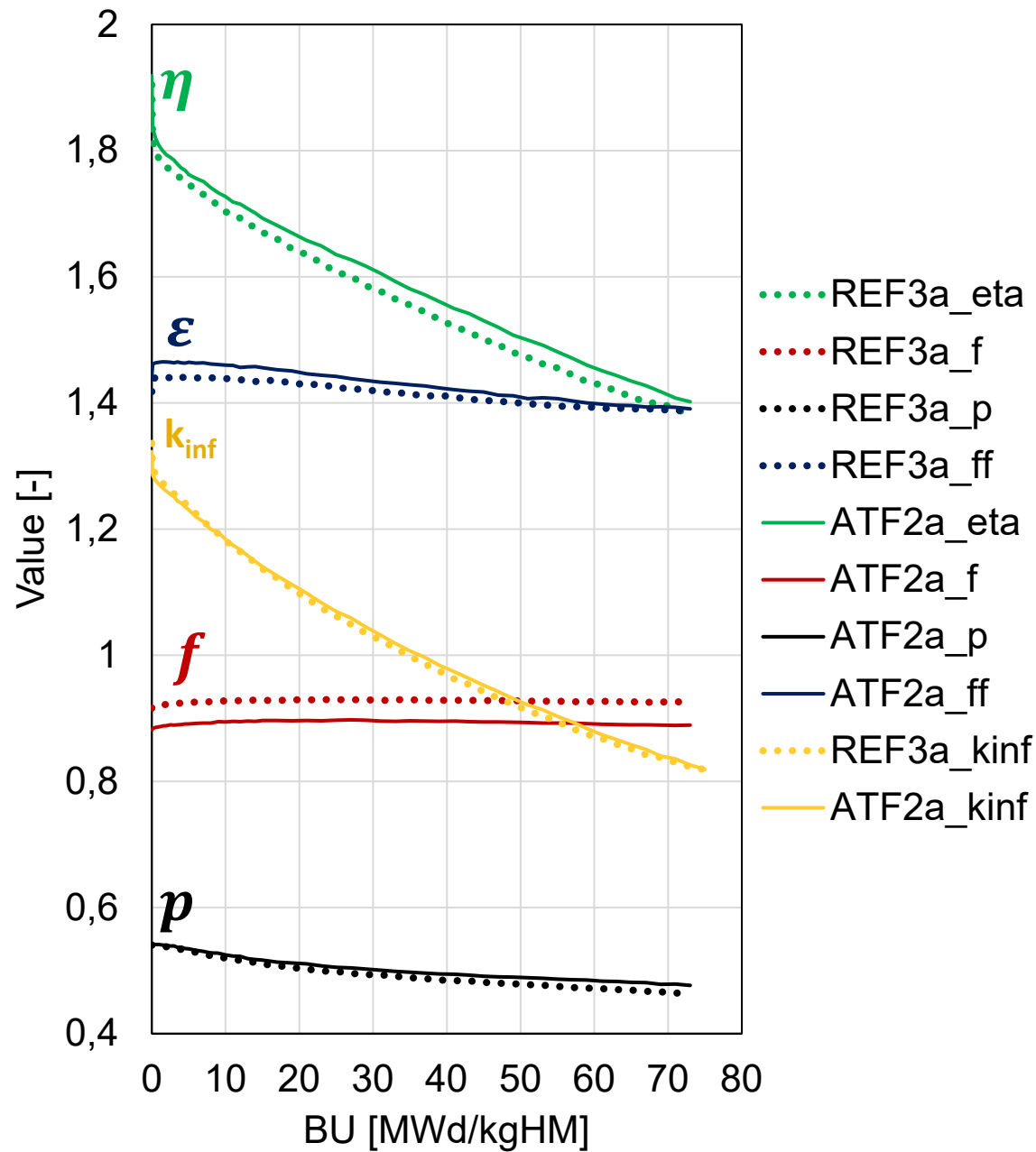
Enrichment  $\blacktriangle$   $\rightarrow$  Flux level  $\blacktriangledown$  + Flux hardening  $\blacktriangle$  (but also hardening  $\blacktriangledown$  due to Moderation  $\blacktriangle$ )

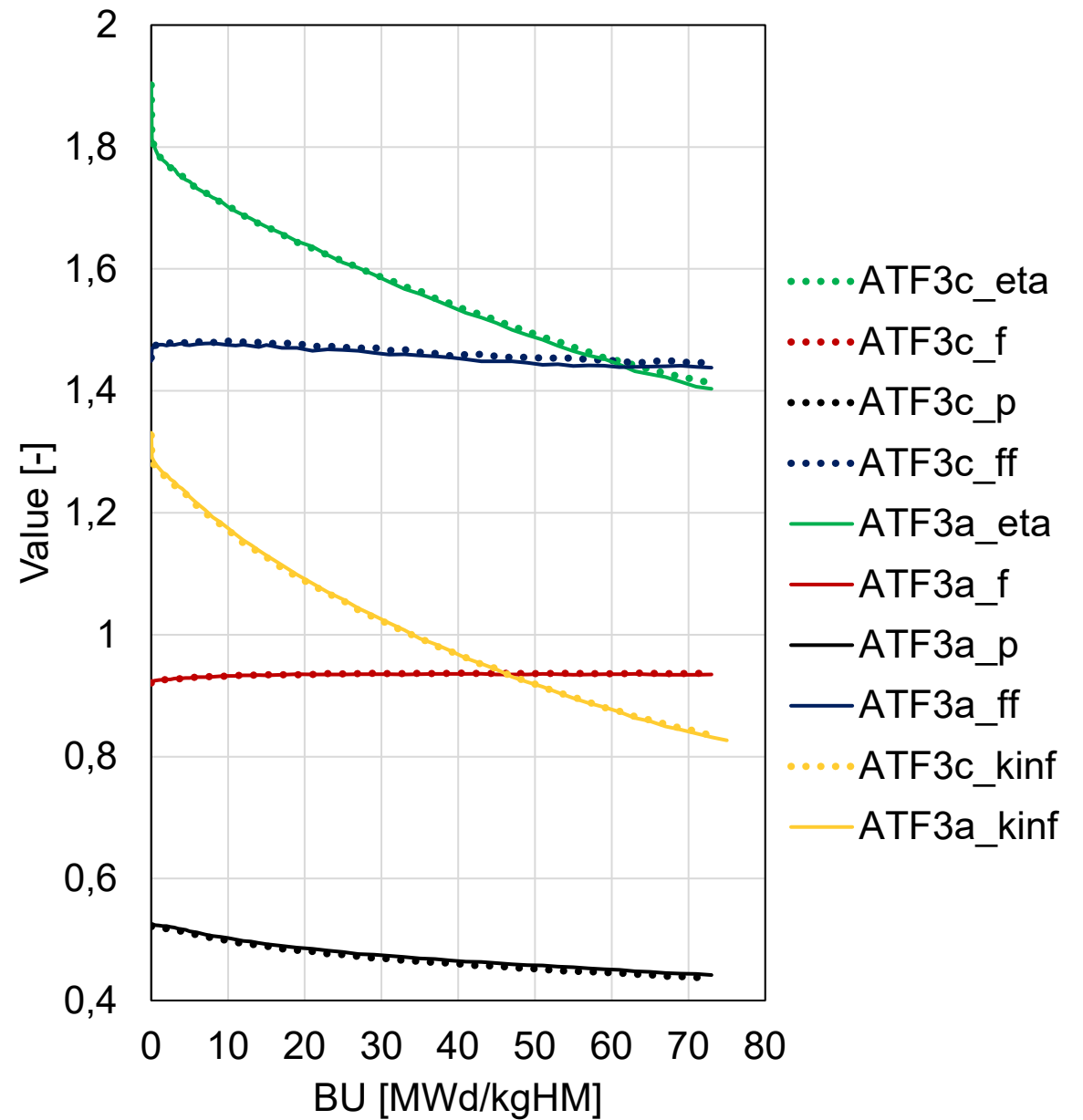
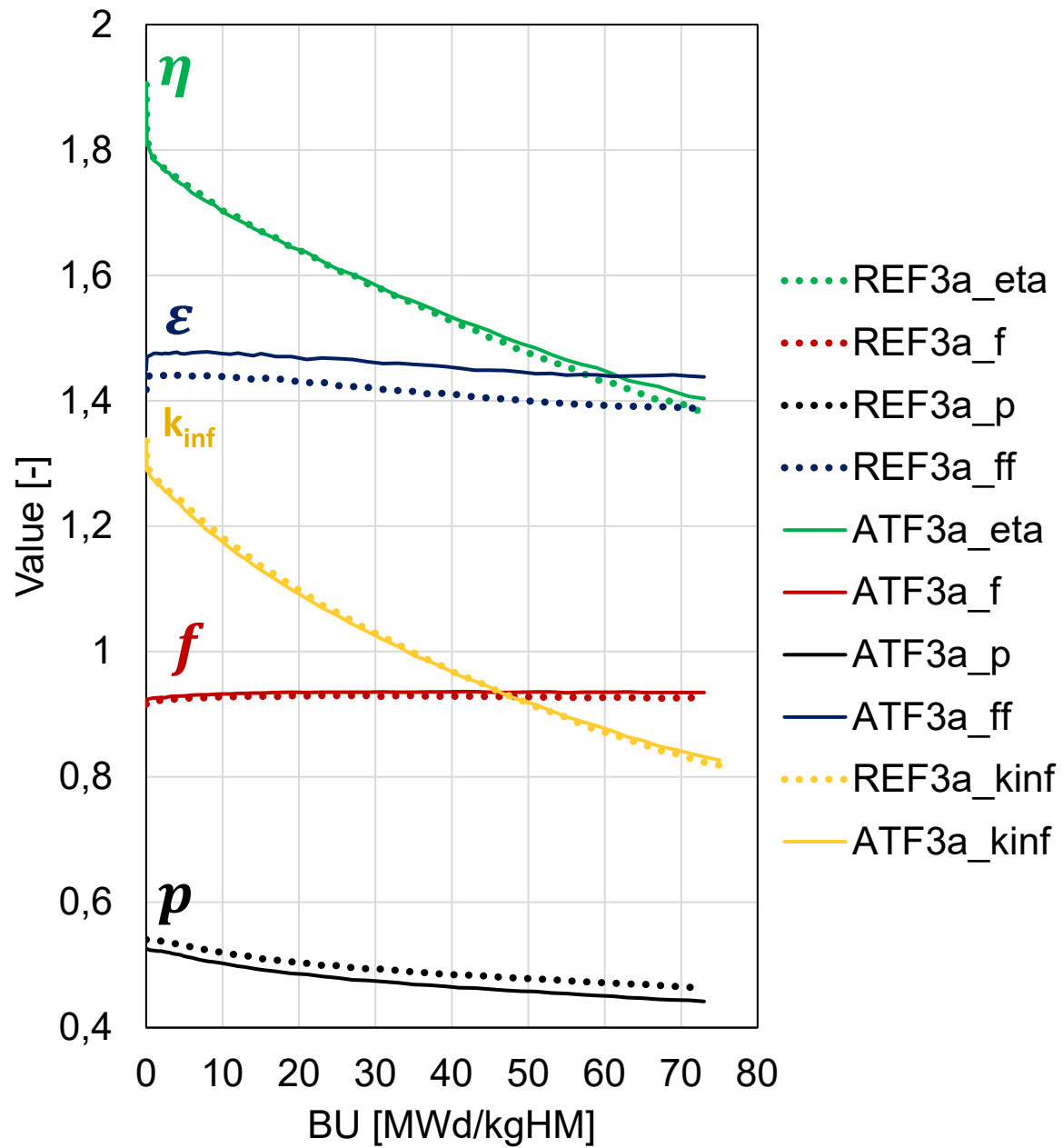
- Higher fuel capture in ATF3a (wrt REF3a).
  - Decreasing fuel capture ratio partly explains increasing reactivity difference.
- Moderation  $\blacktriangledown$   $\rightarrow$  Flux level  $\blacktriangle$  (impacting capture rates)

# **4 factor formula vs BU**

**ATF2a vs REF3a, ATF3a vs REF3a**

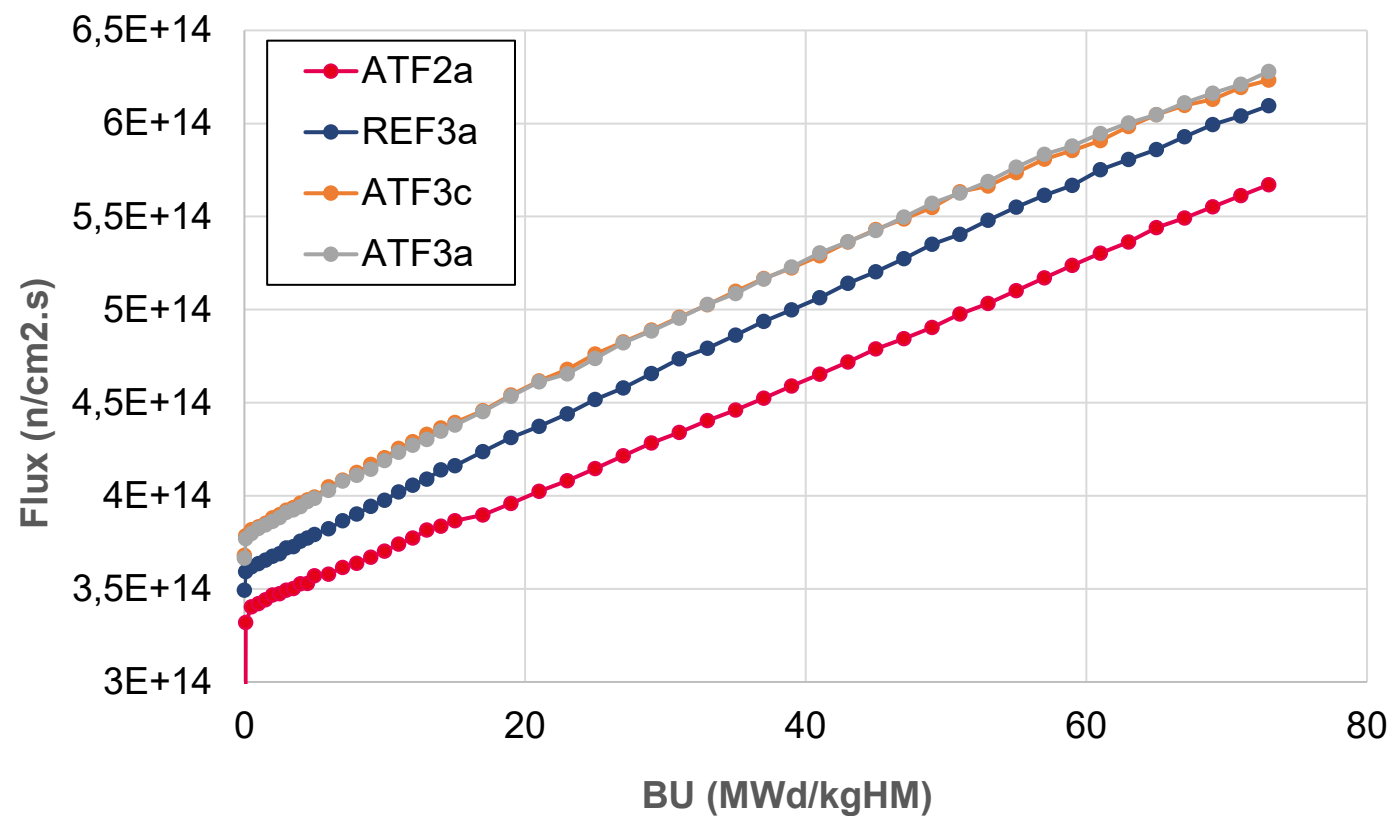






# Flux change with BU

# Flux change with BU (45.7 W/gU<sub>i</sub>, 4.95 gU<sub>i</sub>/cm)



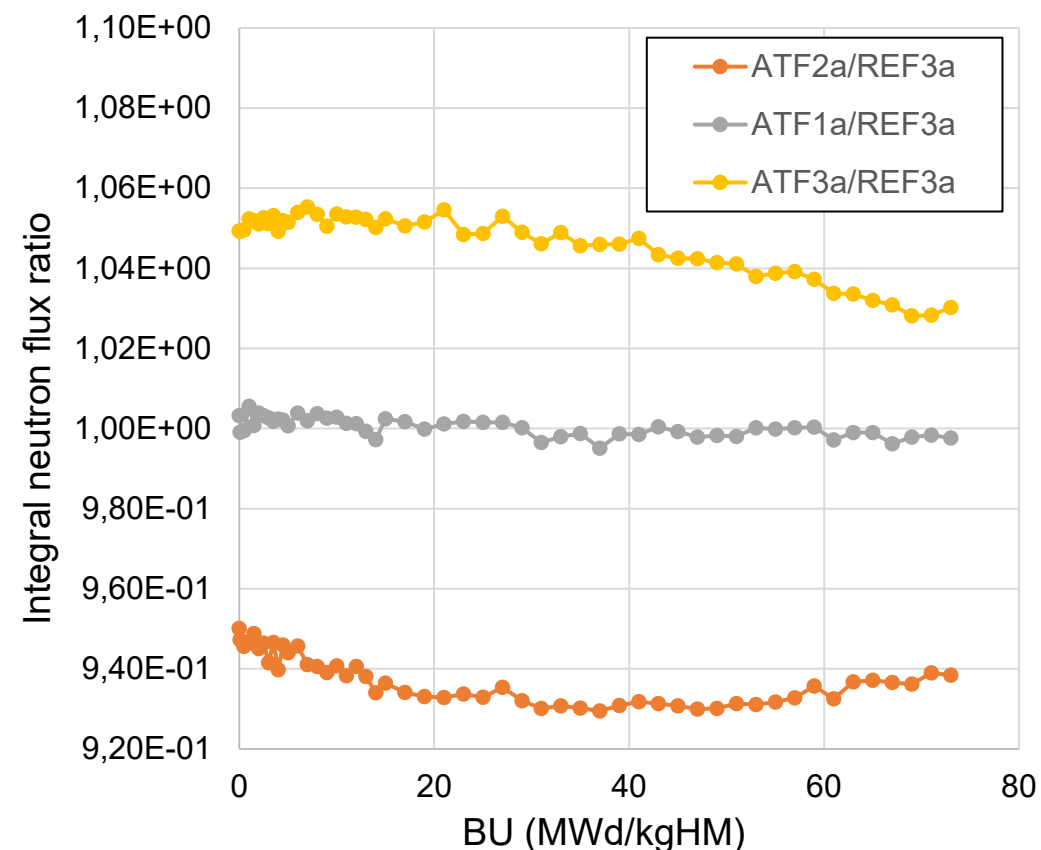
# Spectral shifts

# Flux ratio to REF3a for ATF1a, ATF2a and ATF3a

ATF1a flux level  $\approx$  REF3a flux level

Flux level lowest for **ATF2a** to achieve constant specific power  $\rightarrow$  5.6 wt% and thinnest cladding (better moderation)

**ATF3a** needs highest neutron population (thickest cladding at 5.0 wt%), decreasing flux ratio



# Describing neutron spectrum energy shifts

## Thermal indices

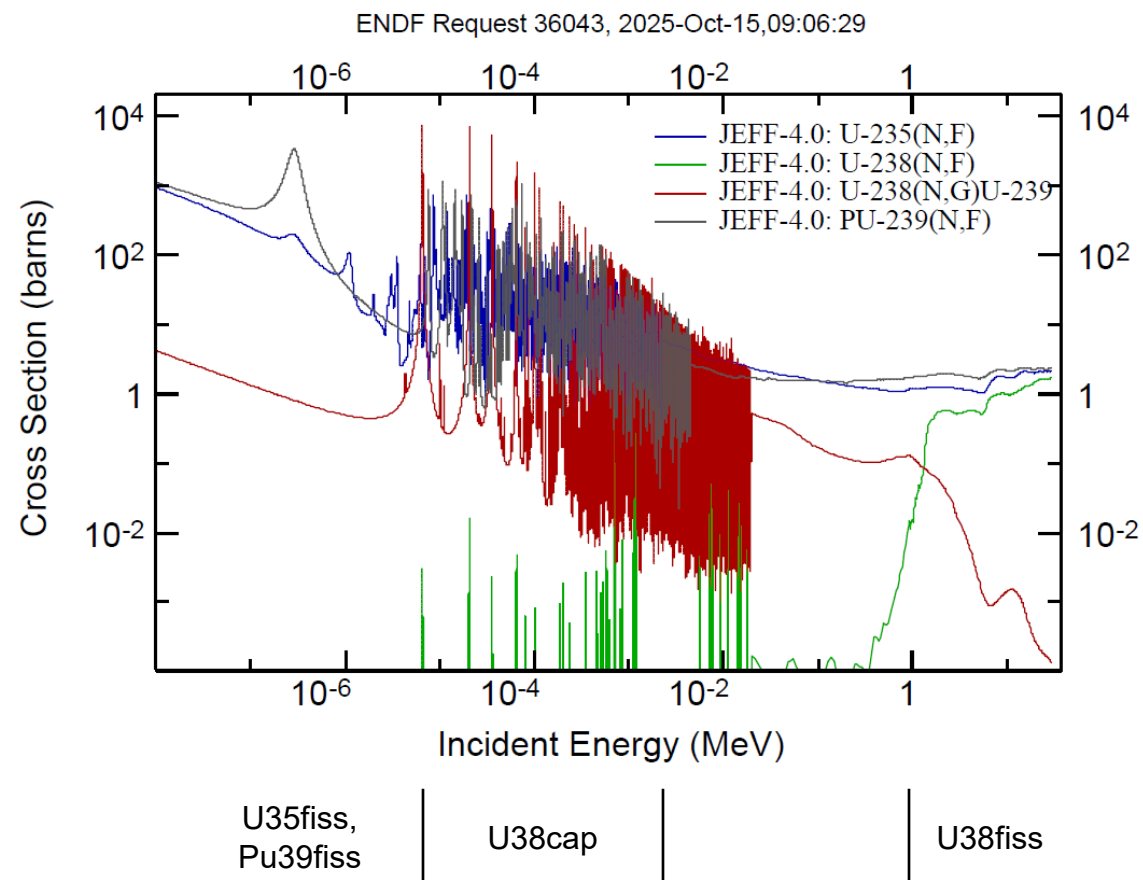
How much fission from P39 and U35 compared to neutrons capture in U38?

- $P39_{fiss}/U38_{cap}$
- $U35_{fiss}/U38_{cap}$

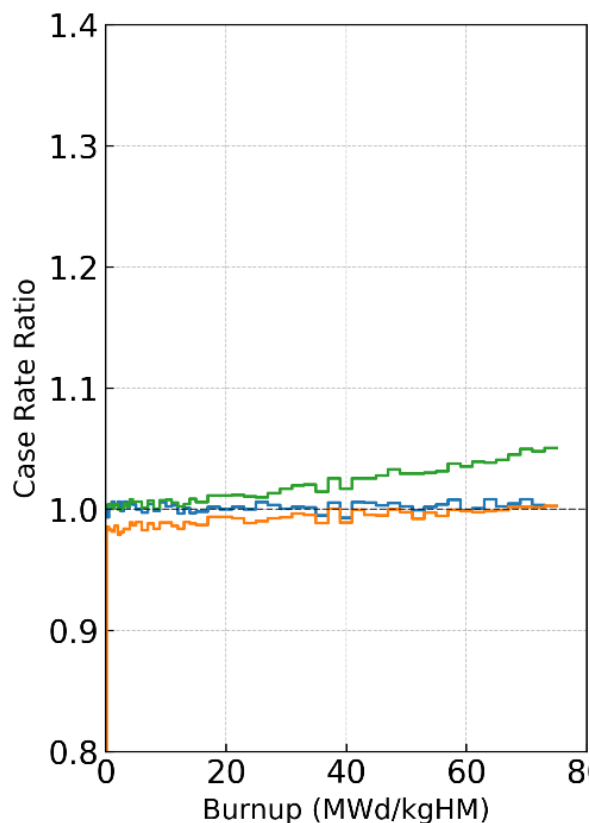
## Fast index

How much U38 threshold fission >1MeV compared to neutron capture in U38?

- $U38_{fiss}/U38_{cap}$

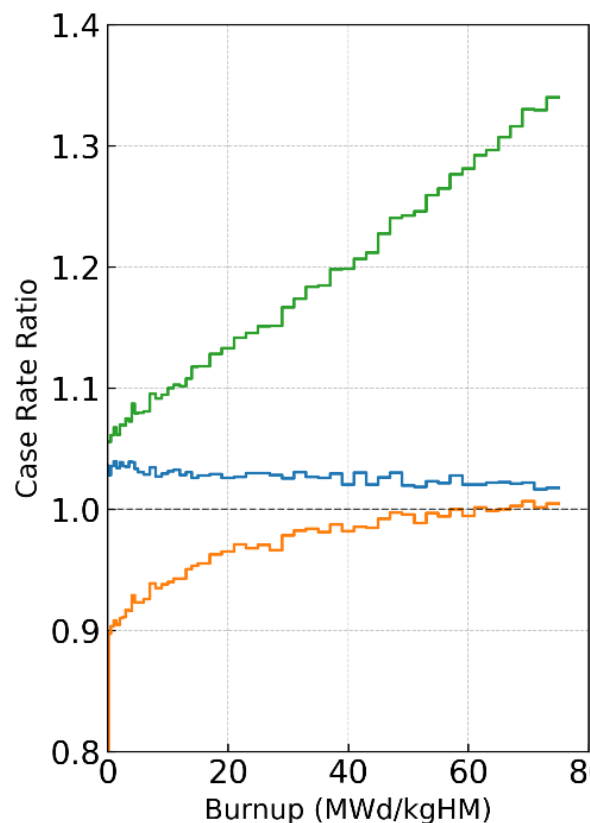


**ATF1a/REF3a**



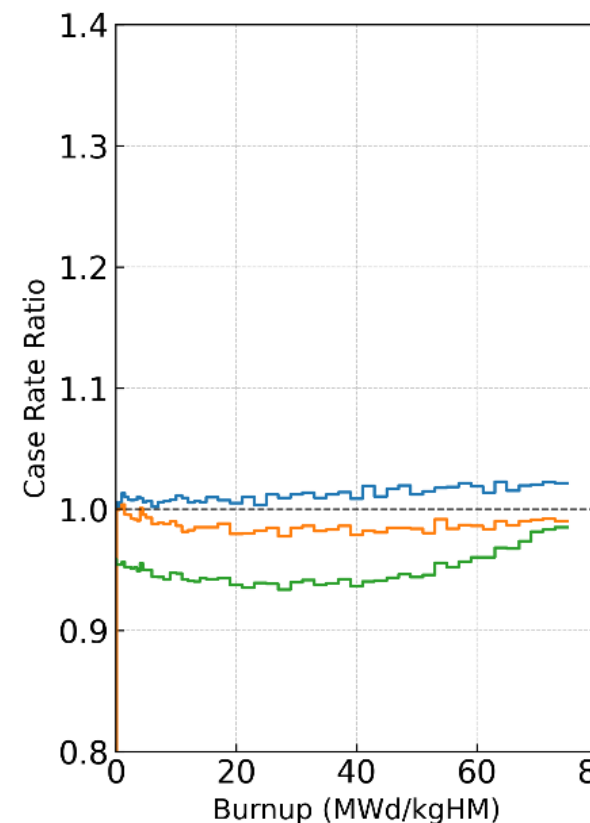
Small differences in SIs.  
U35fiss/U38cap increasing  
(indicates stronger spectrum  
softening of ATF1a).

**ATF2a/REF3a**



ATF2a with higher fast spectrum  
component (U238fiss/U238cap).  
Increasing thermal SI ratios indicate  
stronger thermal softening with BU  
for ATF2a.

**ATF3a/REF3a**



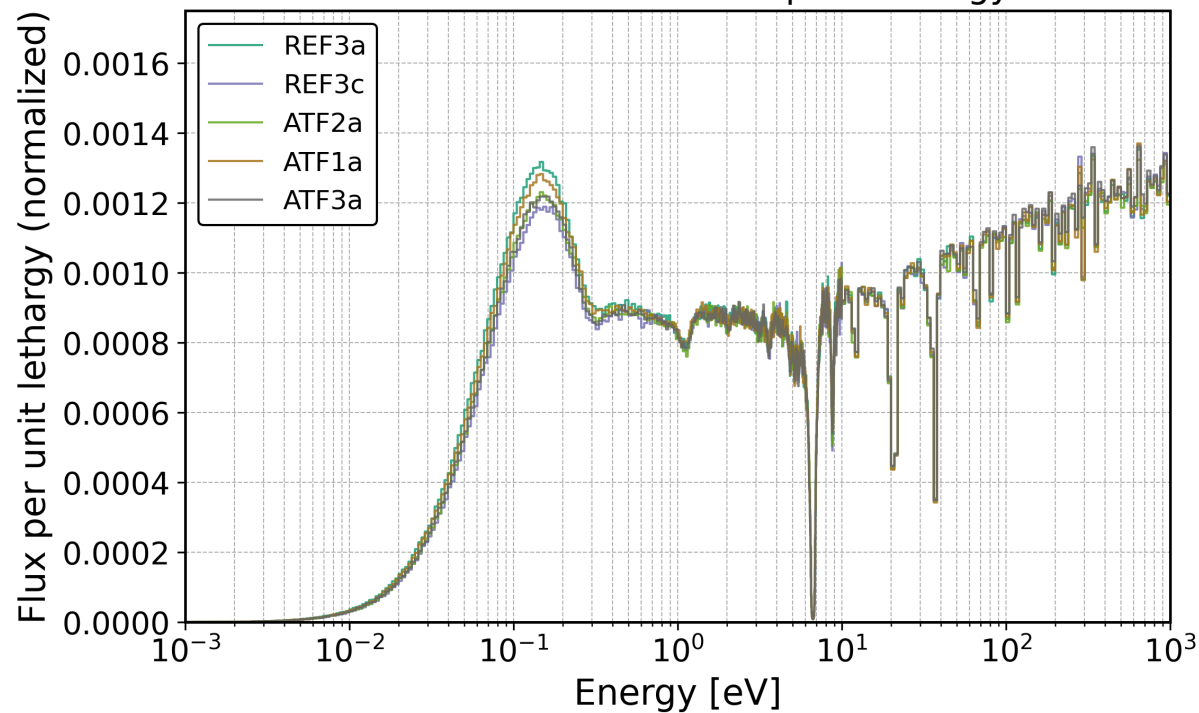
Lower thermal spectrum component of  
ATF3a (worse moderation higher  
U38cap).  
Spectrum hardening (U38fis/U38cap)

P39fiss/U38cap  
U35fiss/U38cap  
U38<sub>fis</sub>/U38<sub>cap</sub>

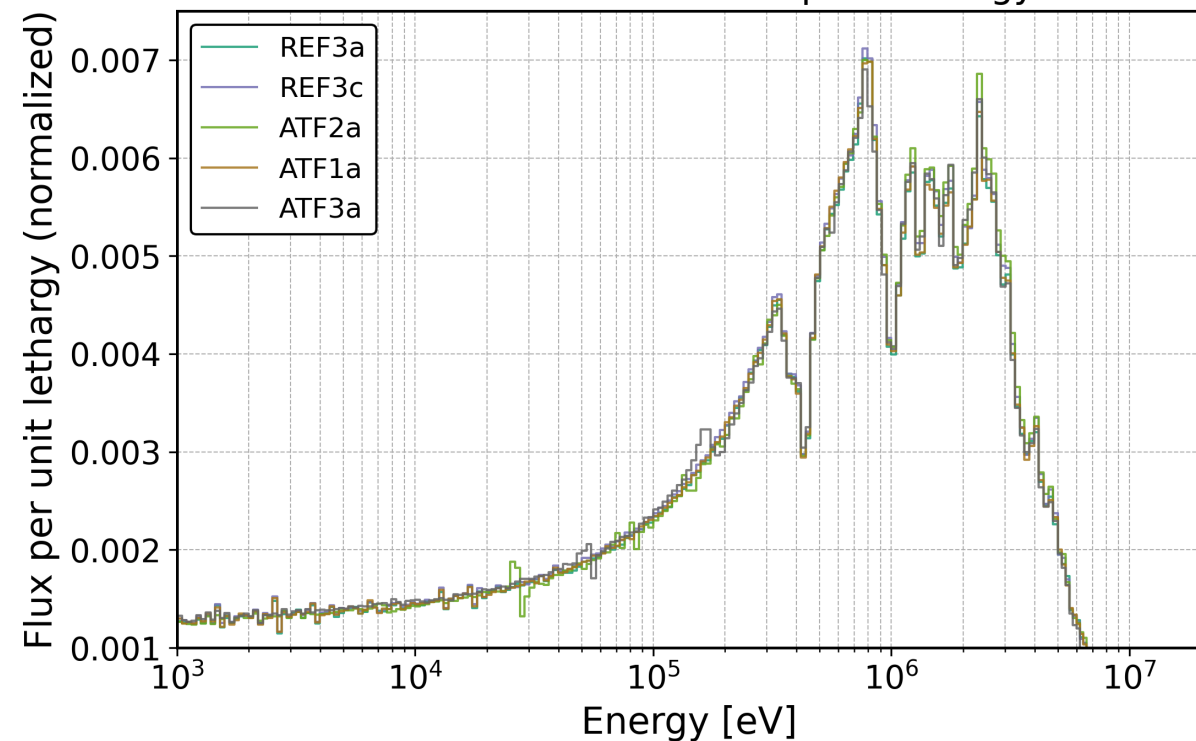


# BOI fuel neutron spectra shape (UKAEA-1102<sup>14</sup>)

SP 004: Normalized Flux per Lethargy



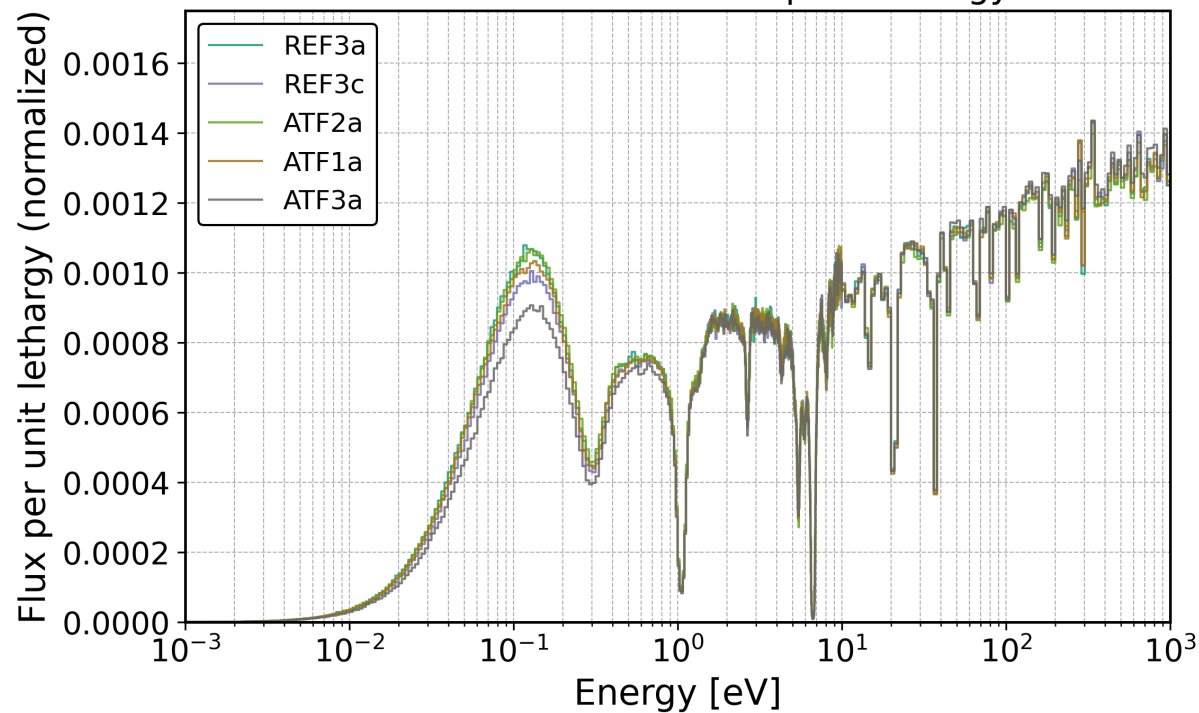
SP 004: Normalized Flux per Lethargy



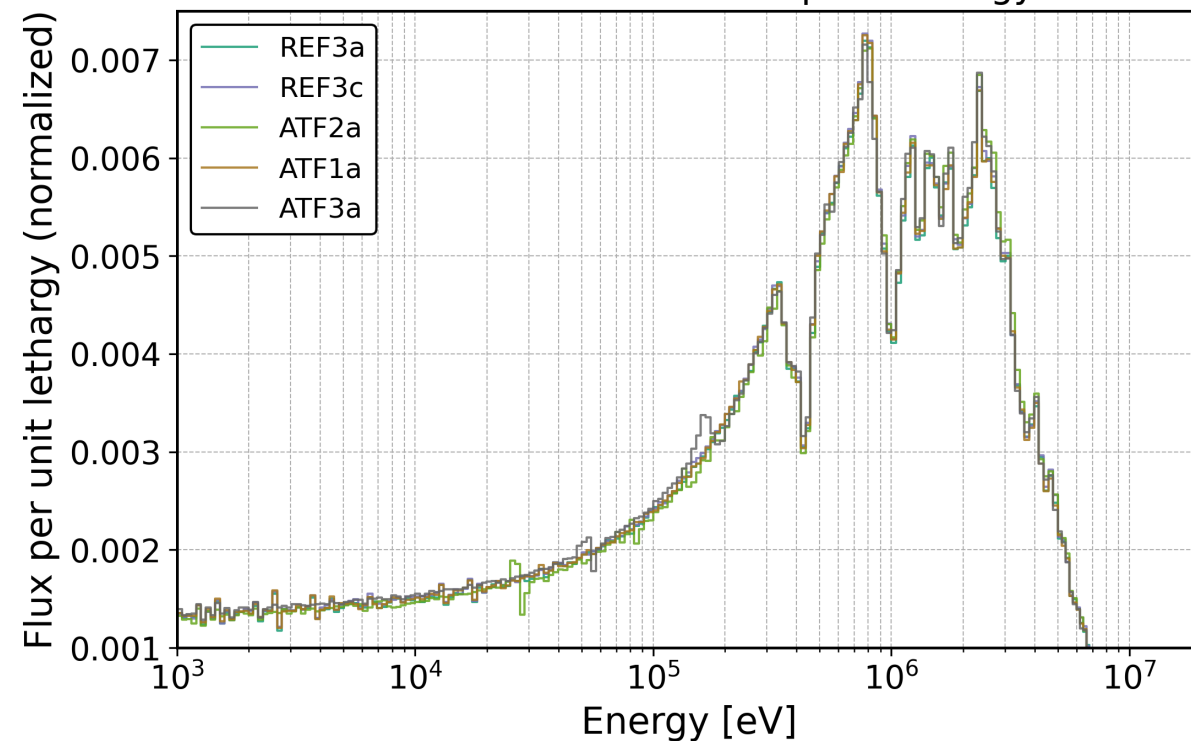
Thermal peak ranking	Case	Enrichment	Moderation
1	REF3a	5.0	0
2	ATF1a	5.1	0
3	ATF3a / ATF2a	5.0 / 5.6	- / +
4	REF3c	5.6	0

# EOI fuel neutron spectra shape (UKAEA-1102<sup>14</sup>)

SP 049: Normalized Flux per Lethargy



SP 049: Normalized Flux per Lethargy



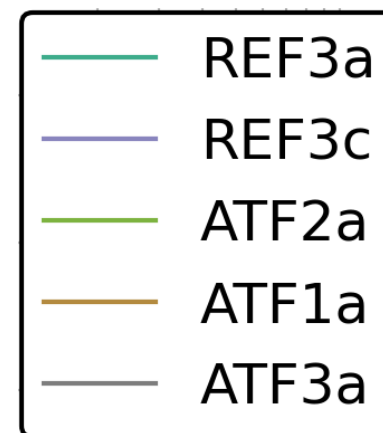
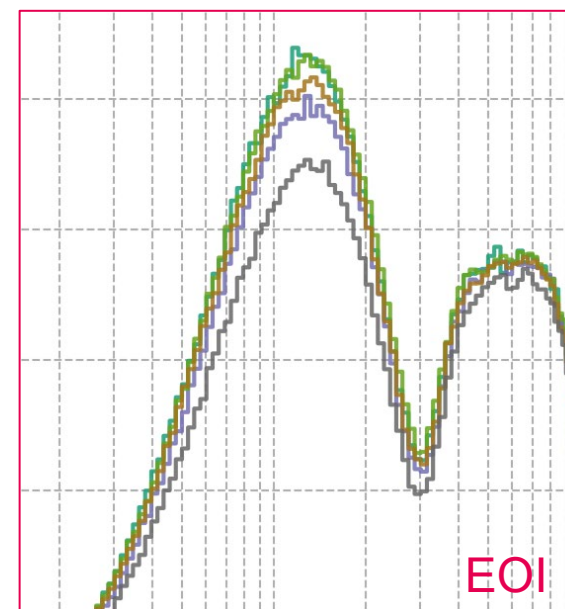
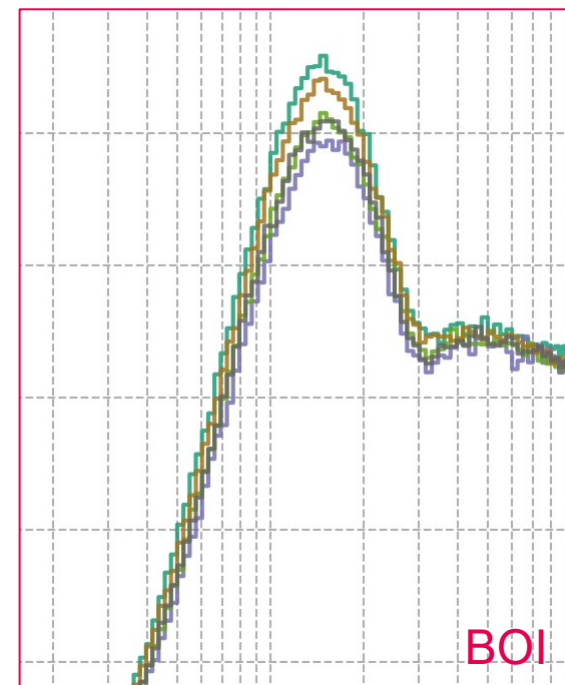
Thermal peak ranking	Case	Enrichment	Moderation
1	REF3a / ATF2a	5.0 / 5.6	0 / +
2	ATF1a	5.1	0
3	REF3c	5.6	0
4	ATF3a	5.0	-

# Spectrum conclusions

Increasing enrichment decreases thermal peak and reduces flux level for defined specific power.

Reducing cladding thickness at 5.6% increases thermal peak (BOI REF3c vs ATF2a) due to improved moderation (also necessitates lower flux level to maintain power)

Thermal peak lowest for 5.0% ATF3a with thickest cladding (BOI/EOI REF3a vs ATF3a): indicates impact of lower moderation.

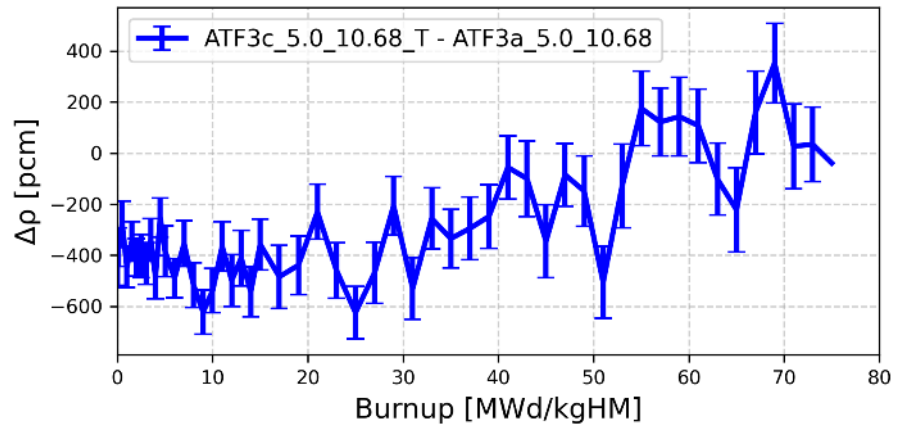
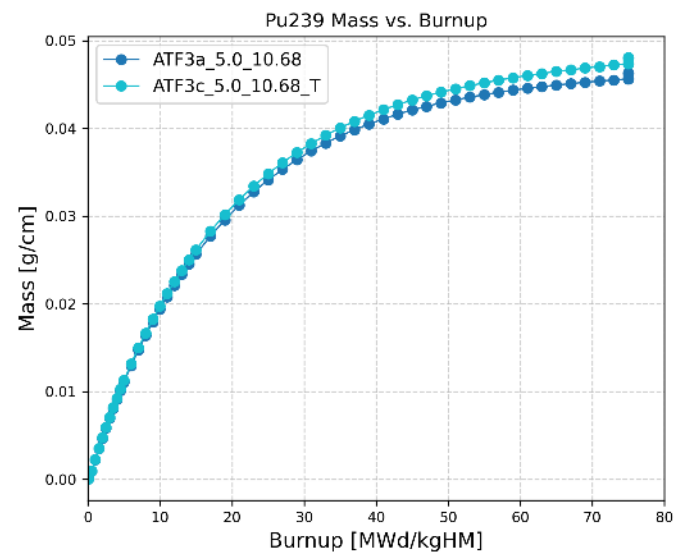
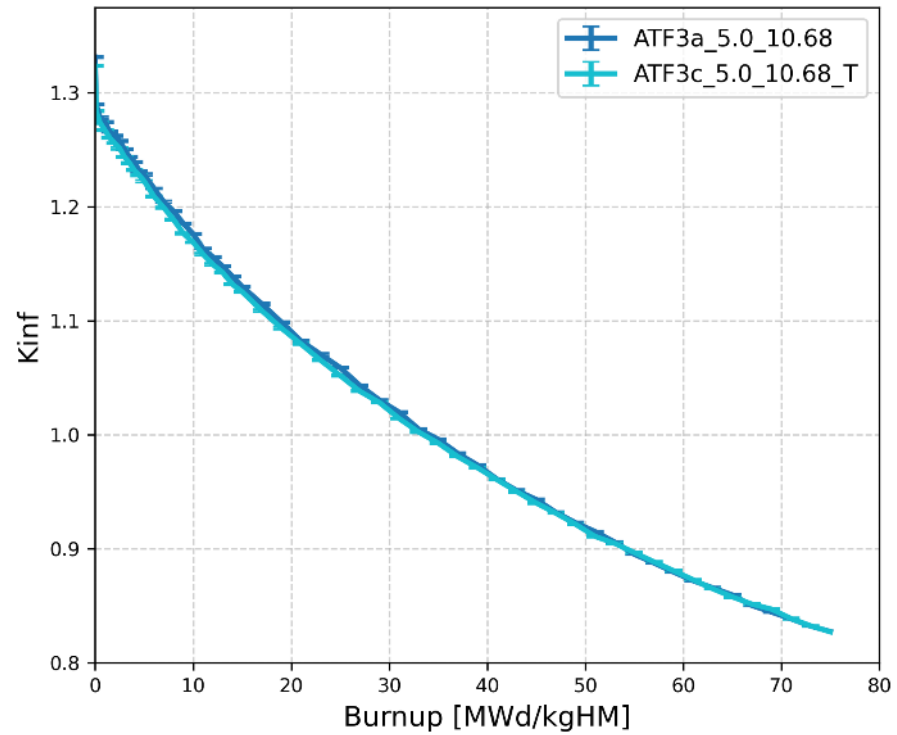
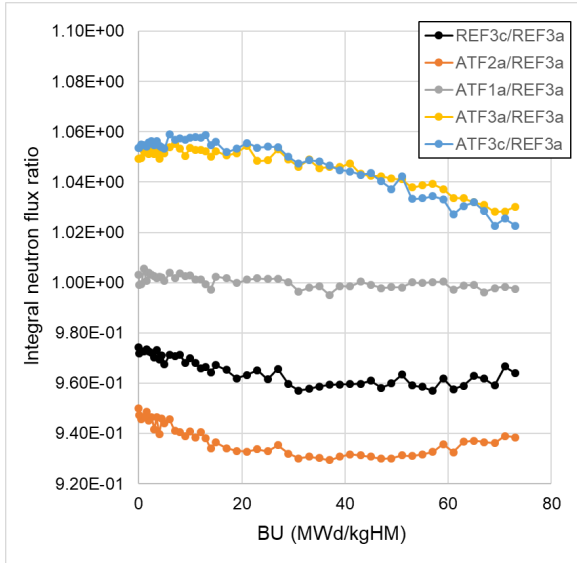
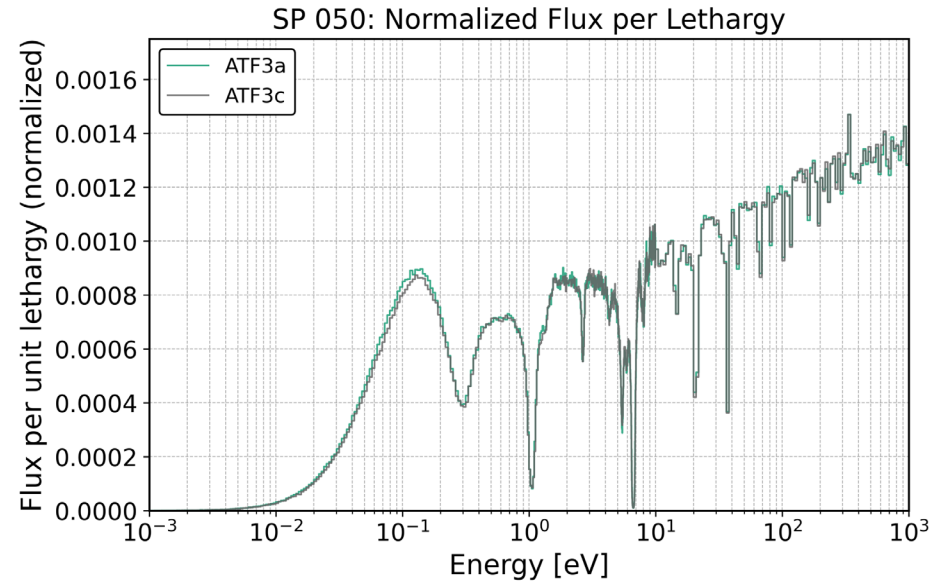




# **ATF3a vs ATF3c**

**600K/900K vs 700K/1100K  
(clad/fuel)**

# ATF3a (600, 900 K) vs ATF3c (700, 1100K)

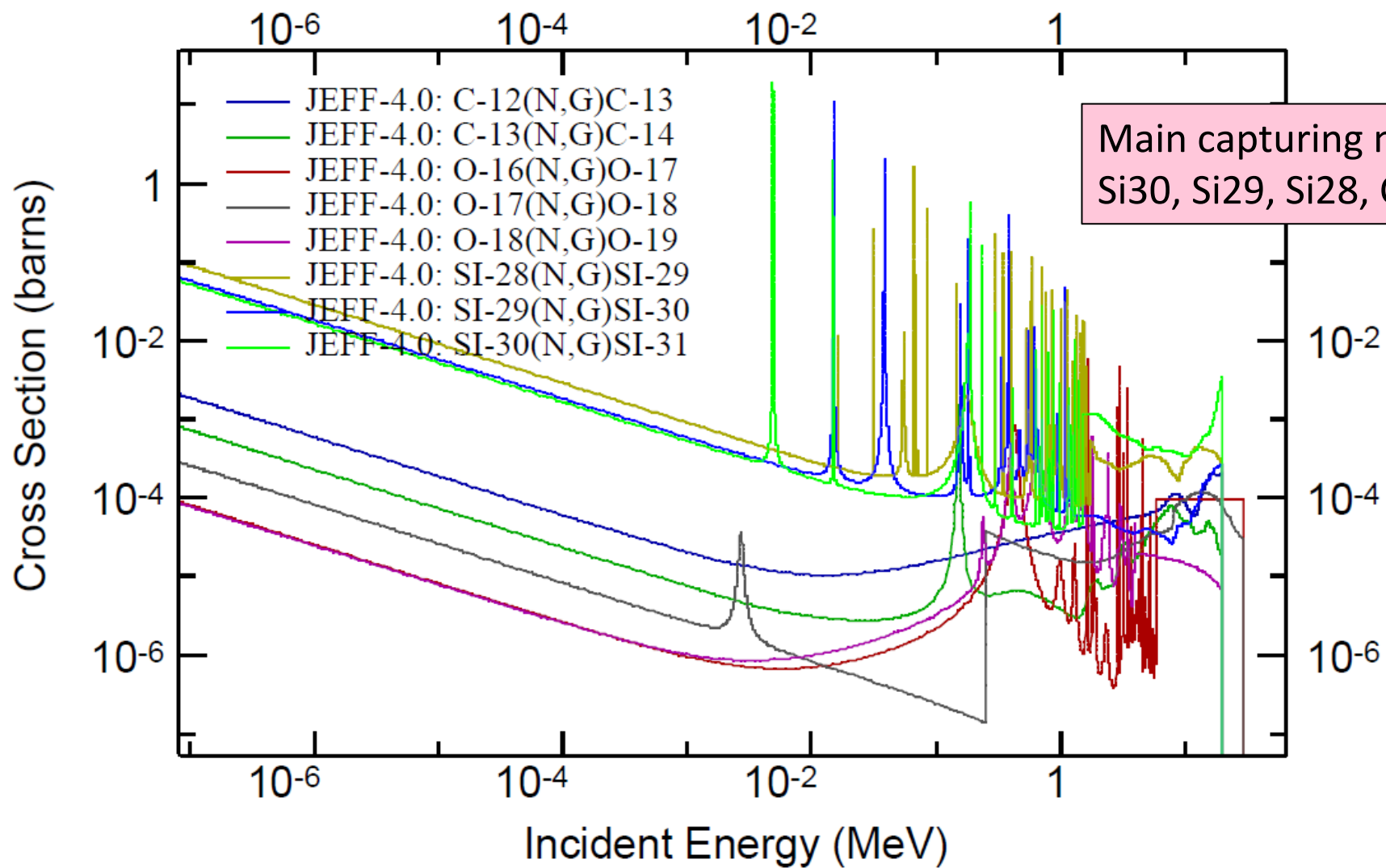




# **JEFF4 cross-sections**

**Silicon and Carbon**

ENDF Request 40453, 2025-Oct-21, 14:41:11





# **JEFF4 vs. JEFF3.3**

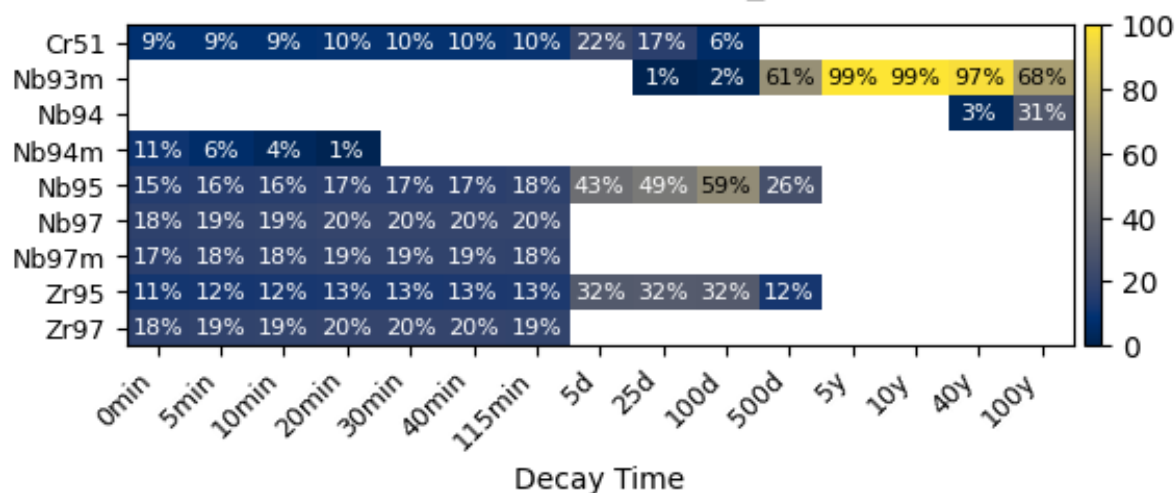
**M5 + 20  $\mu\text{m}$  Cr (pure) ATF1a**

**M5 + 20  $\mu\text{m}$  Cr (with impurities) ATF1b**

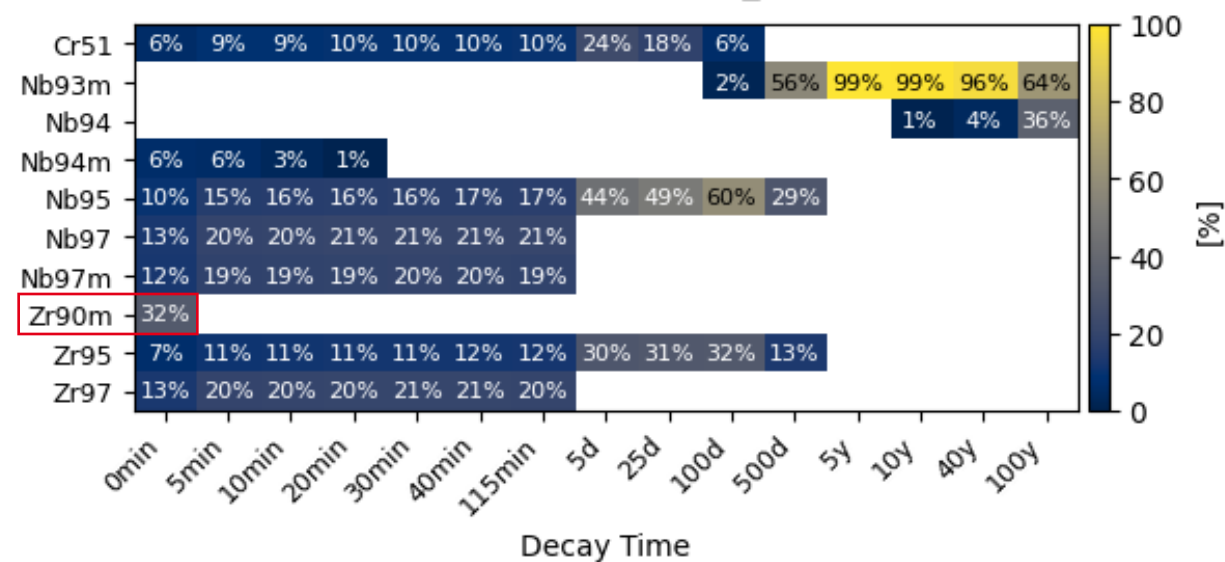


# Nuclear data impact: JEFF-3.3 vs JEFF-4

Activity | ATF1a | jeff33\_300K



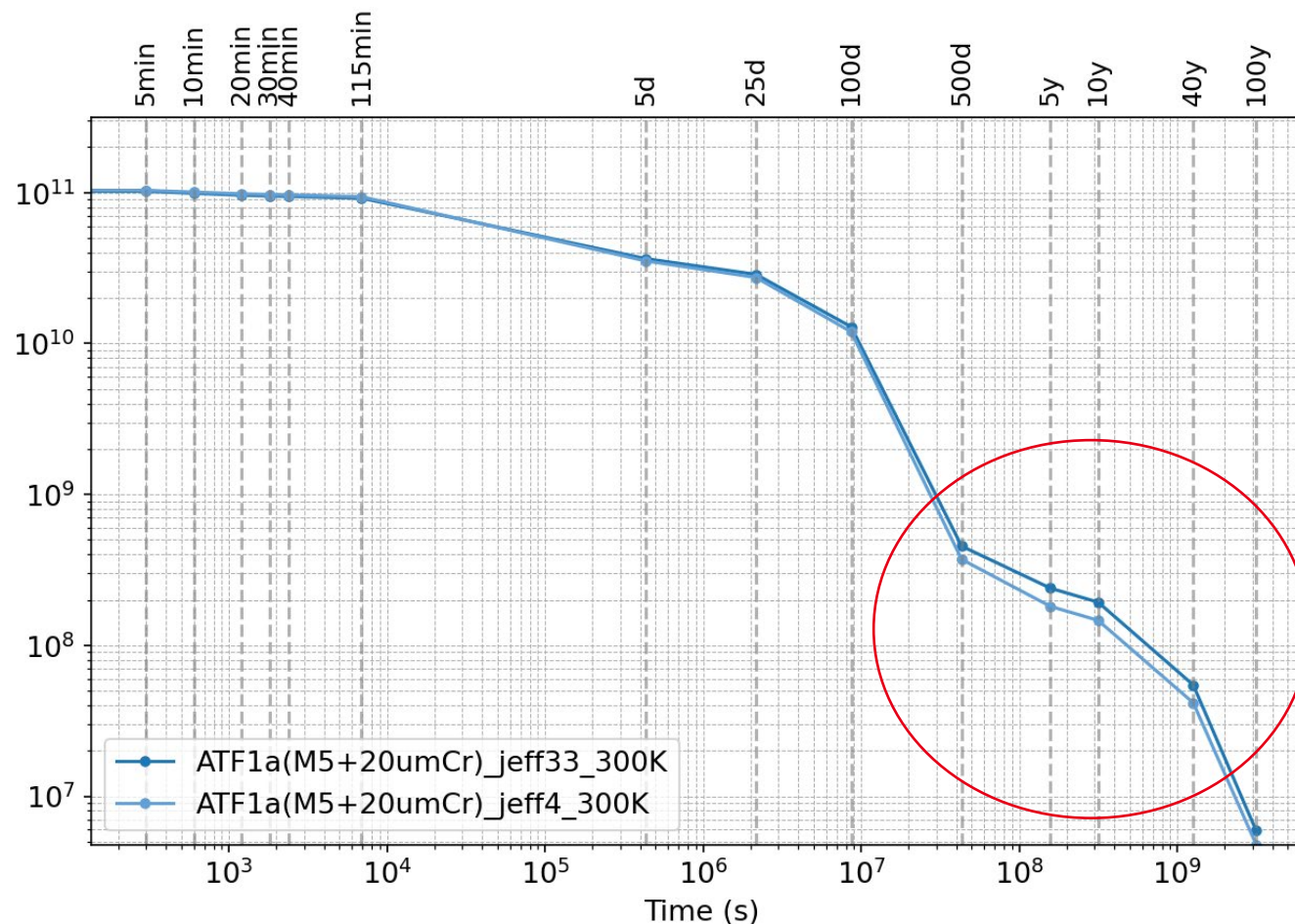
Activity | ATF1a | jeff4\_300K



Relative nuclide contributions to activity vector very similar for JEFF-3.3 vs JEFF-4.

(except for Zr90m at EOI for JEFF-4)

# JEFF-3.3 vs JEFF-4 on total Bq/cm for ATF1a clad



Library impact up to 30 % on total activity (here mainly due to Nb93m).

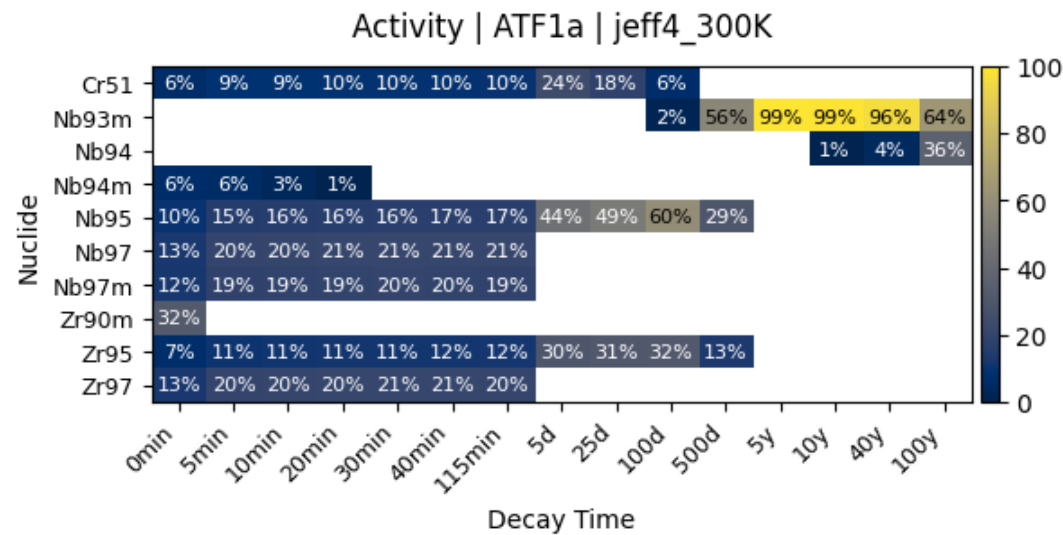
Higher estimation in JEFF-3.3 due to  $\sigma(E)$  difference (TENDL15 vs TENDL23)

Nb93m activity uncertainty (FP-II) with MOI spectrum:

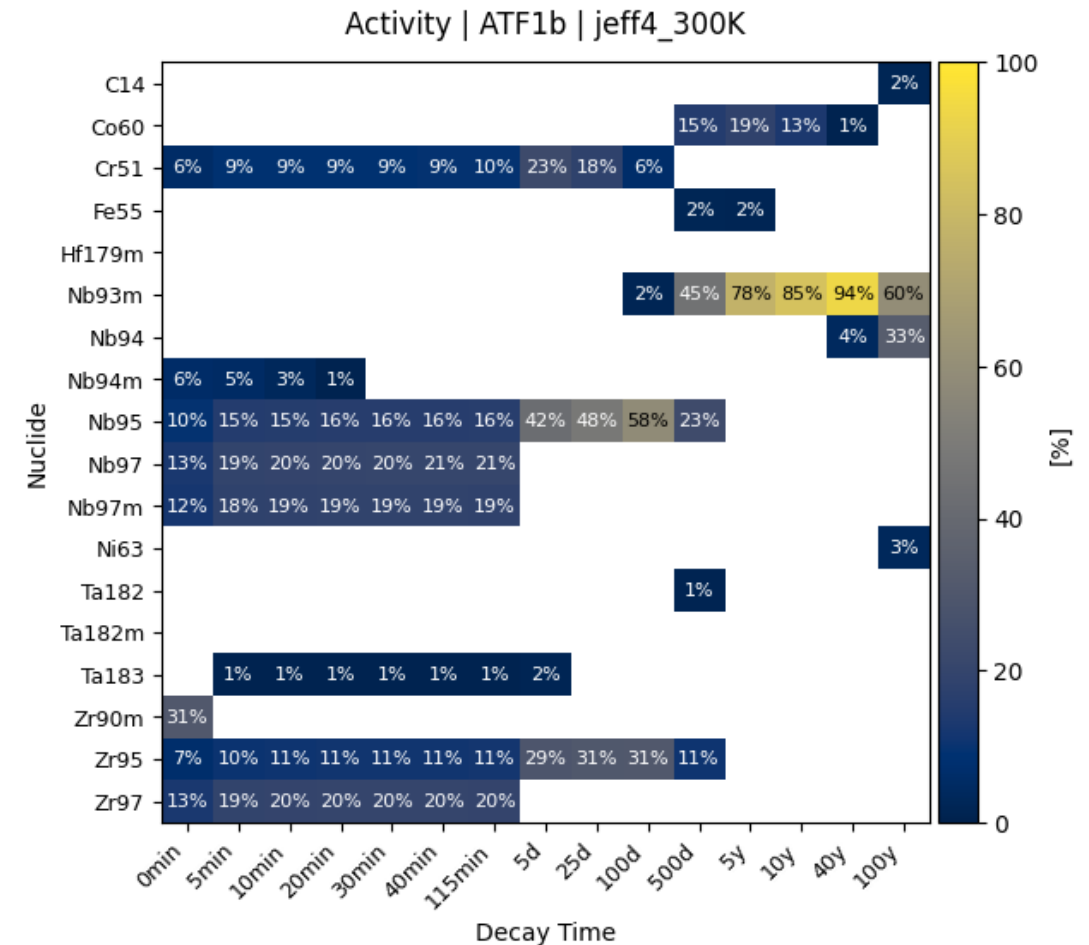
- JEFF-3.3  $\rightarrow$  ~6.6 %
- JEFF-4  $\rightarrow$  ~12.5 %

# Impurity impact: JEFF4

ATF1a



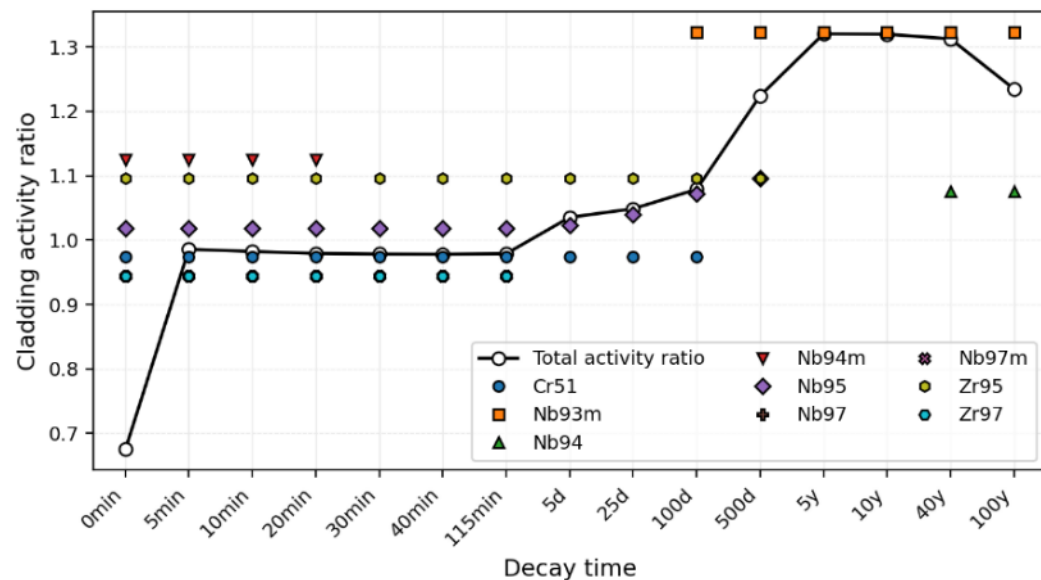
ATF1b



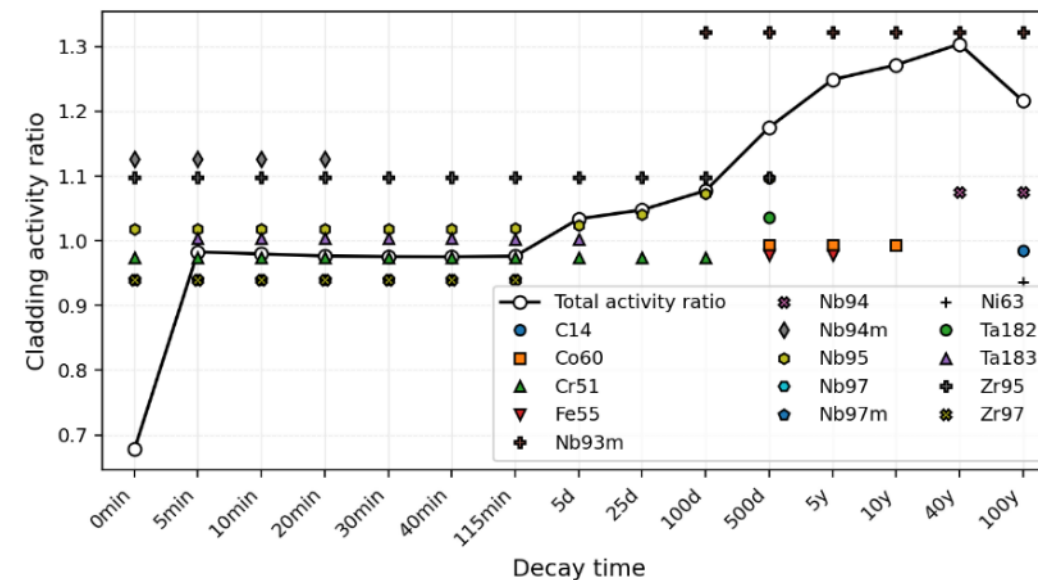
# Nuclear data library impact:

$$\frac{\text{Activity(JEFF3.3)}}{\text{Activity(JEFF4)}}$$

ATF1a



ATF1b (with impurities)



Library impact on nuclide activity is significant (here at 300K)

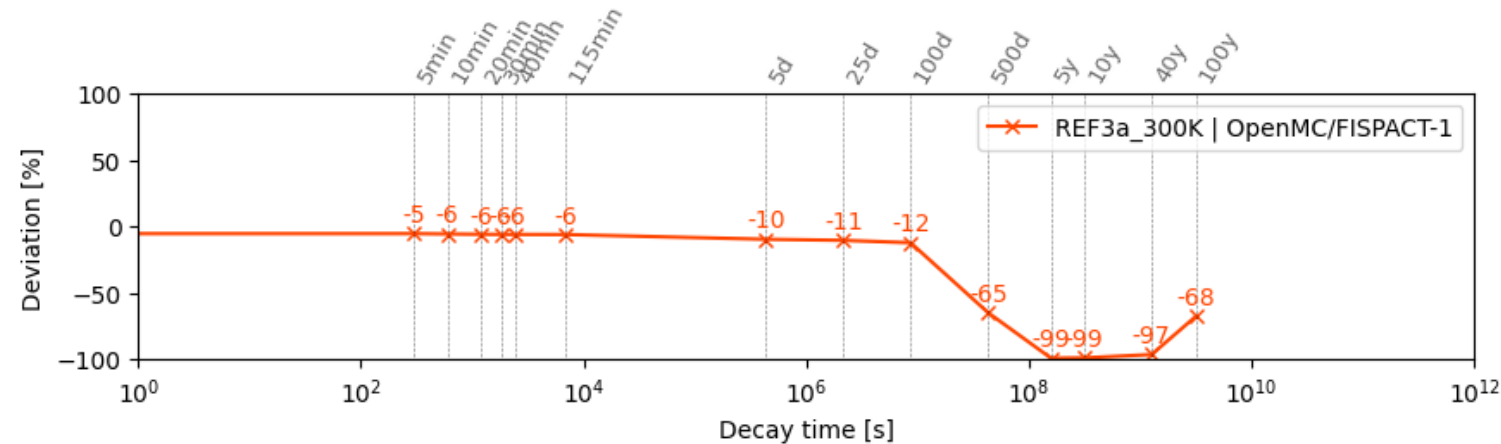
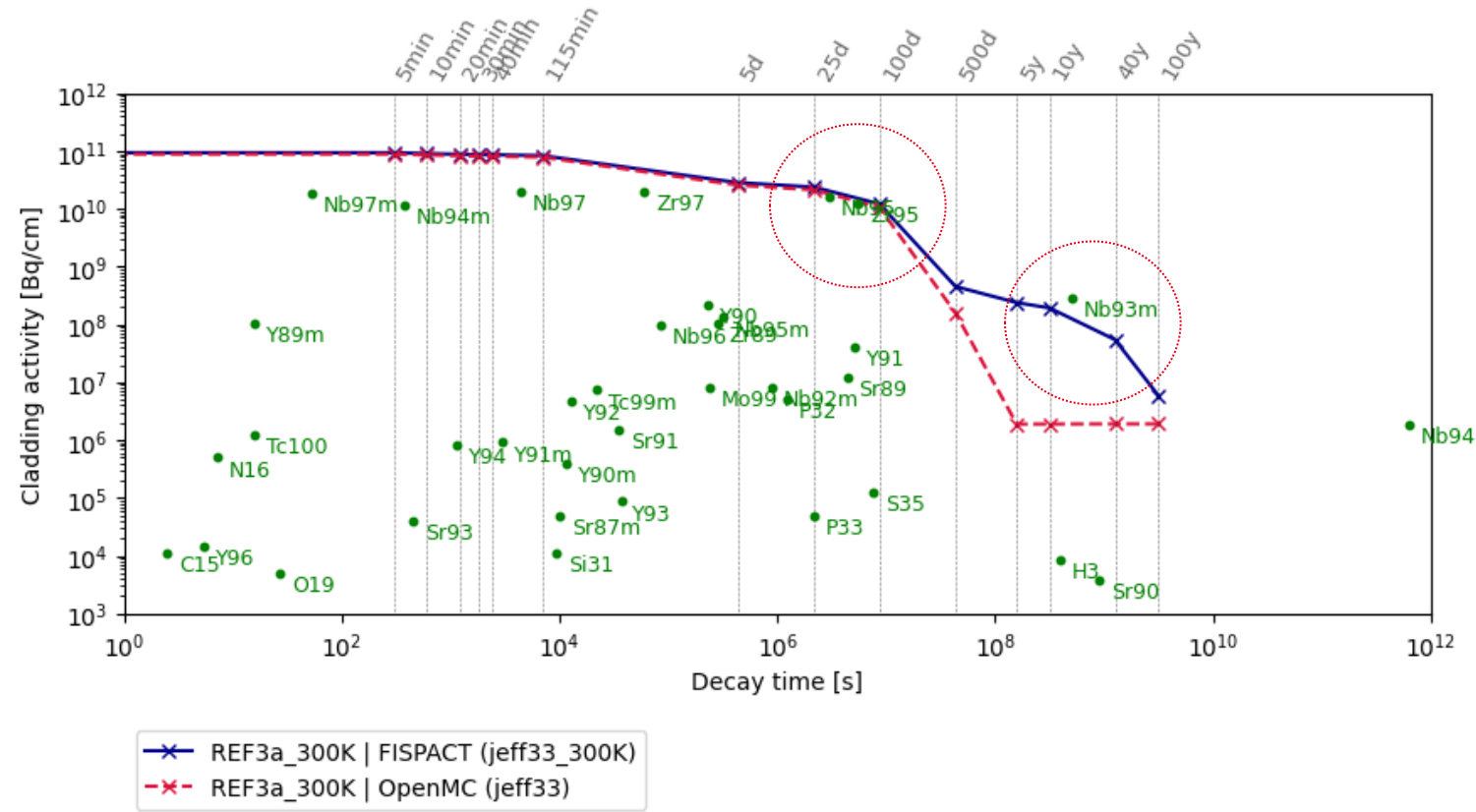
# **OpenMC vs. FP-II**

## **Cladding benchmark**

**Isotopic ratios**

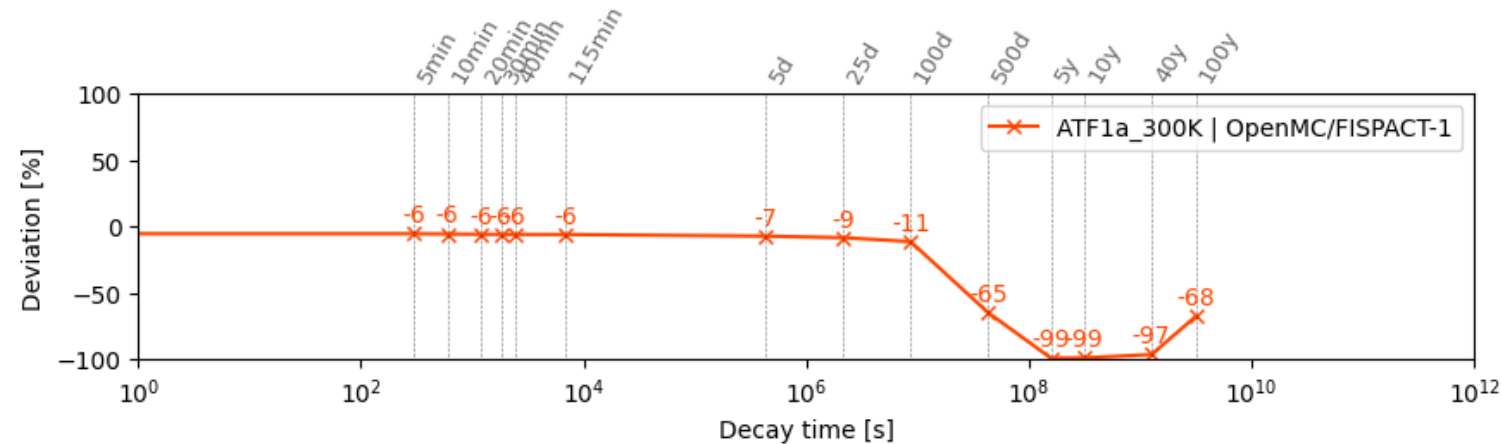
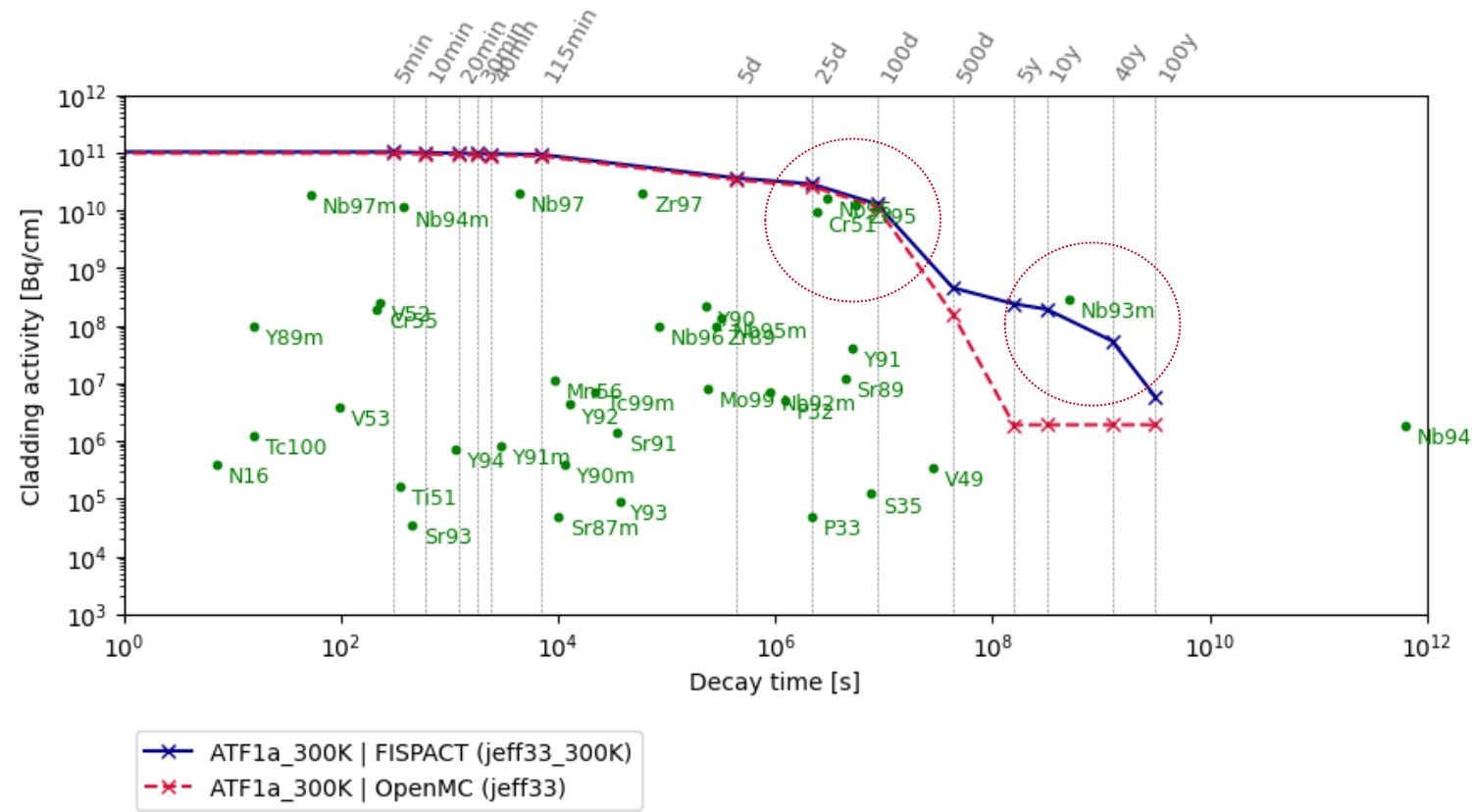
# REF3a\_300K

- Nb93m as a candidate for investigation
- Zr95 and Nb95 at lower decay times



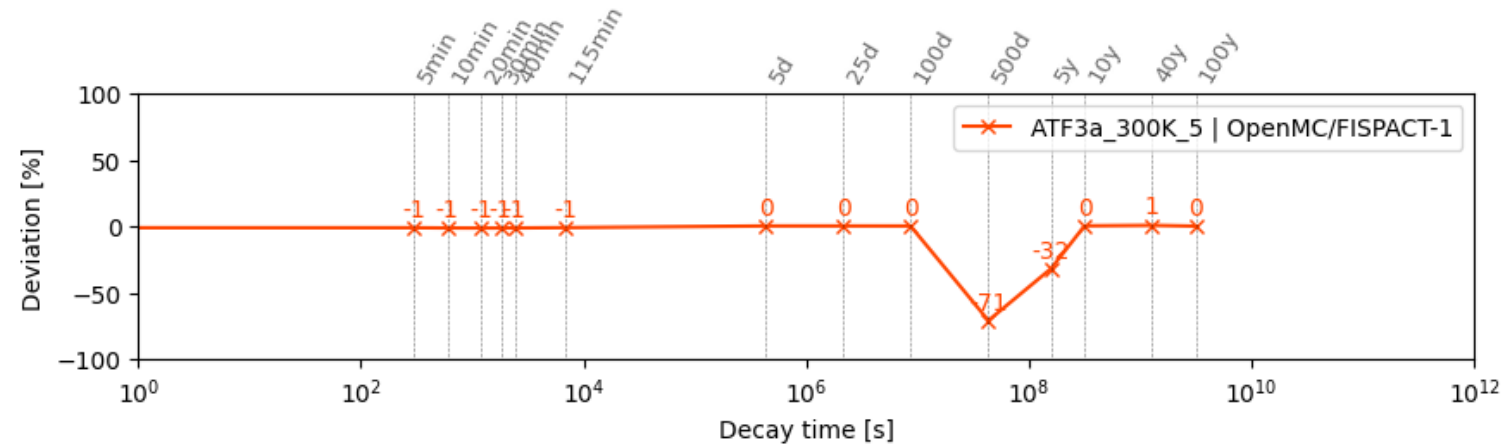
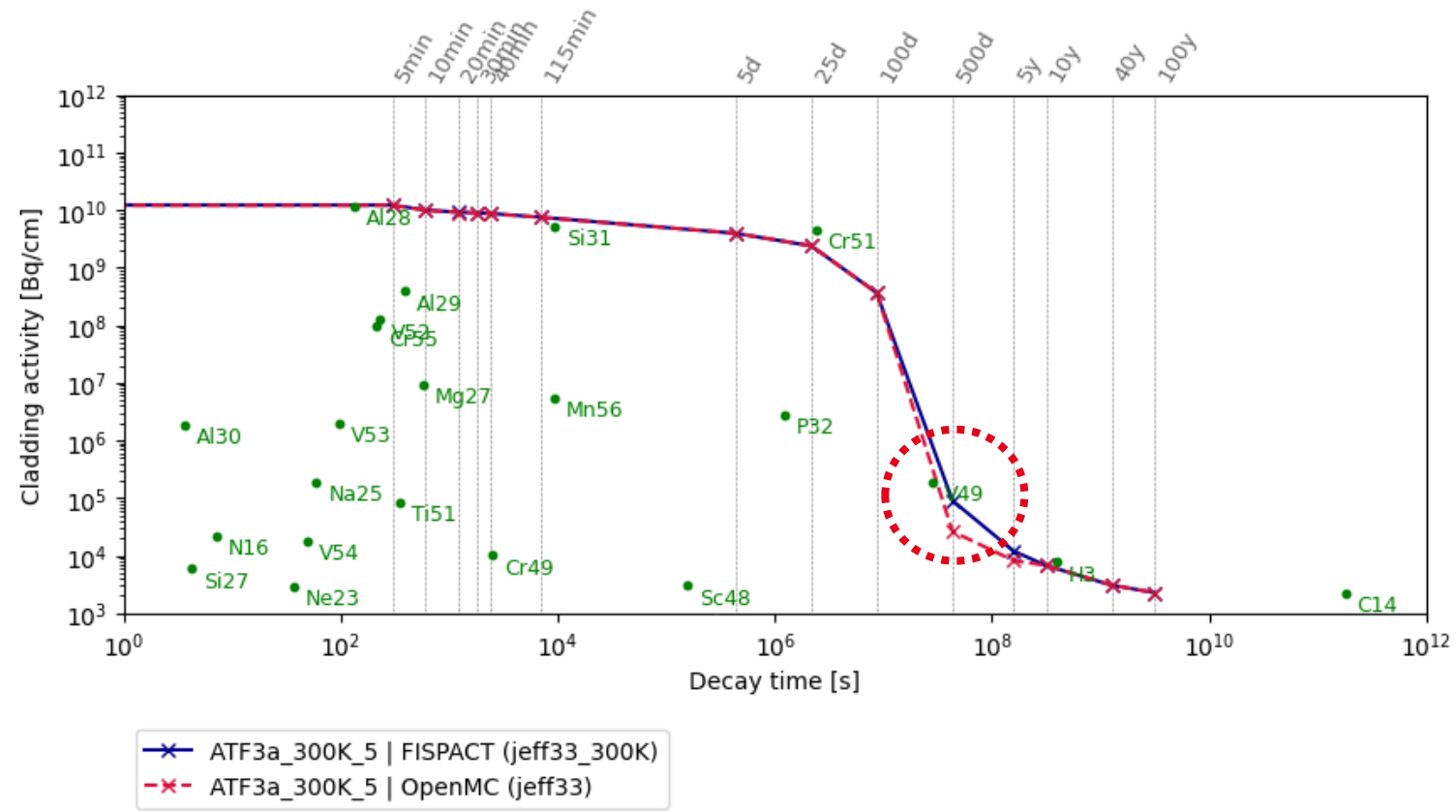
# ATF1a\_300K

- Nb93m as a candidate for investigation
- FP overprediction ~10% Zr95 and Nb95 (see analysis in the following slides)
- Very good agreement for Cr51 (see coming slides)



# ATF3a\_300K

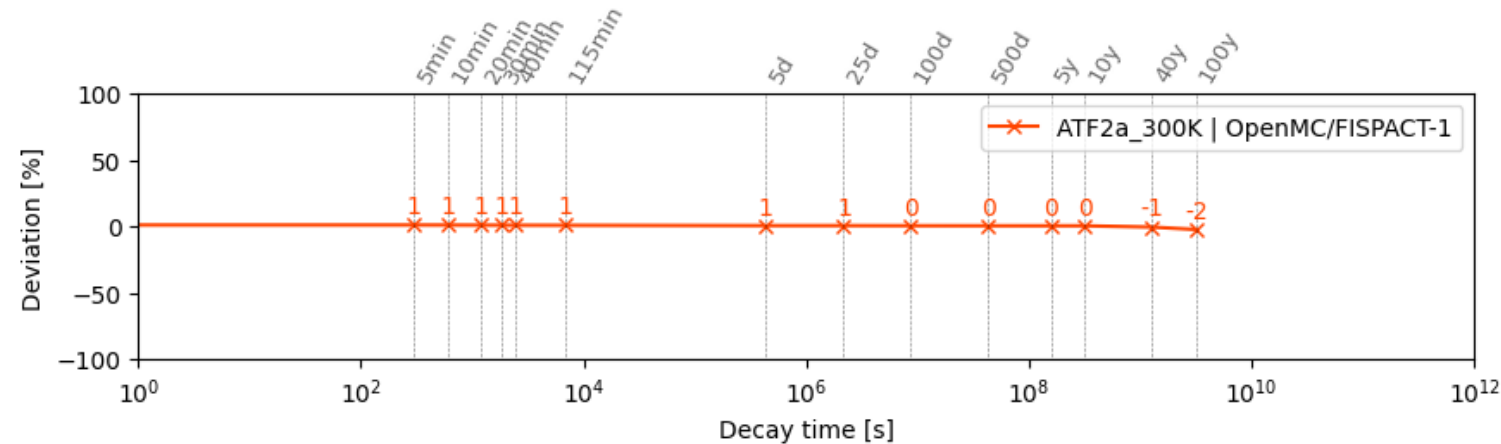
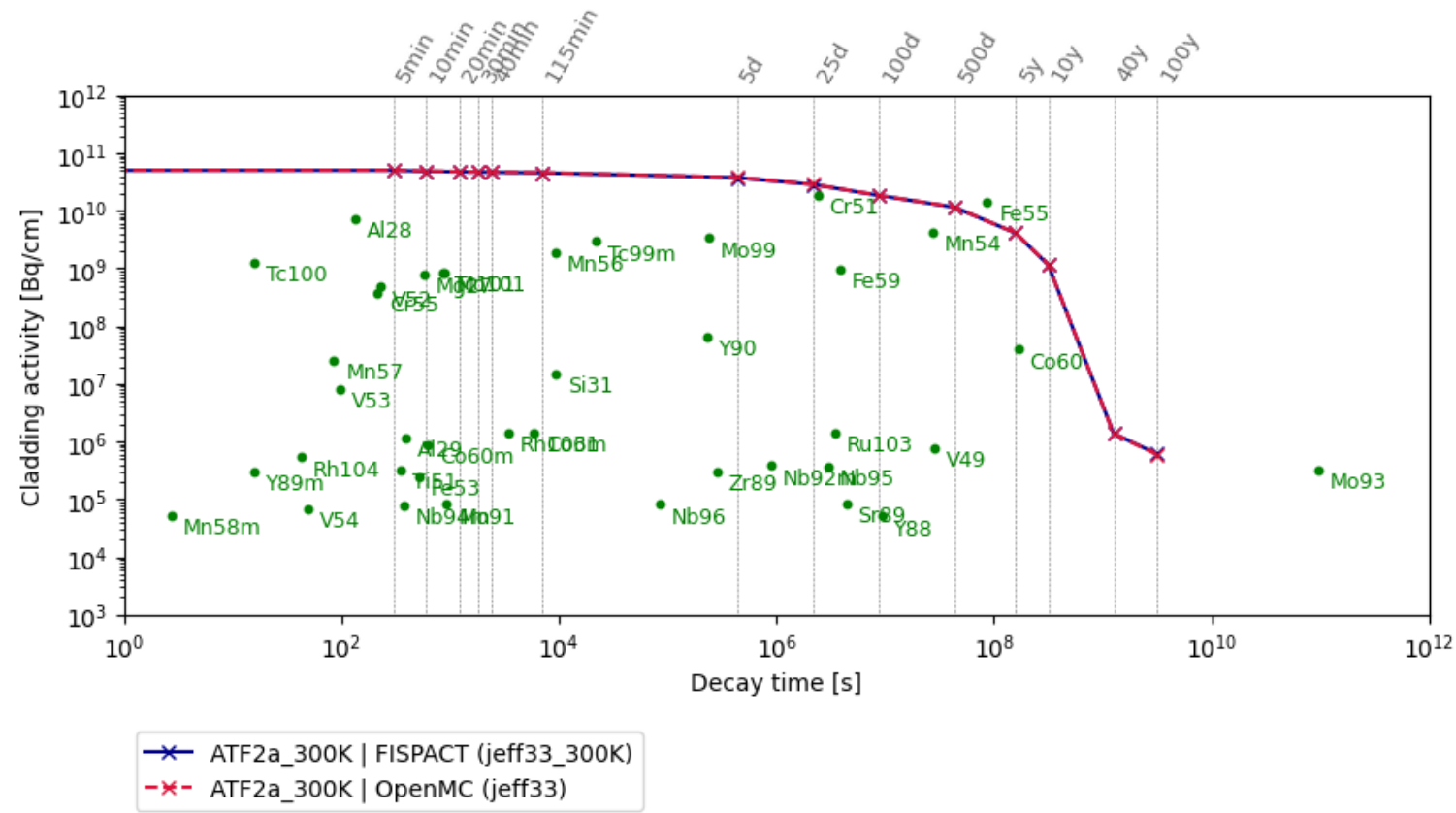
- V49 → candidate for investigation





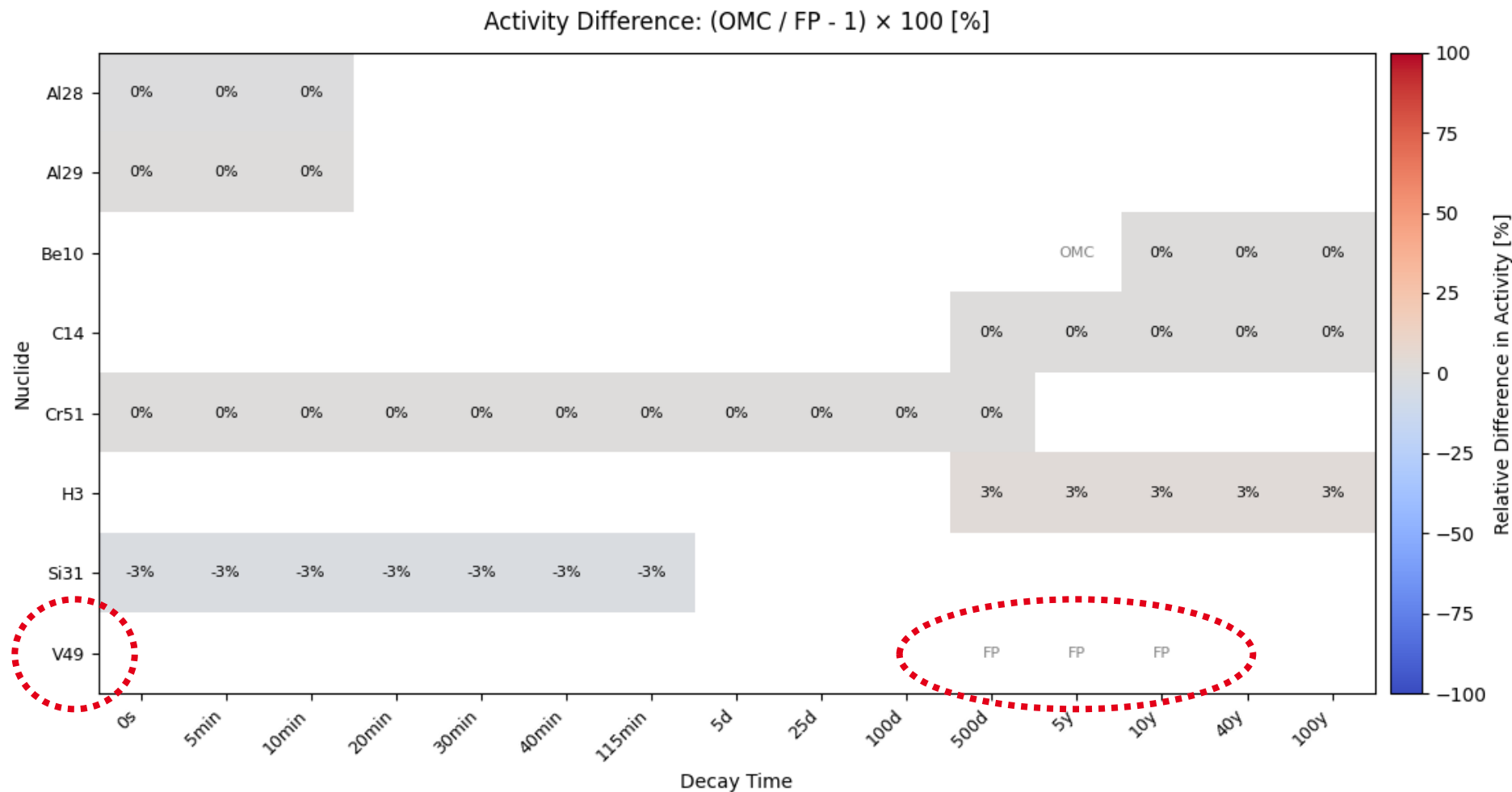
# ATF2a\_300K

- Very good agreement (also on nuclide level, see annex)
- No self-shielding correction in FP
- FP ( $\sigma+\lambda$ ) uncertainty estimate on total activity  $\in [0, 5d] < 2.8\%$



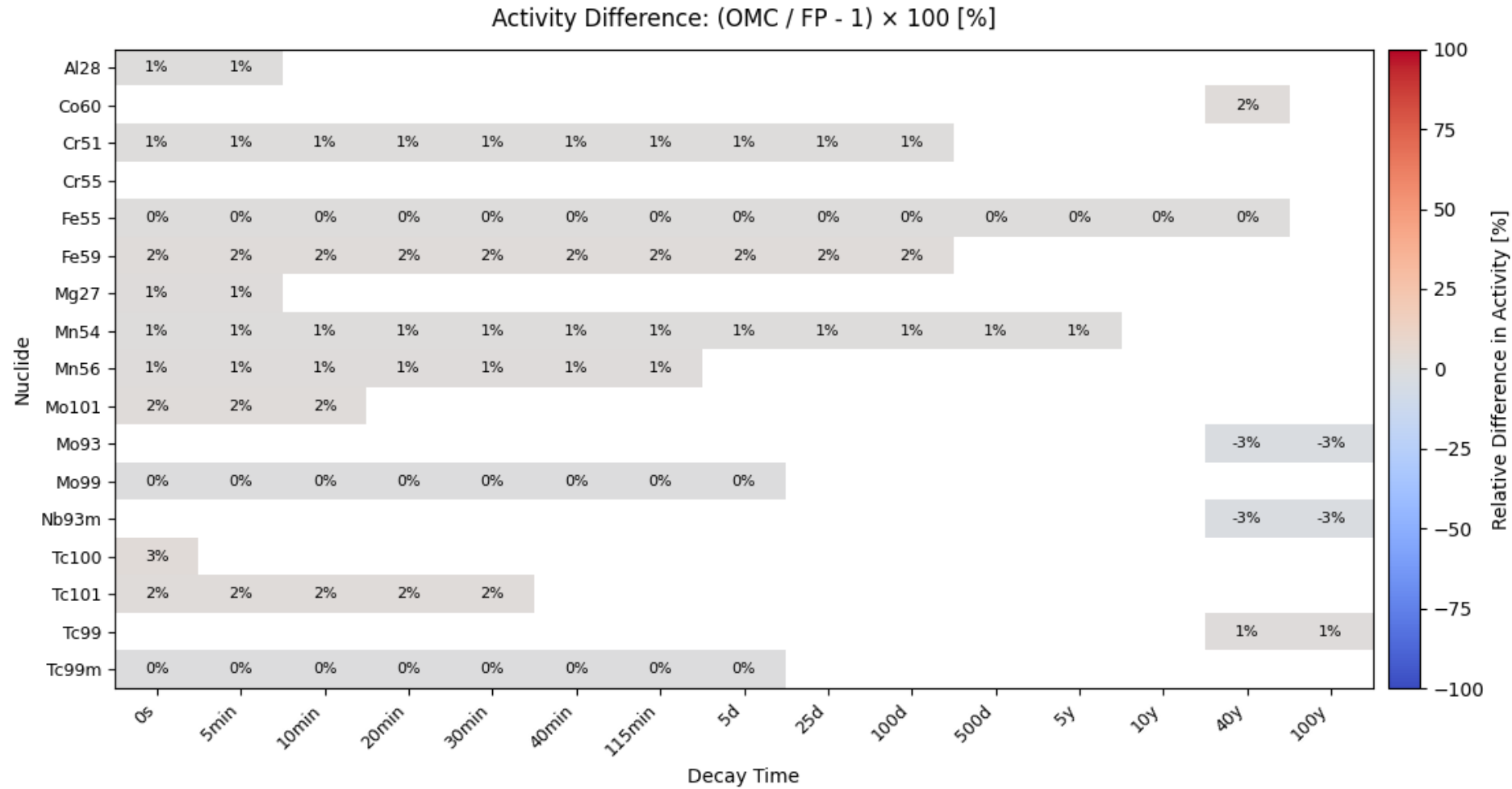
# ATF3a\_300K: OMC/FP-1 (activity)

- Very good agreement except for V49 (only in FP >1%)
- JEFF33  
Cr50(n,anything)V49 in FP-II (MT=5) not implemented in OpenMC depletion chain file
- In TENDL2019<sup>[22]</sup> this is Cr50(n,np)V49



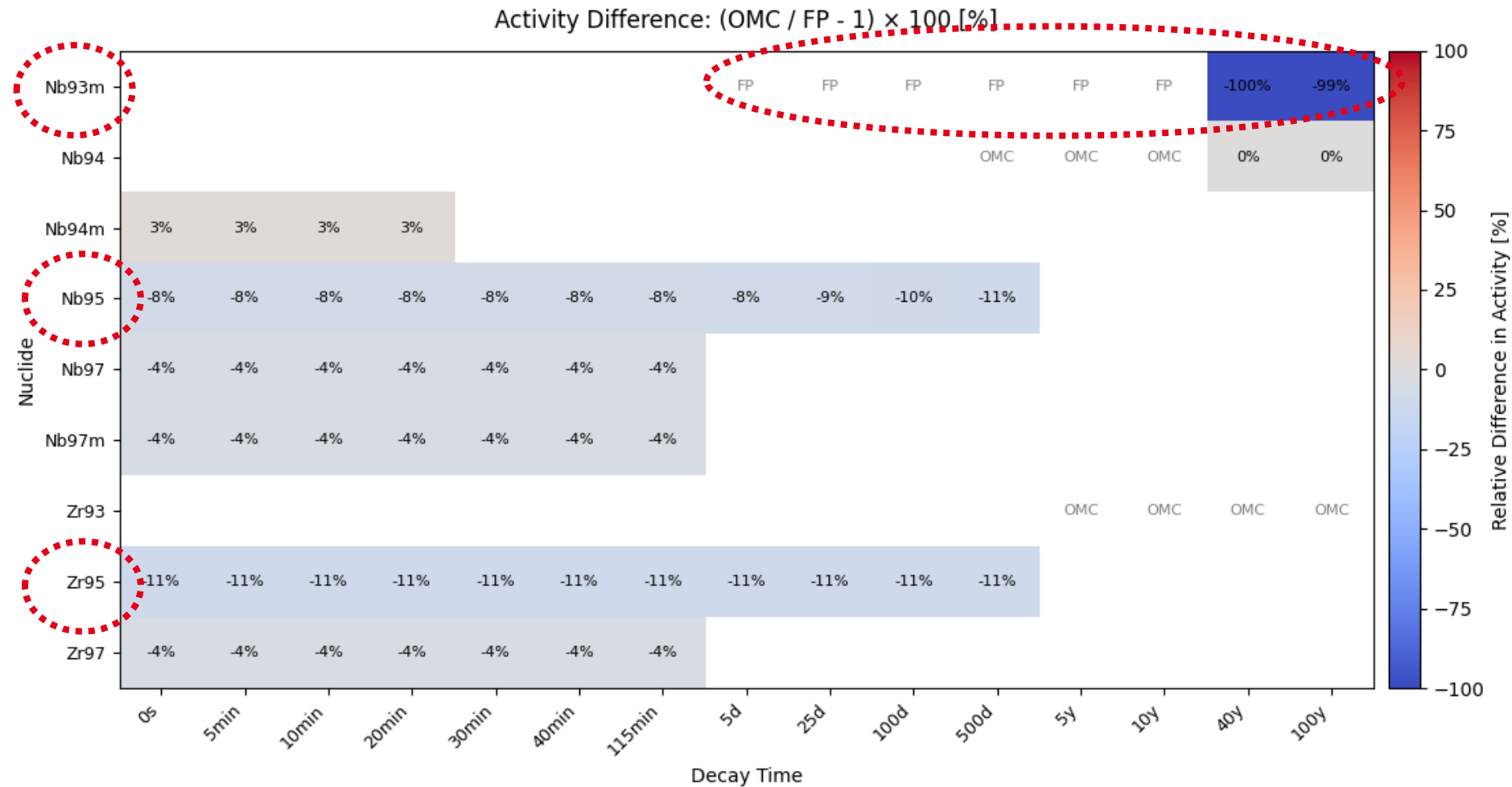
# ATF2a\_300K: OMC/FP-1 (activity)

- No self-shielding
- Very good agreement



# REF3a\_300K: OMC/FP-1 (activity)

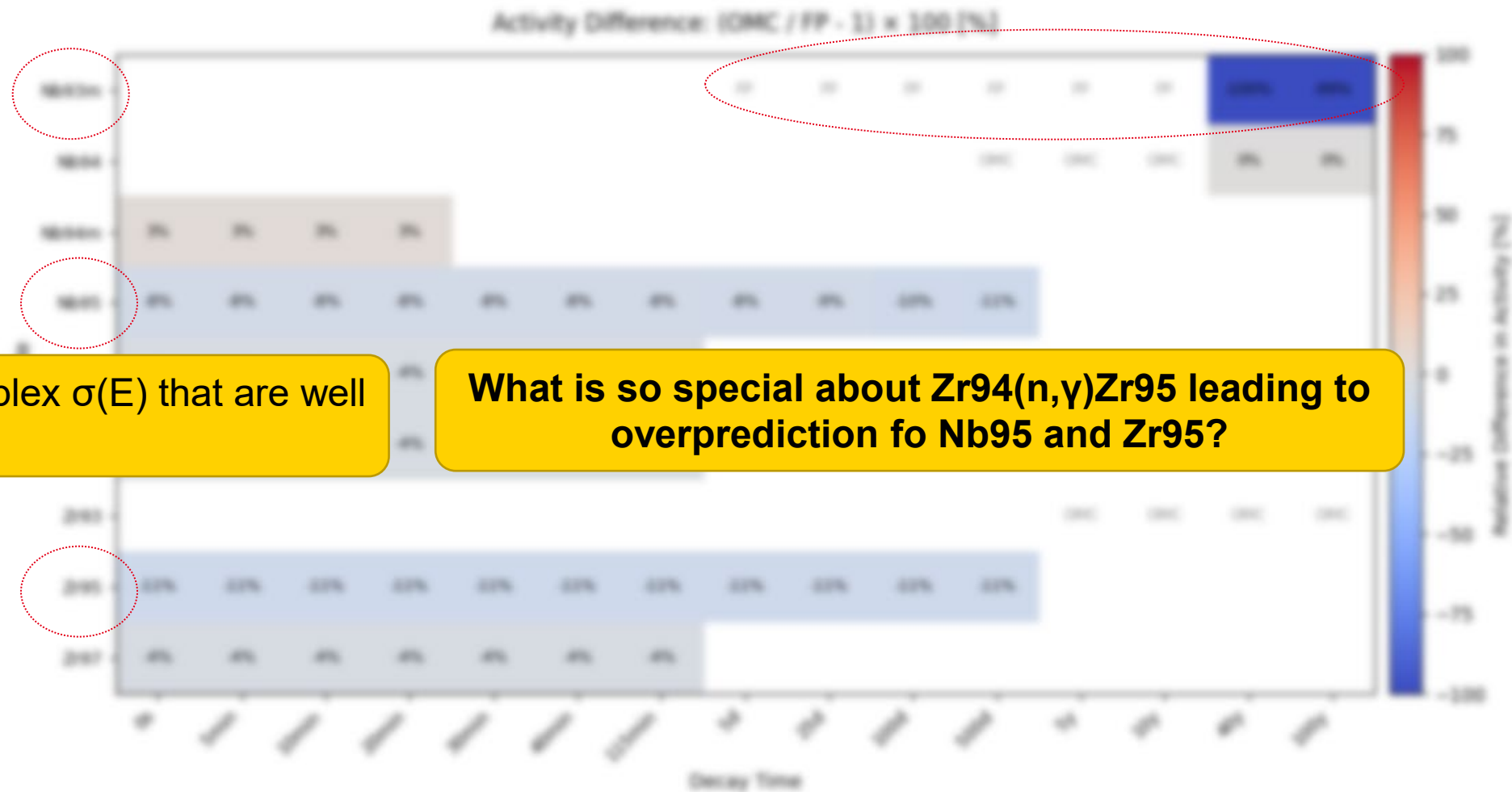
- Nb93(n,n1)Nb93m in FP-II (MT=3) not in OpenMC (inelastic n-scattering into metastable)
- FP overprediction of Zr95 and Nb95



# **Zr95 analysis**

**for REF3a**

# REF3a\_300K: OMC/FP-1 (activity)



# REF3a\_300K: OMC/FP-1 (activity)

Possible impacts on nuclear reactions: here →  $Zr94(n,\gamma)Zr95$

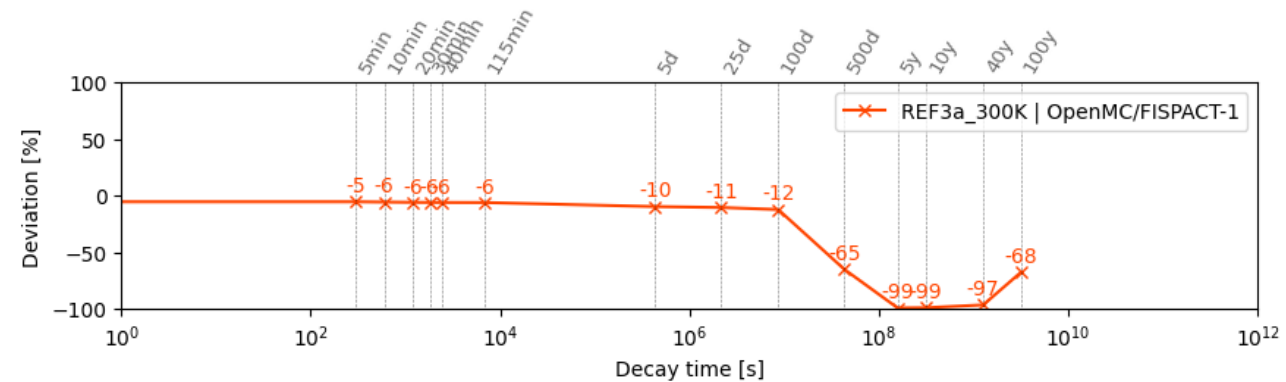
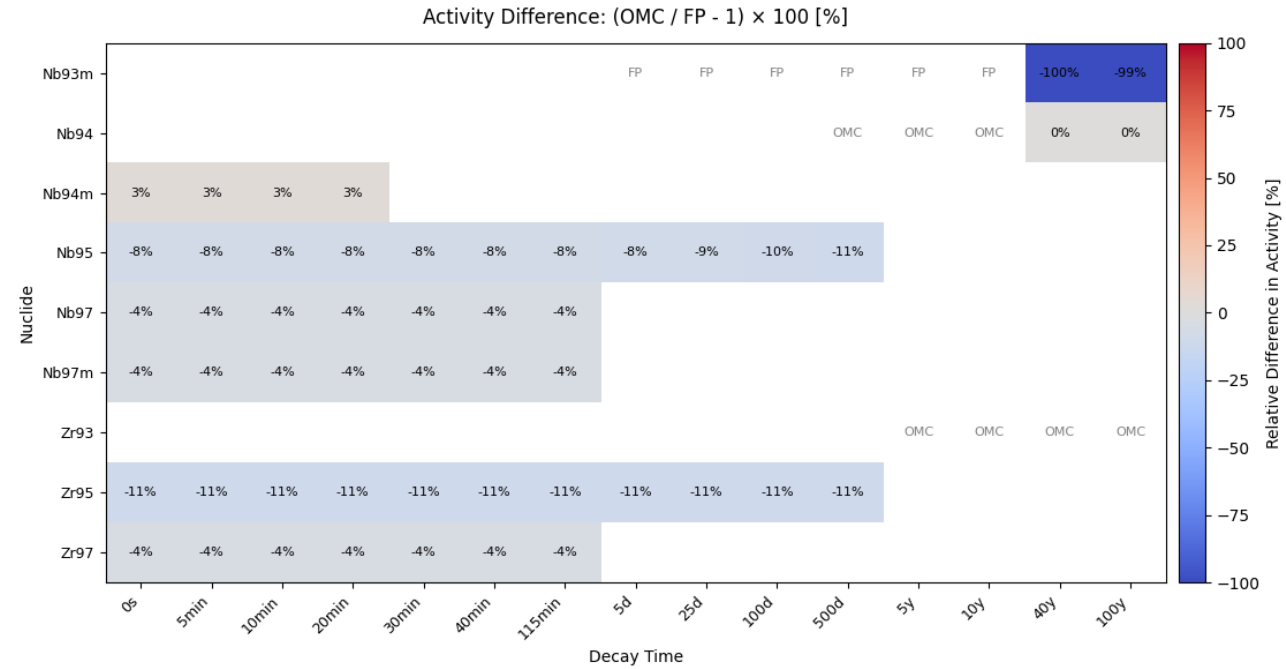
1. CCFE-709 and UKAEA-1102 **group structure vs. continuous  $\sigma$  (E)?**
2. Particular **resonance structure vs. cumulative reaction rate?**
3. Does a **self-shielding** correction in FP help?

## Spoilers:

It is preferred to let FP overestimate the reactions rates (conservatism) and identify such „problematic“ nuclides in the comparison with the continuous energy OpenMC solution.

The particularity of Zr-94 neutron capture and its stronger overprediction in FP remains to be revealed ...

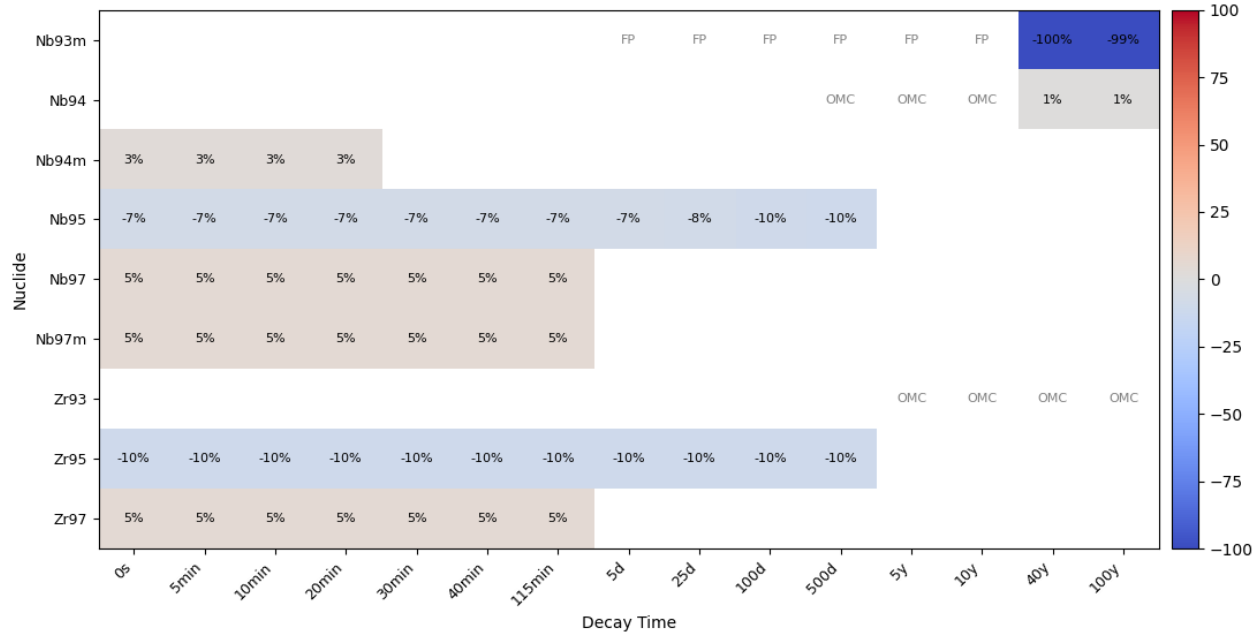
# Self-shielding (SSFGeometry) vs. no self-shielding



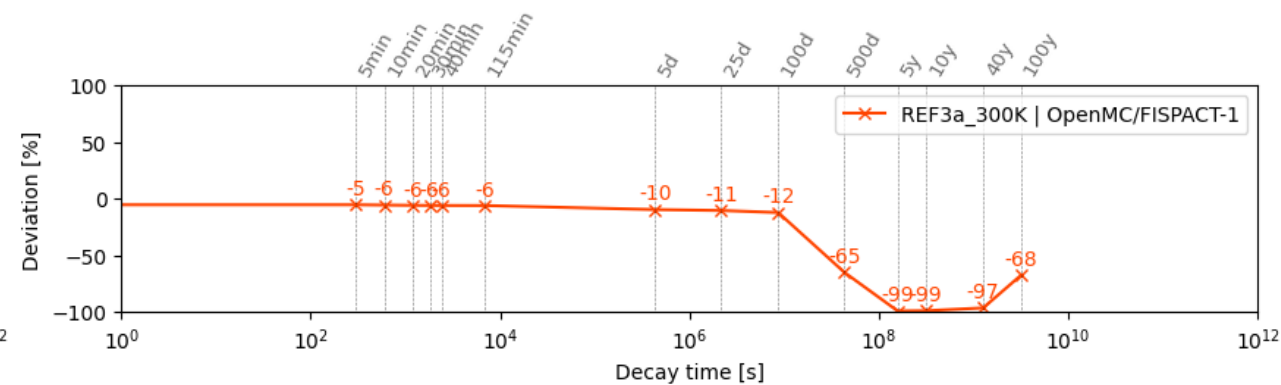
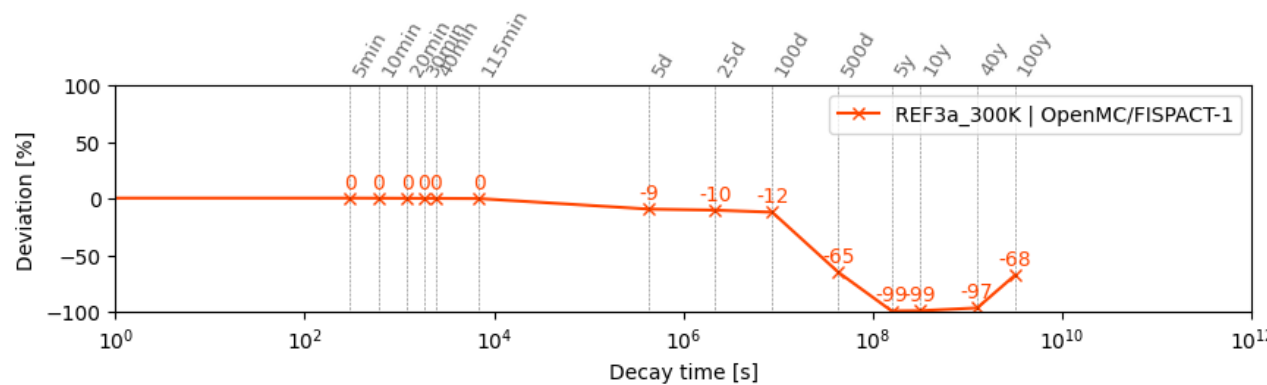
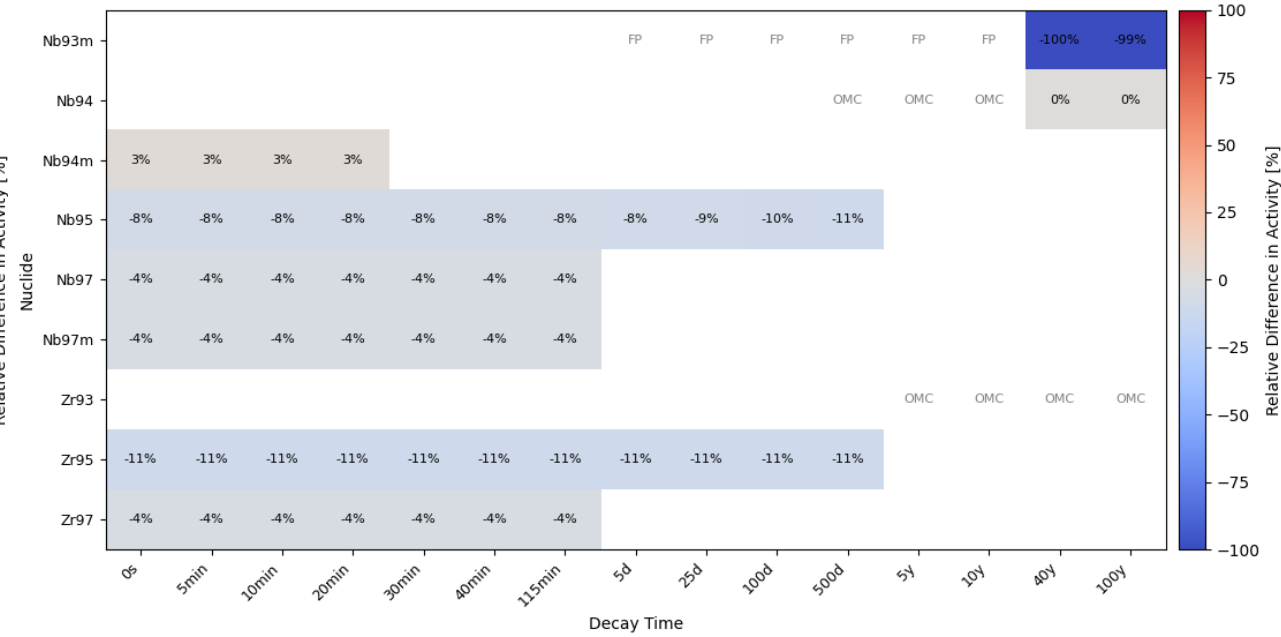


# Self-shielding (SSFGeometry) vs. no self-shielding

Activity Difference:  $(\text{OMC} / \text{FP} - 1) \times 100$  [%]



Activity Difference:  $(\text{OMC} / \text{FP} - 1) \times 100$  [%]

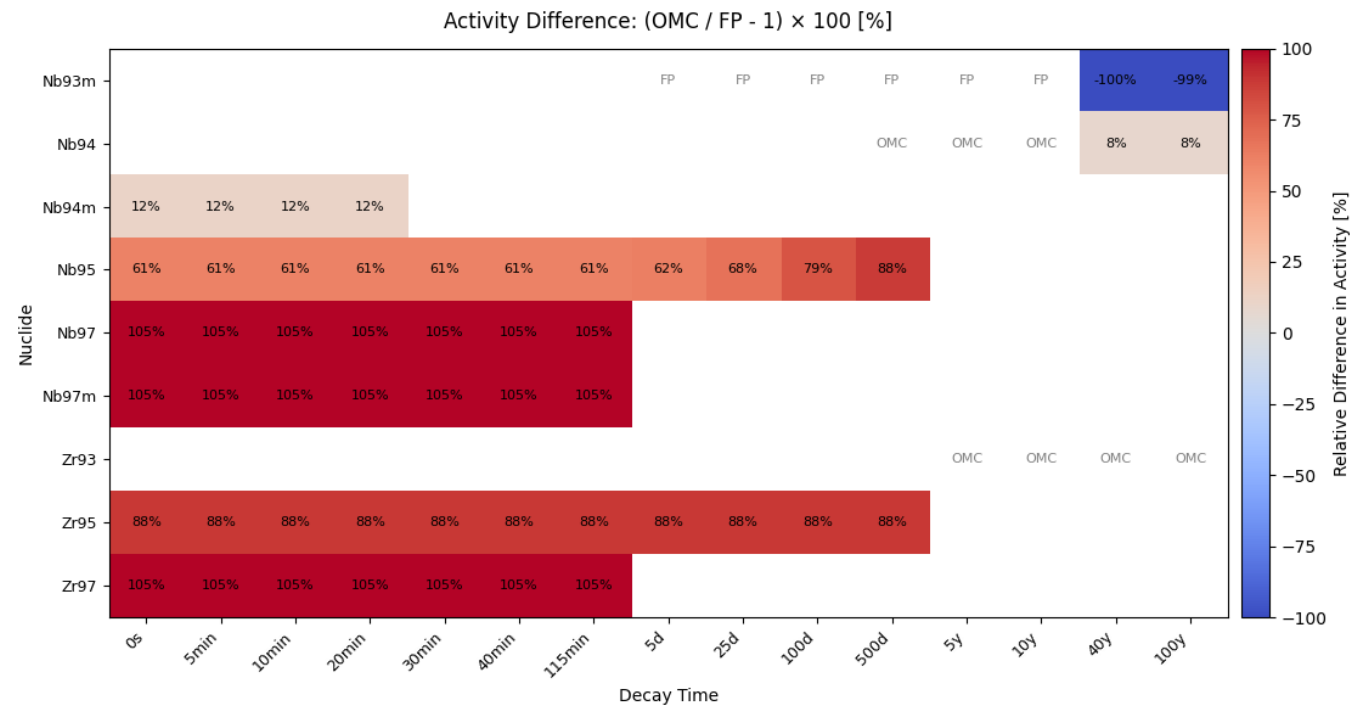


# Self-shielding (SSFGeometry) vs. no self-shielding

- Impact of SSFGeometry self-shielding model in FP-II visible on some nuclides (correction for resolved resonances without significant overlap)
- $Zr94(n,g)Zr95$  reaction rate not changed much (do tricky resonances overlap?)
- Self-shielding model (extended, calibrated correlation by irradiation experiments for simple geometries) is supposed to grasp „*geometry effect*“ of self-shielding
- „*Geometry effect*“: cannot be fully separated from energy self-shielding effect, but generally describes how the activation of a material lump is not homogenous through the body (e.g. Pu-239 build-up in pellet rim)
- Here: thin cladding and OpenMC track length cell-averaged neutron spectrum corresponds to average neutron spectrum in the cladding cell → geometry effect should already be covered in average

# Self-shielding (ProbTable) vs. no self-shielding

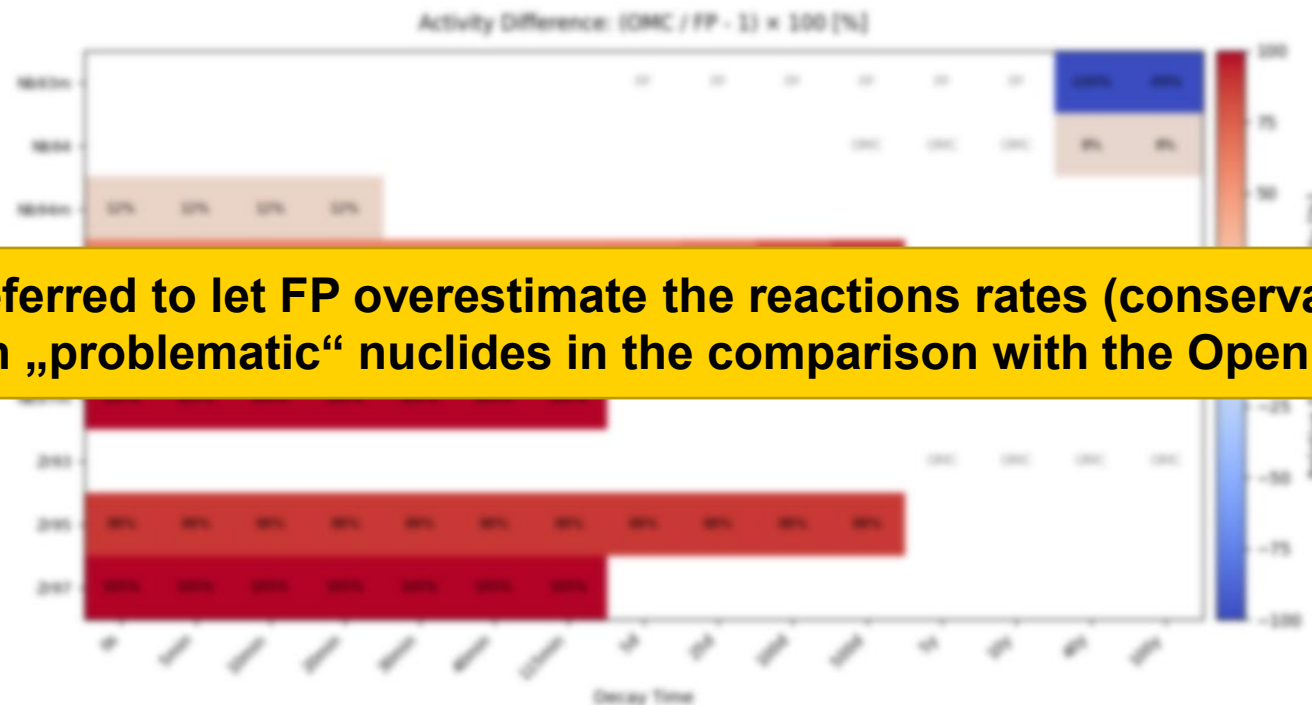
- Other self-shielding model in FP (ProbTable, see below) leads to very strong over-shielding (also reported in literature<sup>[26]</sup>)
- Possibility to use SSFDILUTION to artificially adapt the dilution cross-section in specific energy groups is cumbersome...



Strong over-shielding in FP with ProbTable SF when using accurately tallied spectra from OpenMC

# Self-shielding (ProbTable) vs. no self-shielding

- Other self-shielding model in FP (ProbTable, see below) leads to very strong over-shielding (also reported in literature<sup>[26]</sup>)
- Possibility to use SSFDILUTION to artificially adapt the dilution cross-section in specific energy groups is cumbersome...



→ It is preferred to let FP overestimate the reactions rates (conservatism) and identify such „problematic“ nuclides in the comparison with the OpenMC solution.

# Nuclide resonance structure vs. reaction rate

Having a look at

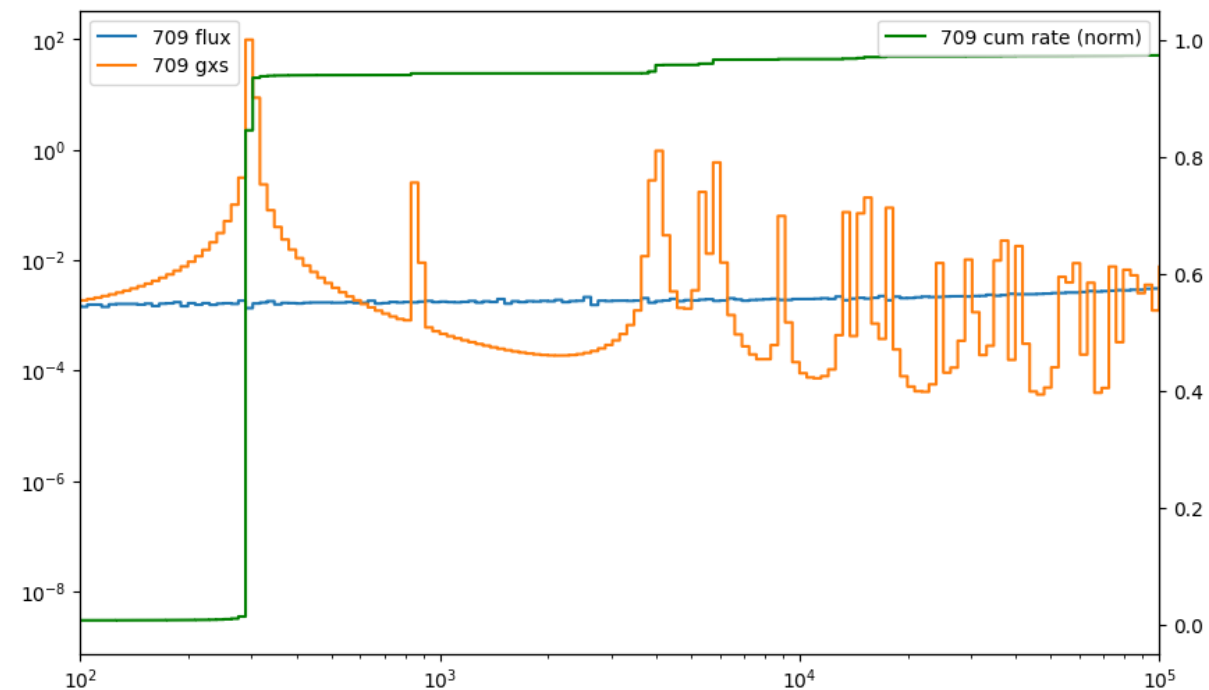
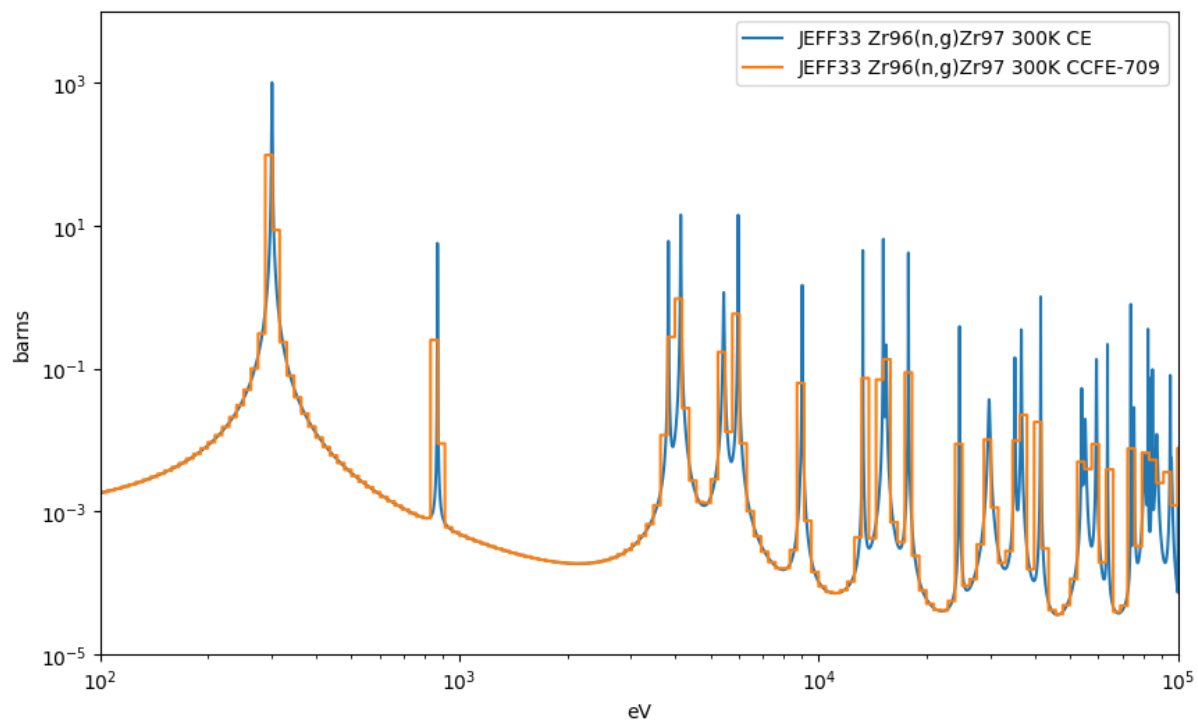
- nuclear resonance structure and its energy discretization in the group structure and cumulative reaction rate

First, looking at nuclides that are well predicted by FP (compared to OpenMC)

Nb93(n,g)Nb94m:	$\Delta \sim 3\%$
Zr96(n,g)Zr97:	$\Delta \sim 4\%$
Si30(n,g)Si31:	$\Delta \sim 3\%$
C13(n,t)B11:	$\Delta \sim 3\%$ on $^3\text{H}$
Zr94(n,g)Zr95:	$\Delta \sim 11\%$

# Zr96(n,g)Zr97:

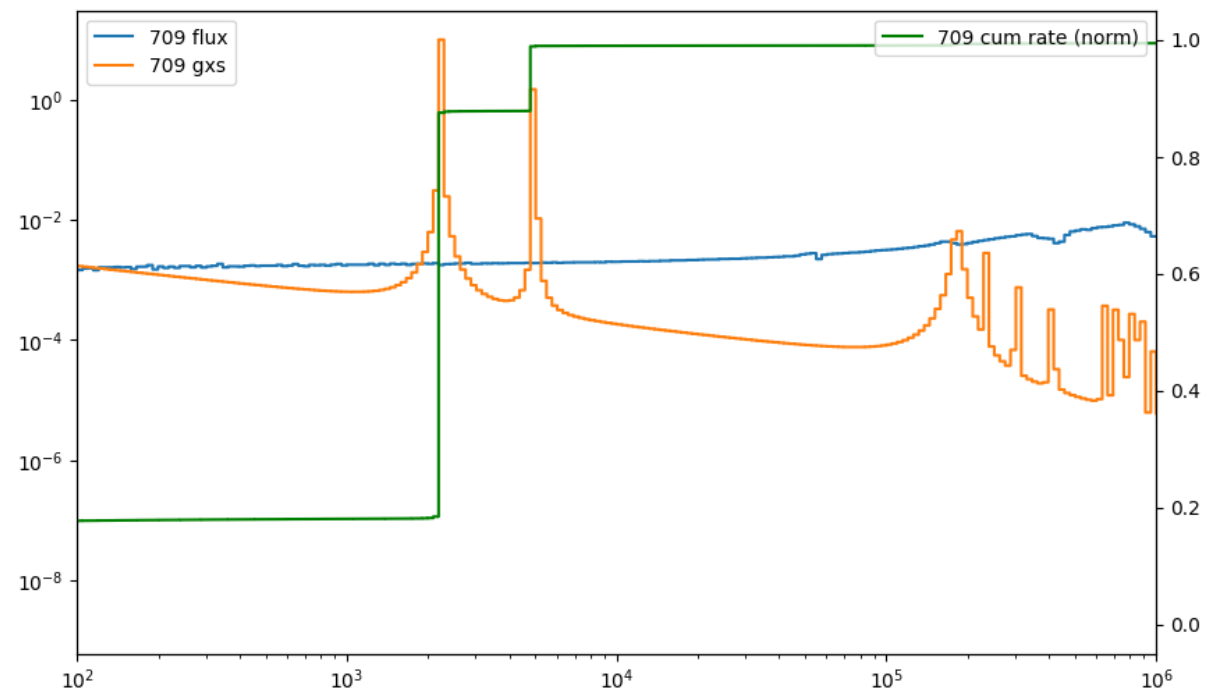
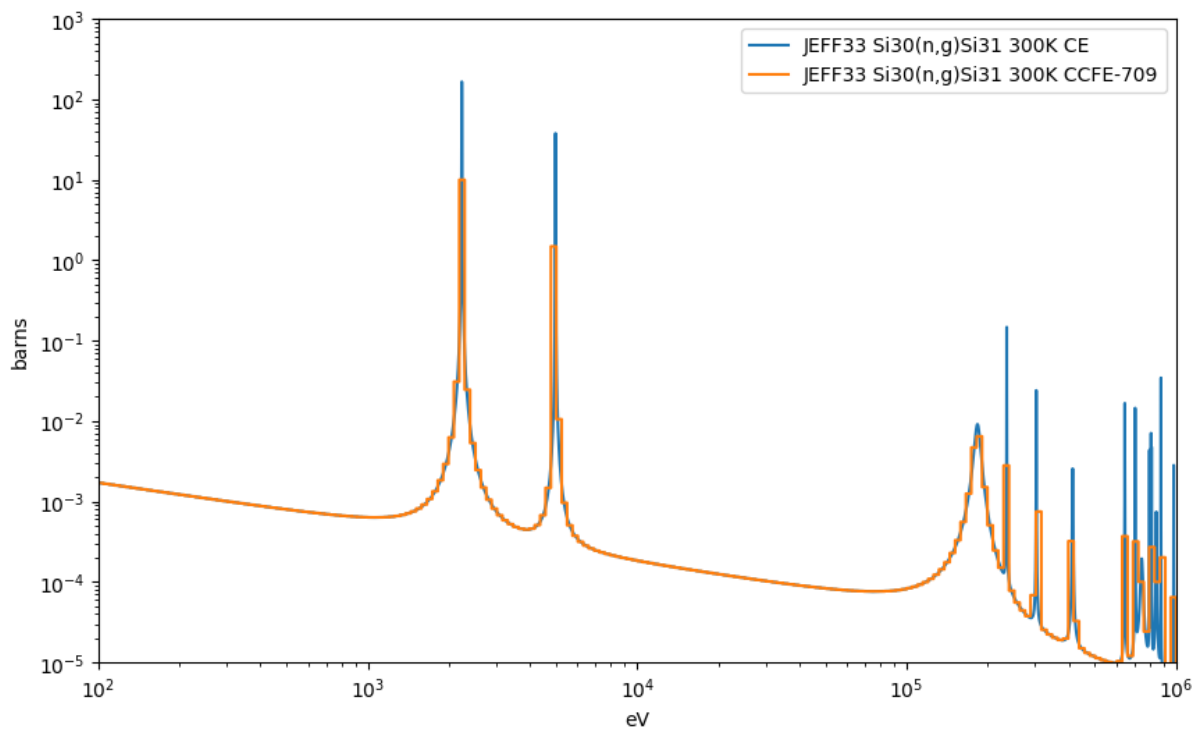
$\Delta \sim 4\%$  on Zr97



One major resonance  $\sim 200\text{-}300$  eV  $> 95\%$  of cumul. rate

# Si30(n,g)Si31:

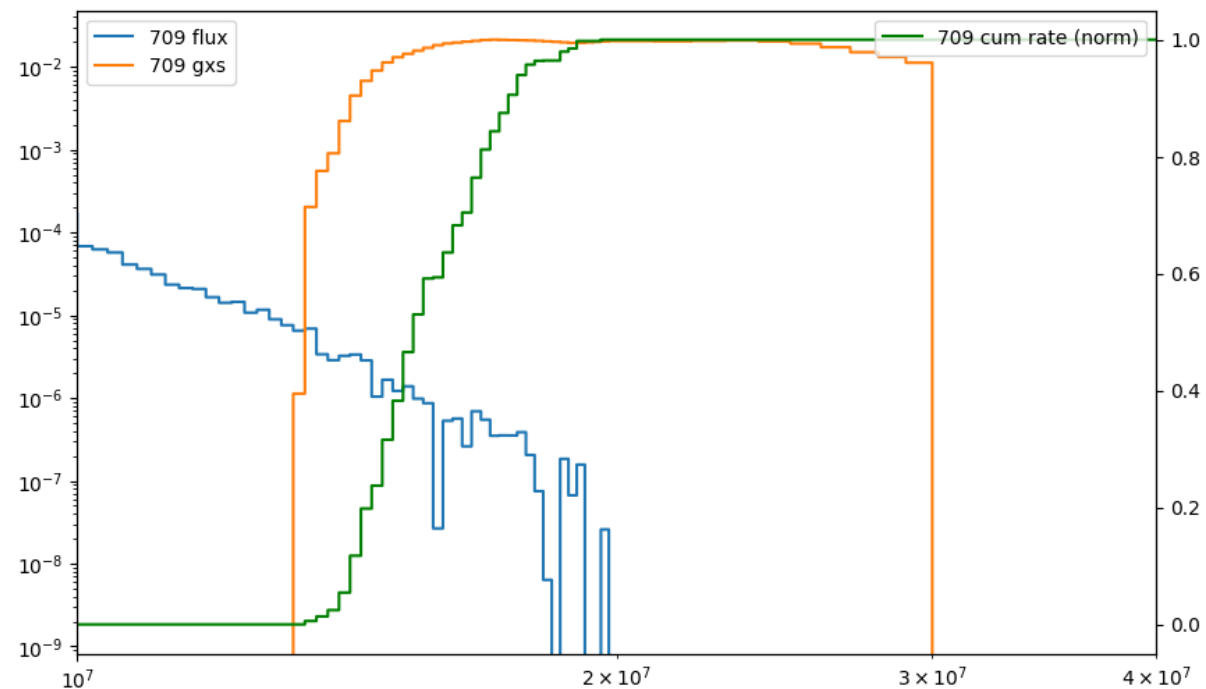
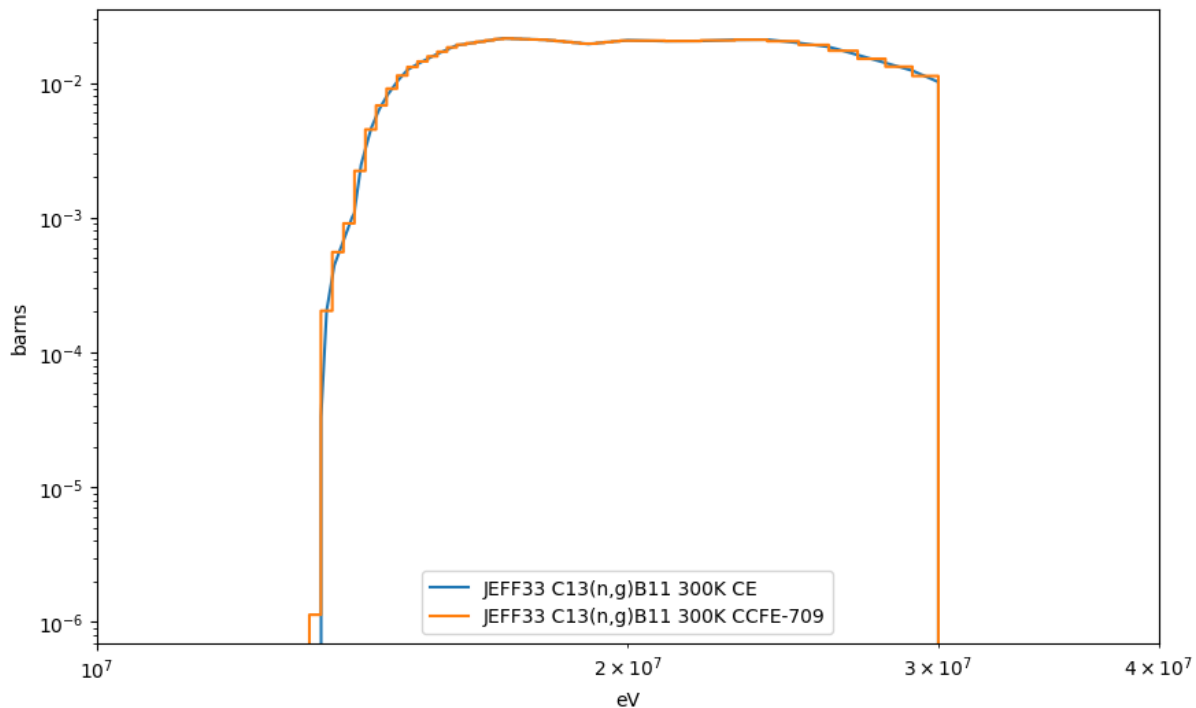
$\Delta \sim 3\%$  on Si31



Two major resonances (~2 and ~5 keV) > 99% of cumul. rate

# C13(n,t)B11:

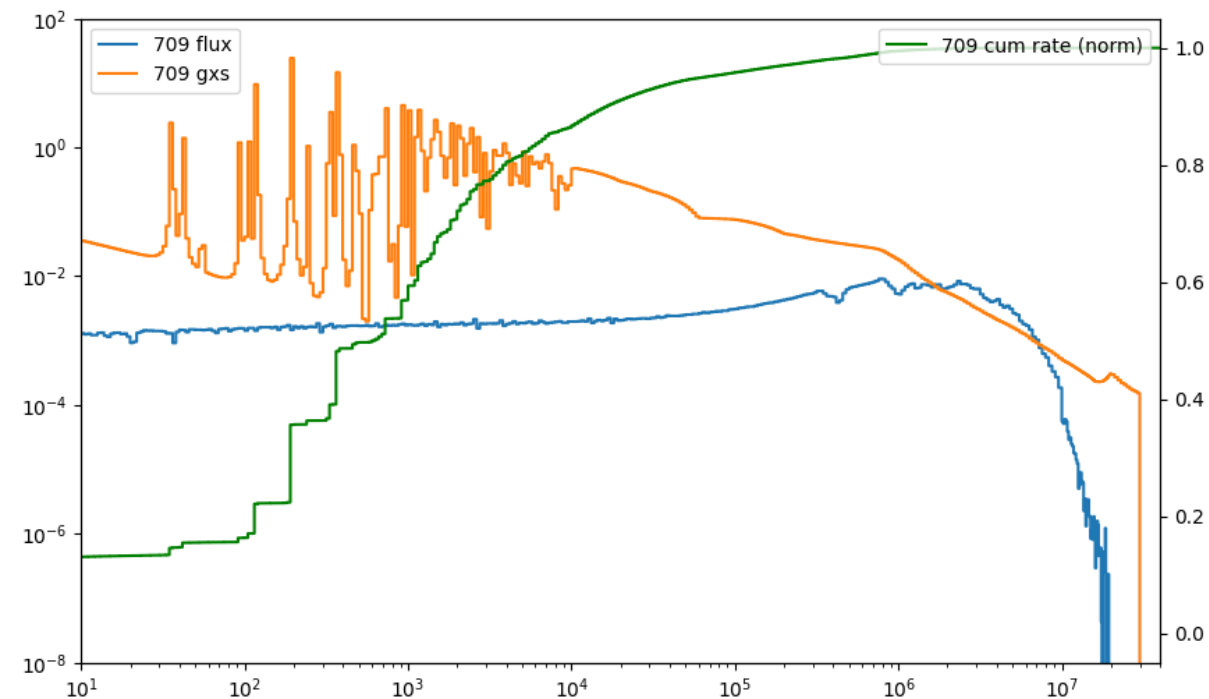
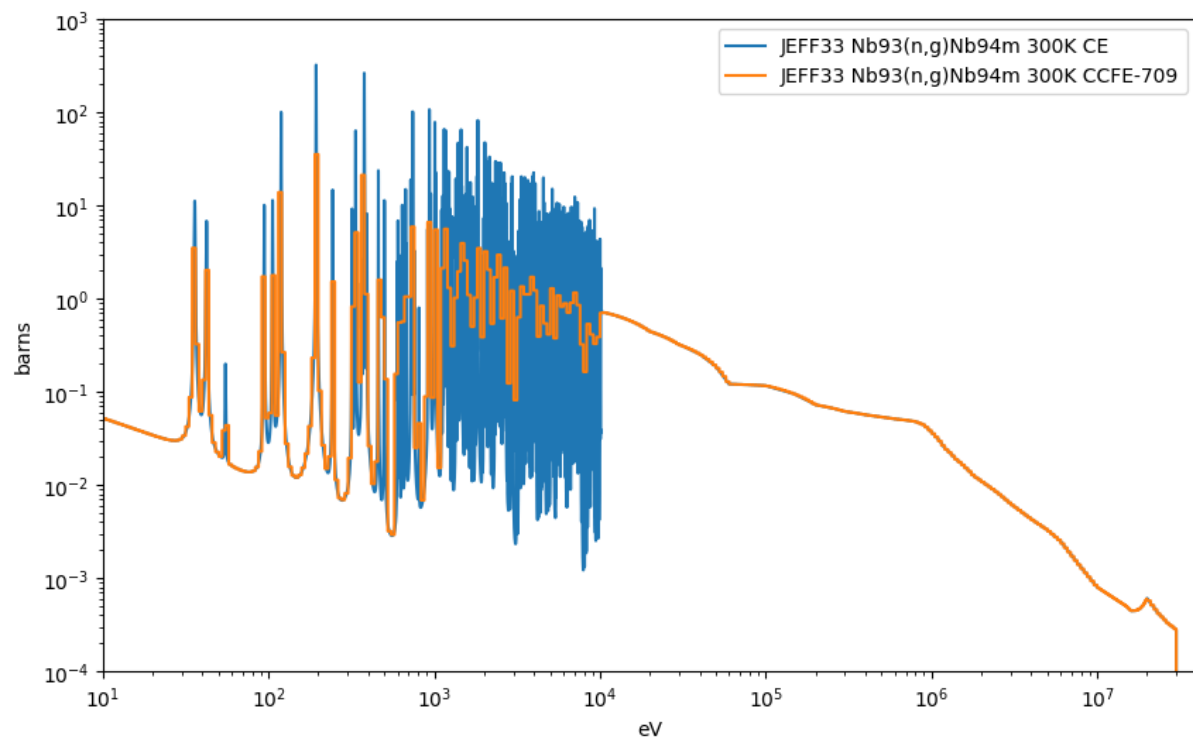
$\Delta \sim 3\%$  on H3



Threshold reaction well predicted even though neutron tail with low statistics.



# Nb93(n,g)Nb94m: $\Delta \sim 3\%$ on Nb94m

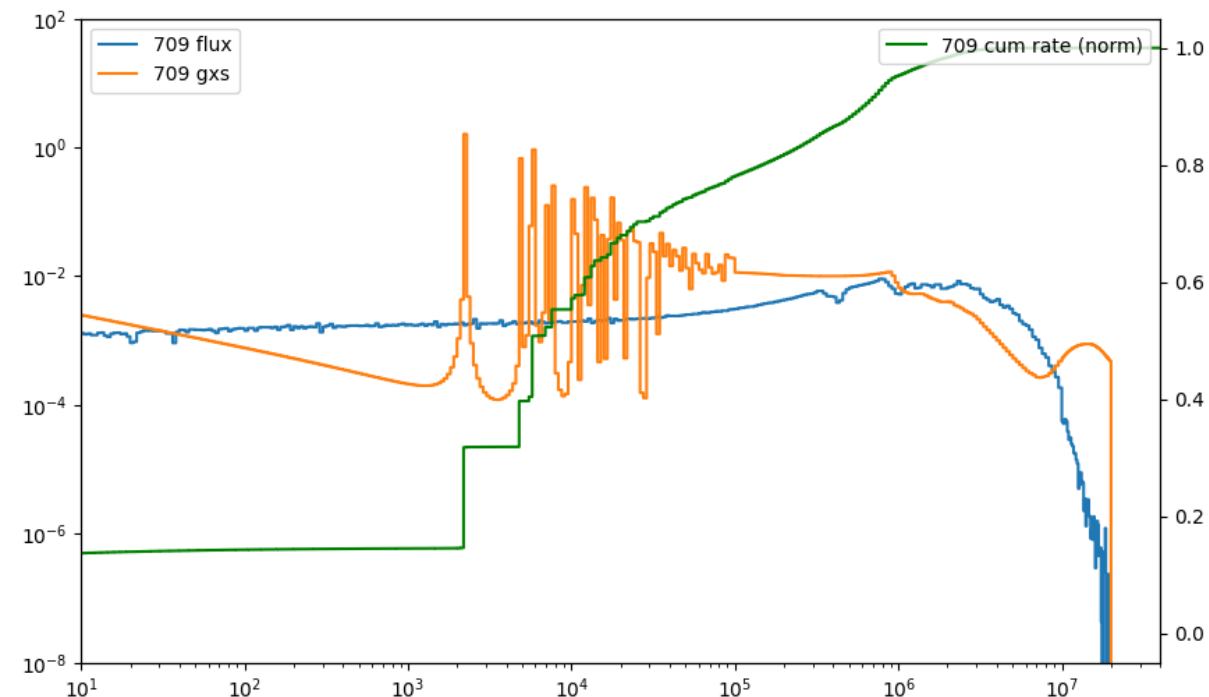
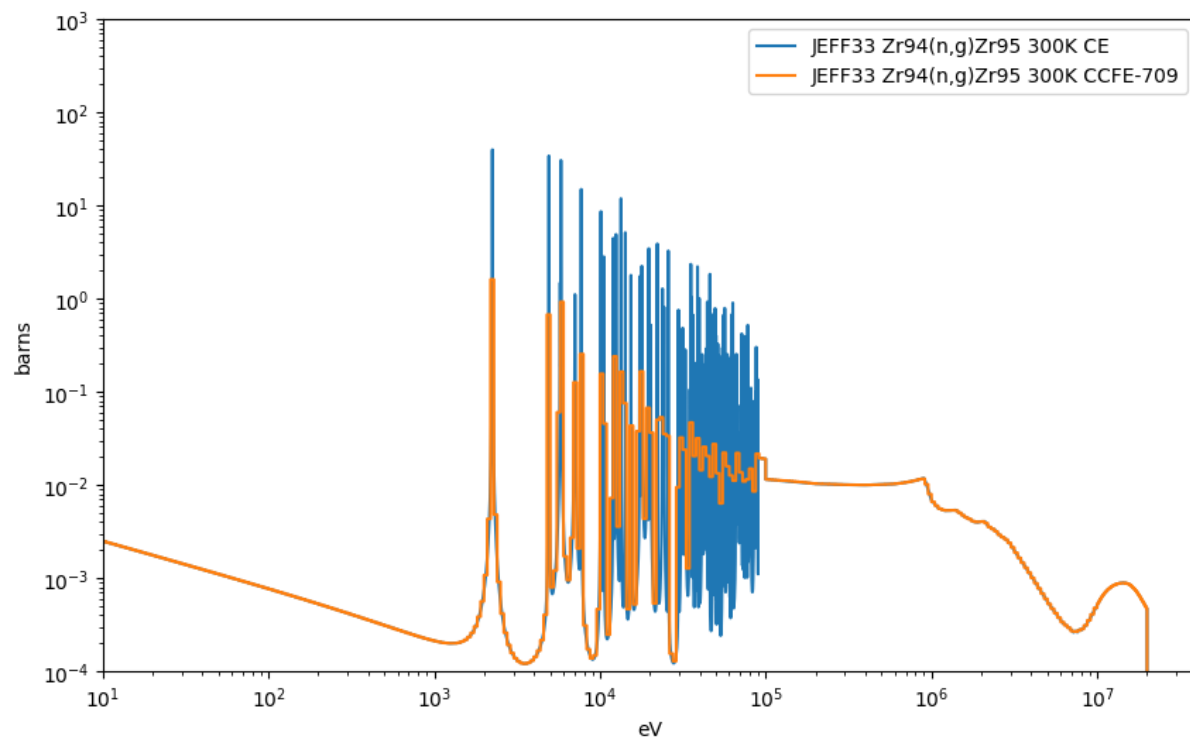


RRR: >50 % of reaction rate with several resonances form 20 to 1000 eV

URR: remaining part from 1000 eV to 10 MeV

# Zr94(n,g)Zr95:

$\Delta \sim 11\%$  on Zr95



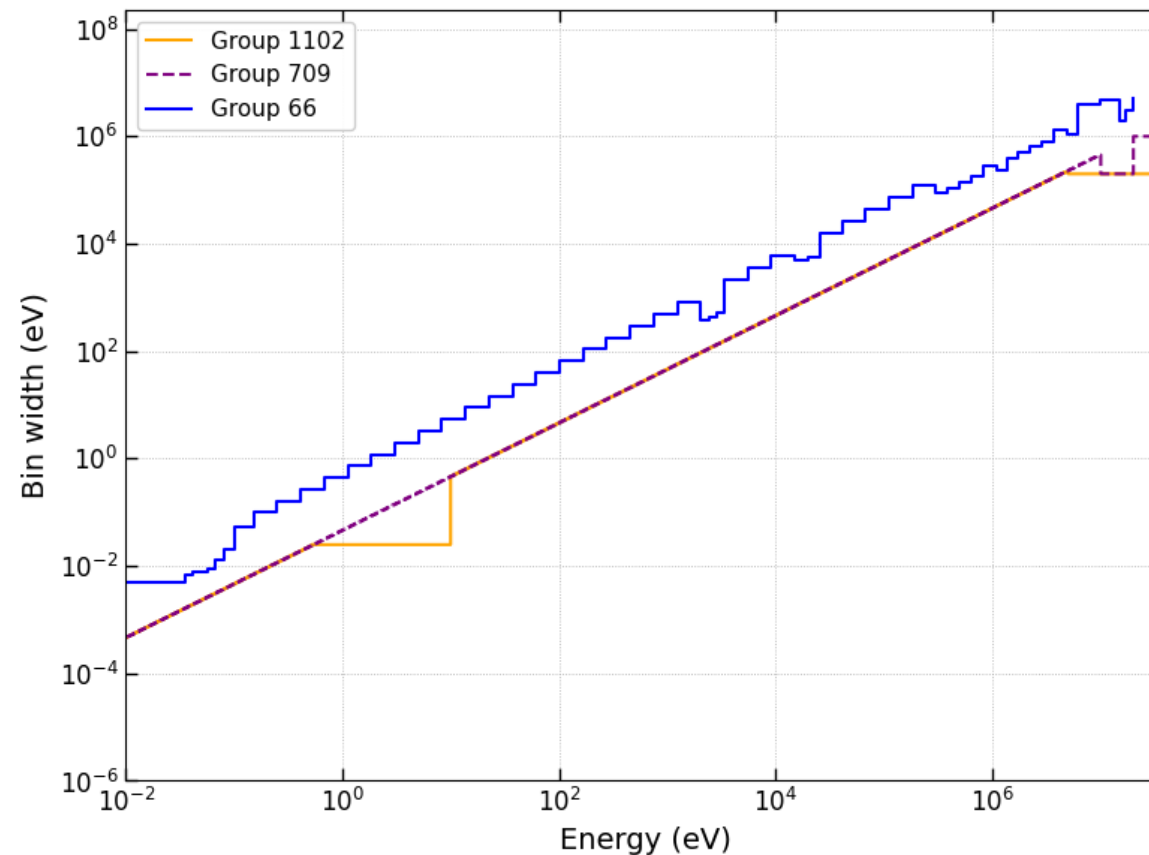
RRR: >50 % of reaction rate with several resonances from 2 to 10 keV

URR: remaining part from 10 keV to 30 MeV

# Energy bin width vs group structure

- No difference for 709 and 1102 group structure in RRR of  $Zr94(n,g)Zr95$  from 2 to 10 keV
- No difference for 709 and 1102 group structure in URR of  $Zr94(n,g)Zr95$  up to 40 MeV

→ **1102 group would very likely not perform “better”**



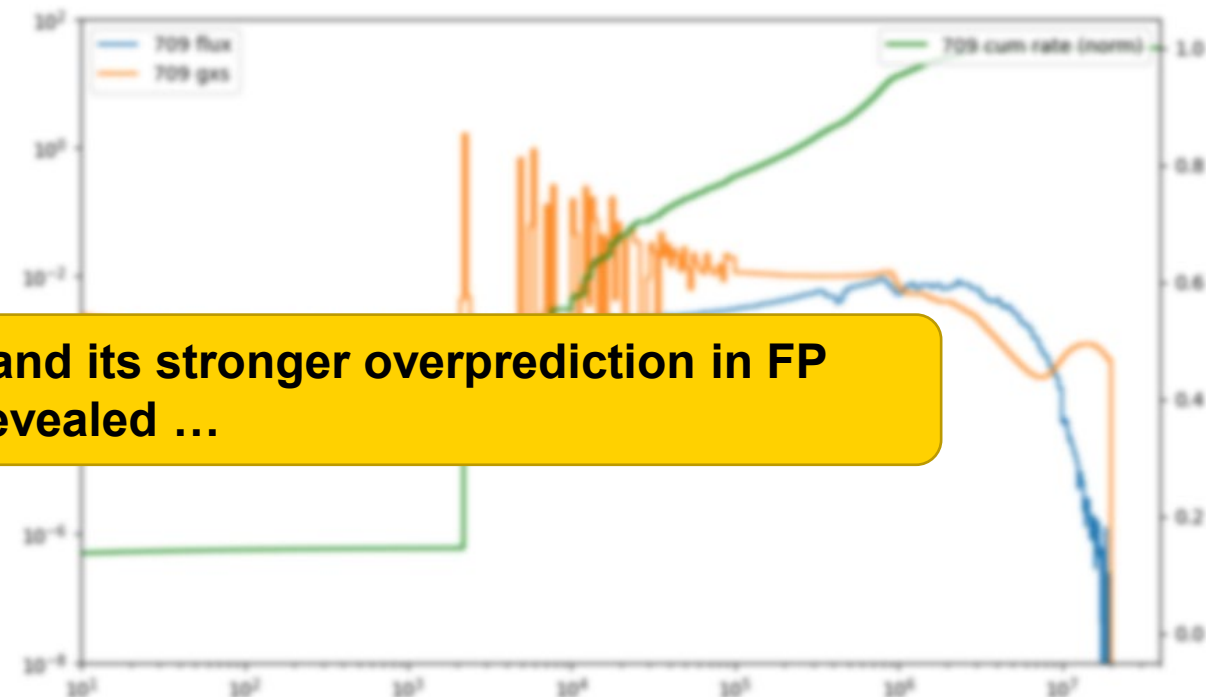
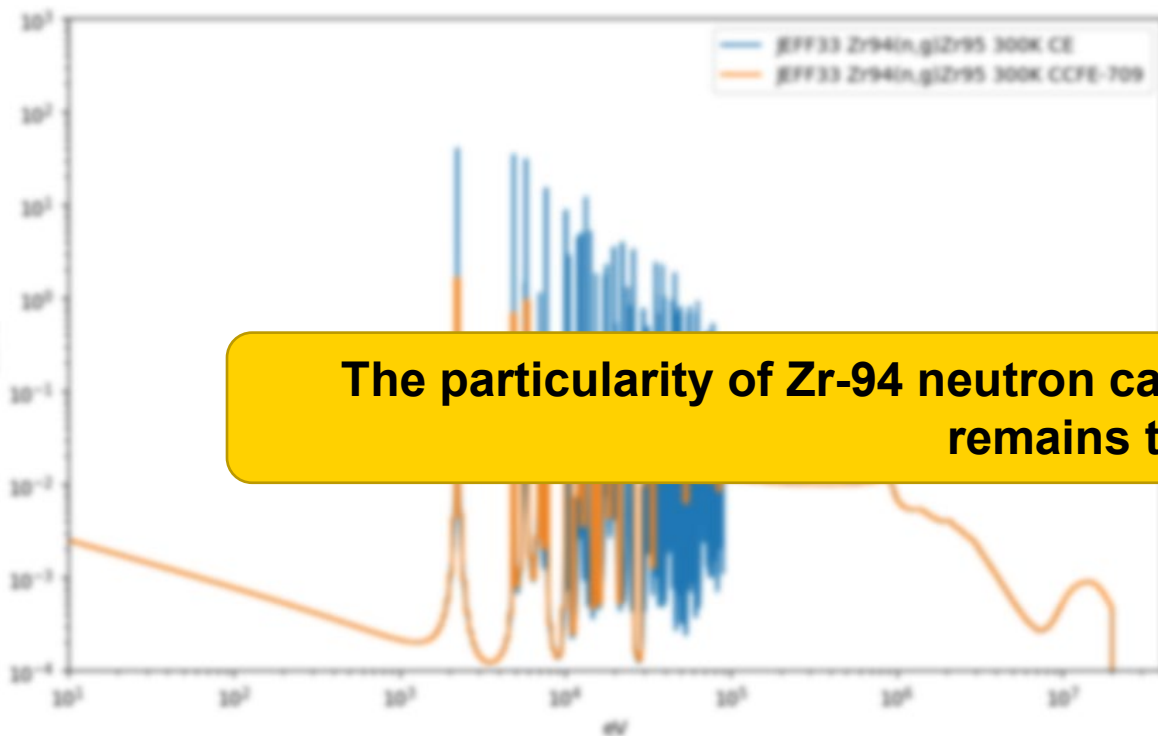
# Uncertainty (FP pathway analysis)

- REF3a example (MOI spectra, jeff-3.3 300 K)
- Estimated uncertainty at the end of irradiation (FP path analysis)

<b>Total activity:</b>	<b>1.61 %</b>
Nb97:	3.641%
Nb95:	3.910 %
Zr97:	3.826 %
Nb97m:	3.826 %
Zr95:	5.195 % (less than 11% diff to OpenMC)
Nb94m:	3.093 %

# Zr94(n,g)Zr95:

$\Delta \sim 11\%$  on Zr95



The particularity of Zr-94 neutron capture and its stronger overprediction in FP remains to be revealed ...

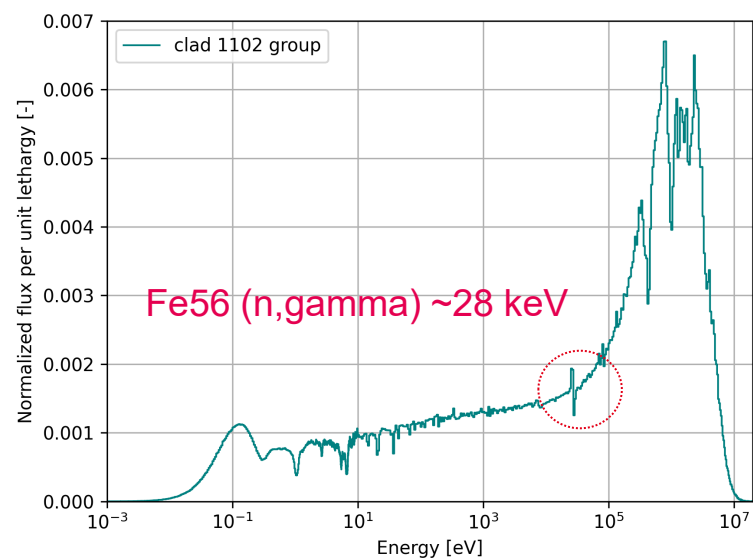
# Conclusions OpenMC vs Fispact-II

- **CE OpenMC solution as reference** except for reactions that cannot be yet included in the depletion chain file for describing the inventory change (Nb93m, V49) ...72 hours per sim  
→ Knowledge about such nuclides through FP-II
- **FP path analysis:** Identification of all relevant paths to dominant nuclides, adding reactions of interest on the nuclide-specific level to the OpenMC depletion chain file → e.g. (n,np) for Cr50 only.  
→ Complementary modelling also to estimate inventory uncertainties
- **FP includes all available reactions from ND library**, but library (+SSF) not readily available at temperature of interest (“[...] scripts and processes defined by the UK Atomic Energy Authority [...]” → 3 more ND codes: NJOY, PREPO and CALENDF) ...minutes per sim
- **OpenMC→FP-II workflow:** Using OpenMC tallied spectra with BU in FP evades “constant branching ratios” through collapse of the BU-specific spectrum with nuclear cross-sections

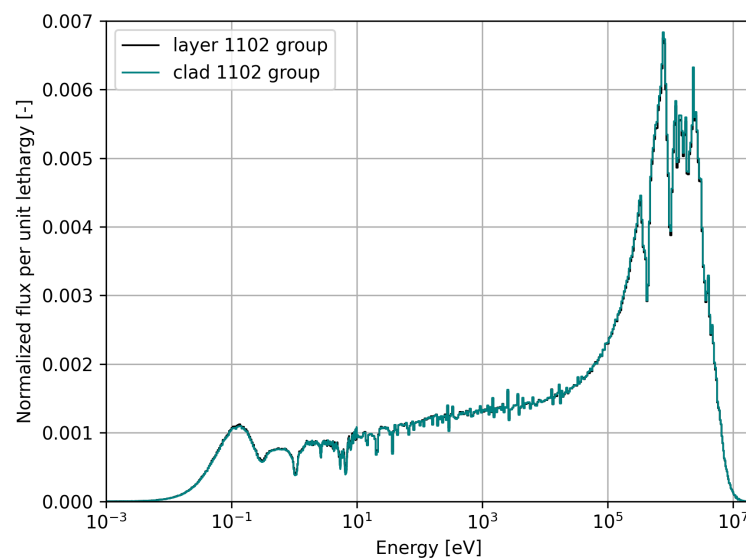
# **More ATF cladding metrics from FP-II**

# Tallied clad spectra in OpenMC for use in FP (here: MOI)

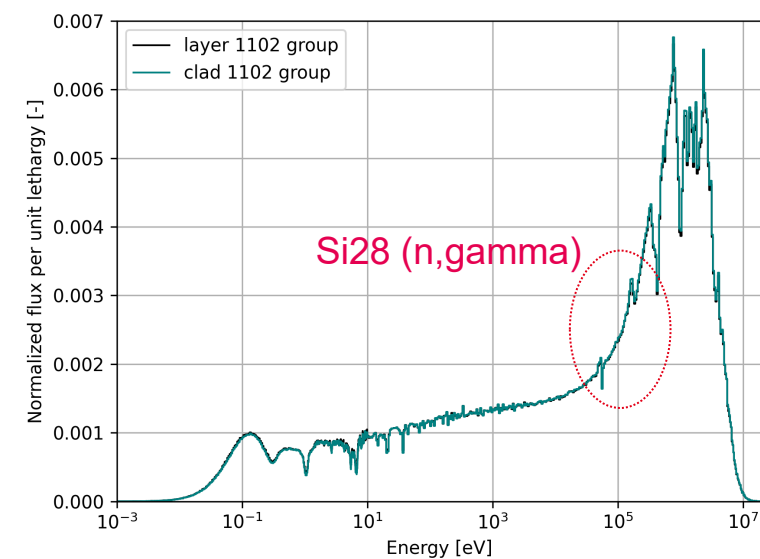
## FeCrAl



## M5+20μmCr

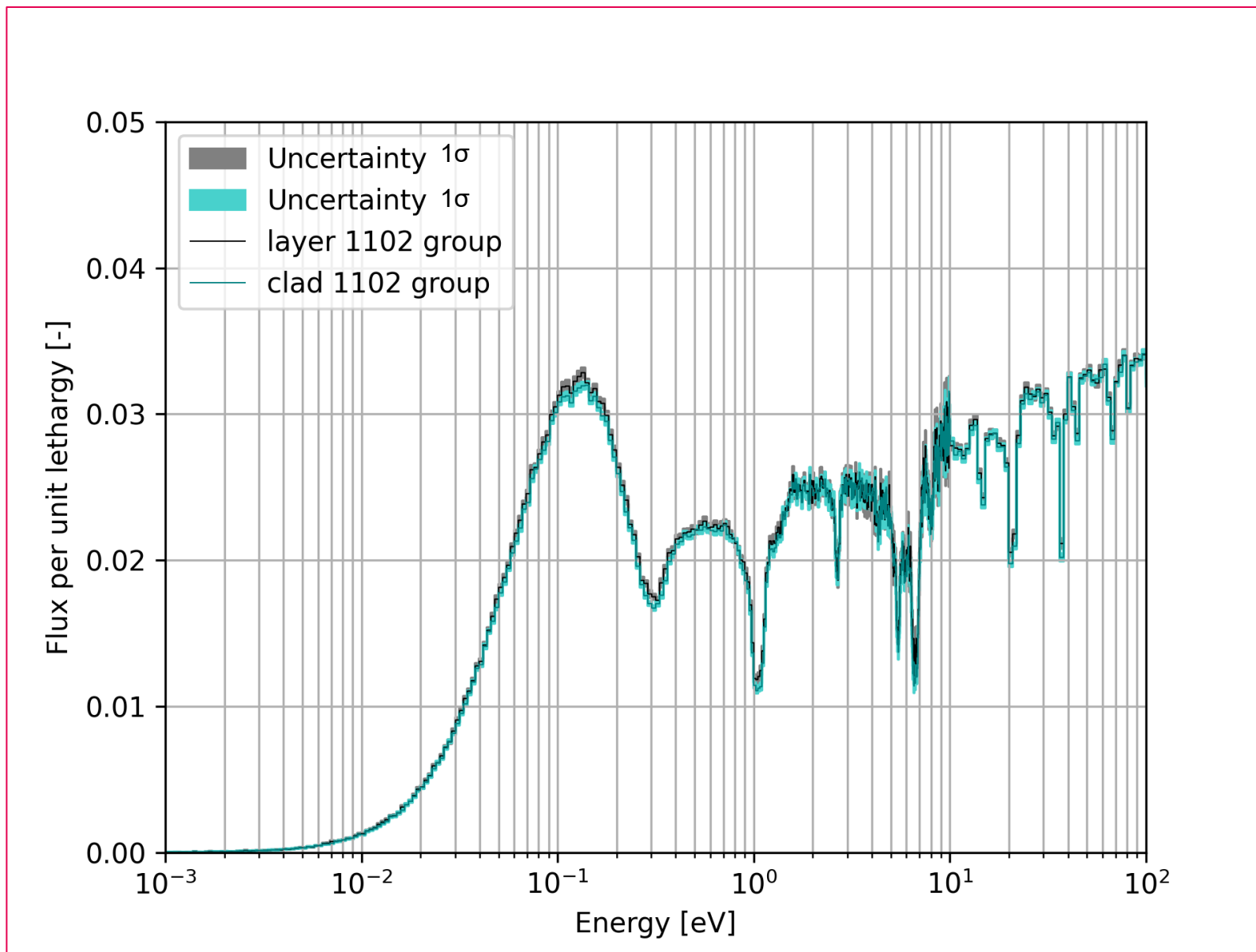


## SiC+10μmCr





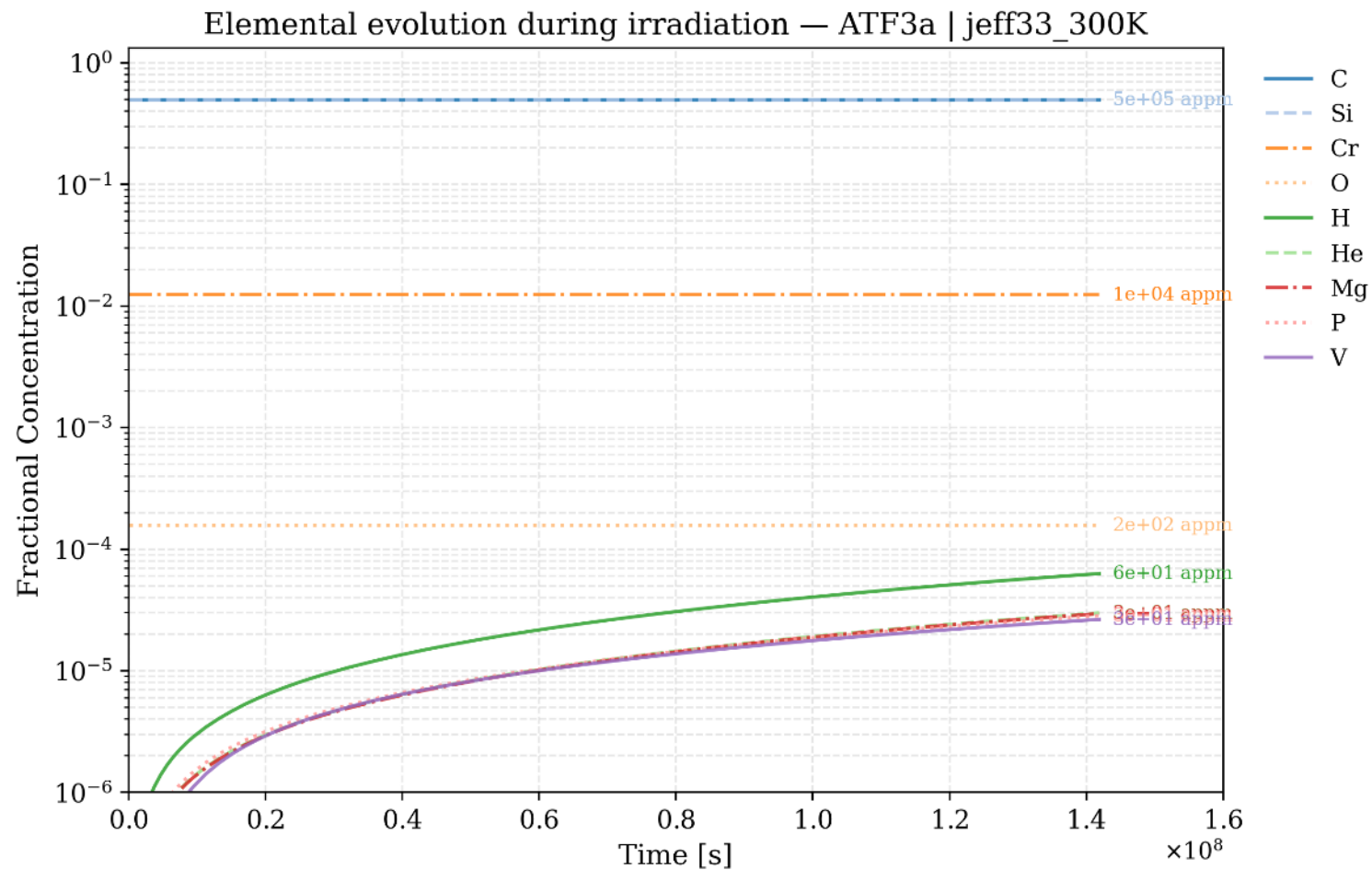
# M5+20 $\mu$ mCr (here: MOI)





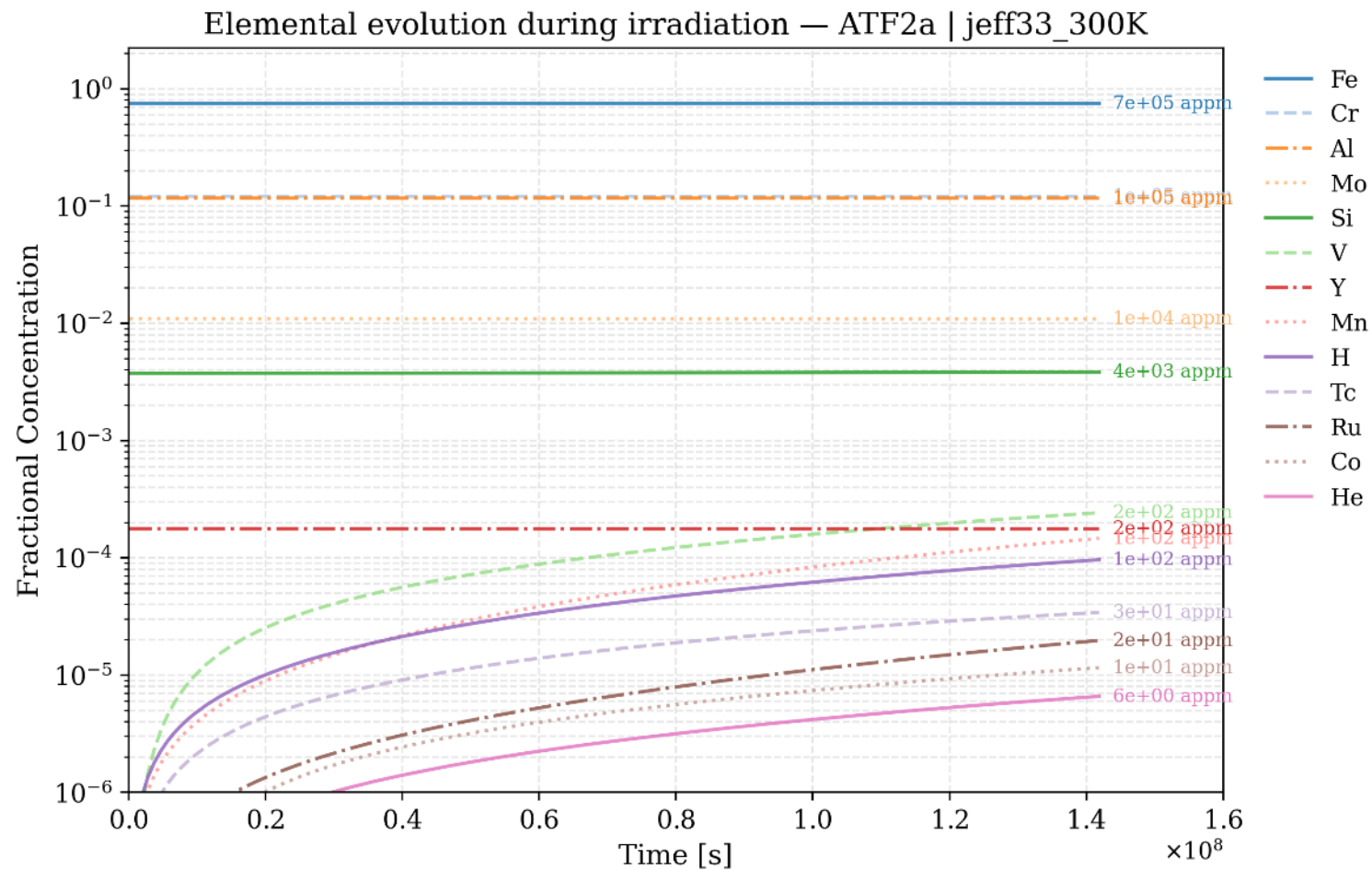
# SiC+Cr: Evolution of elemental appm (>1appm)

	ATF3a
H	6e+01
V	3e+01
He	3e+01
P	3e+01
Mg	3e+01



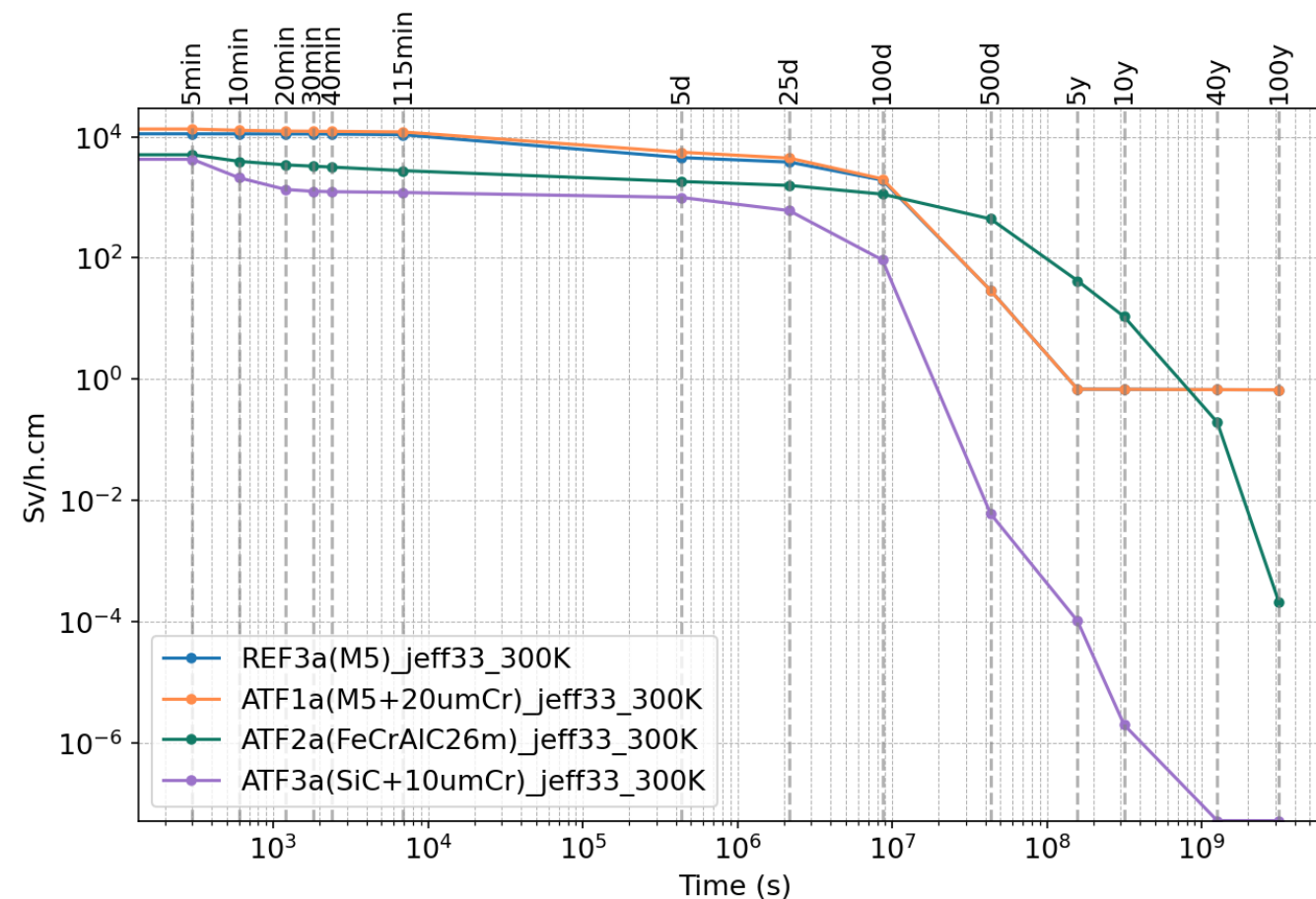
# FeCrAl: Evolution of elemental appm (>1appm)

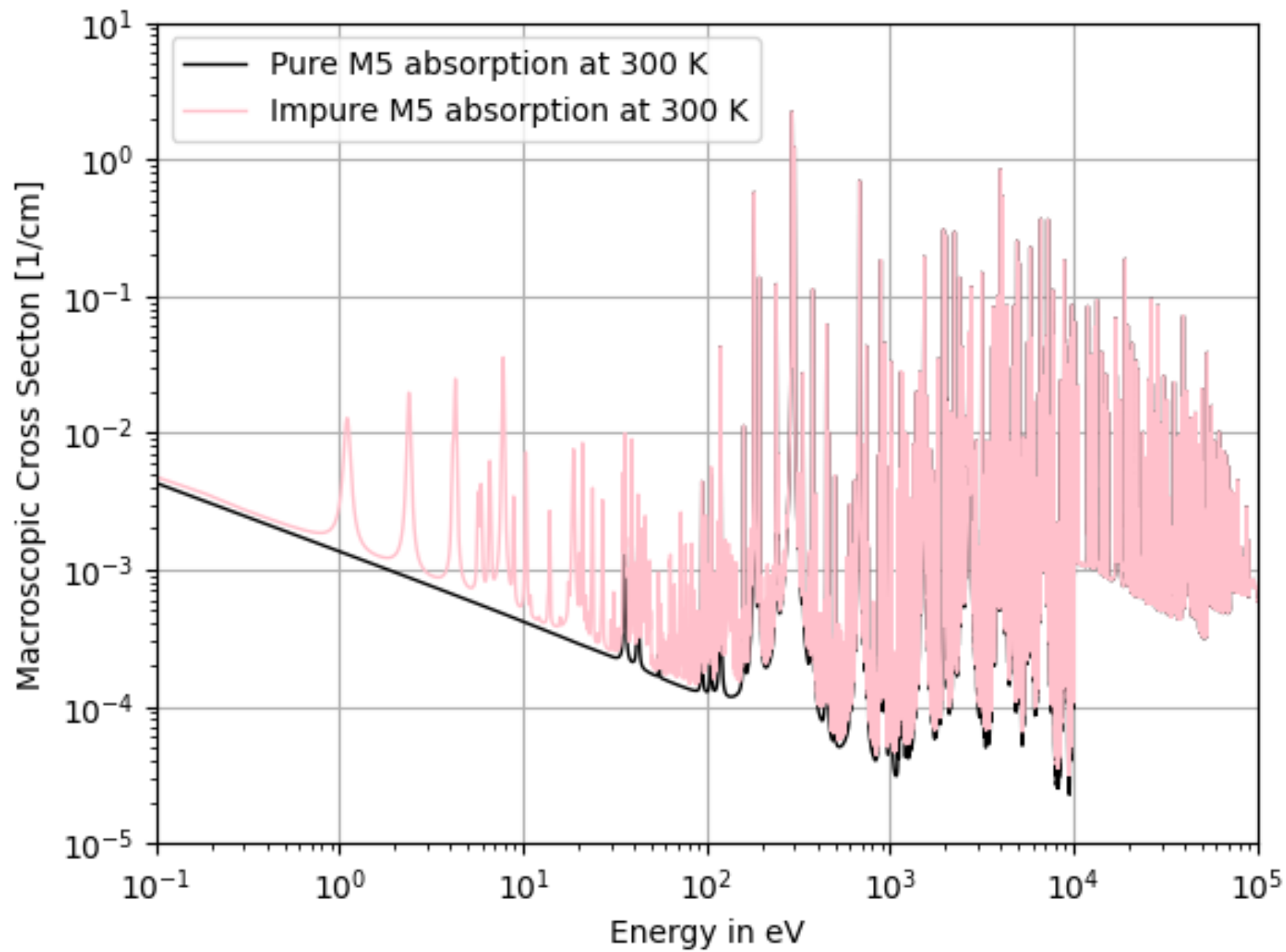
	ATF2a
V	2e+02
Mn	1e+02
H	1e+02
Tc	3e+01
Ru	2e+01
Co	1e+01
He	7e+00

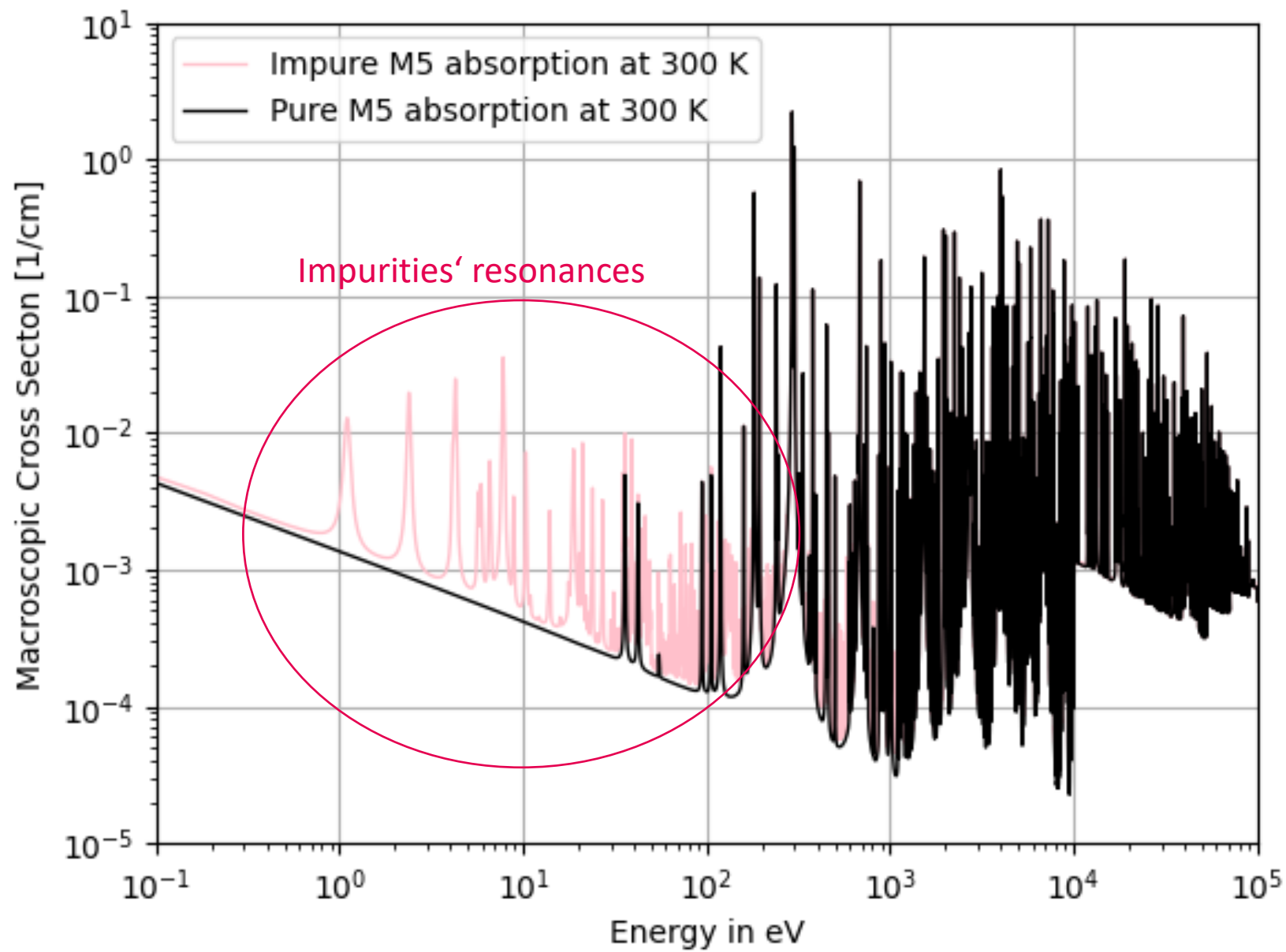


# Contact dose rate semi-infinite slab (jeff-3.3)

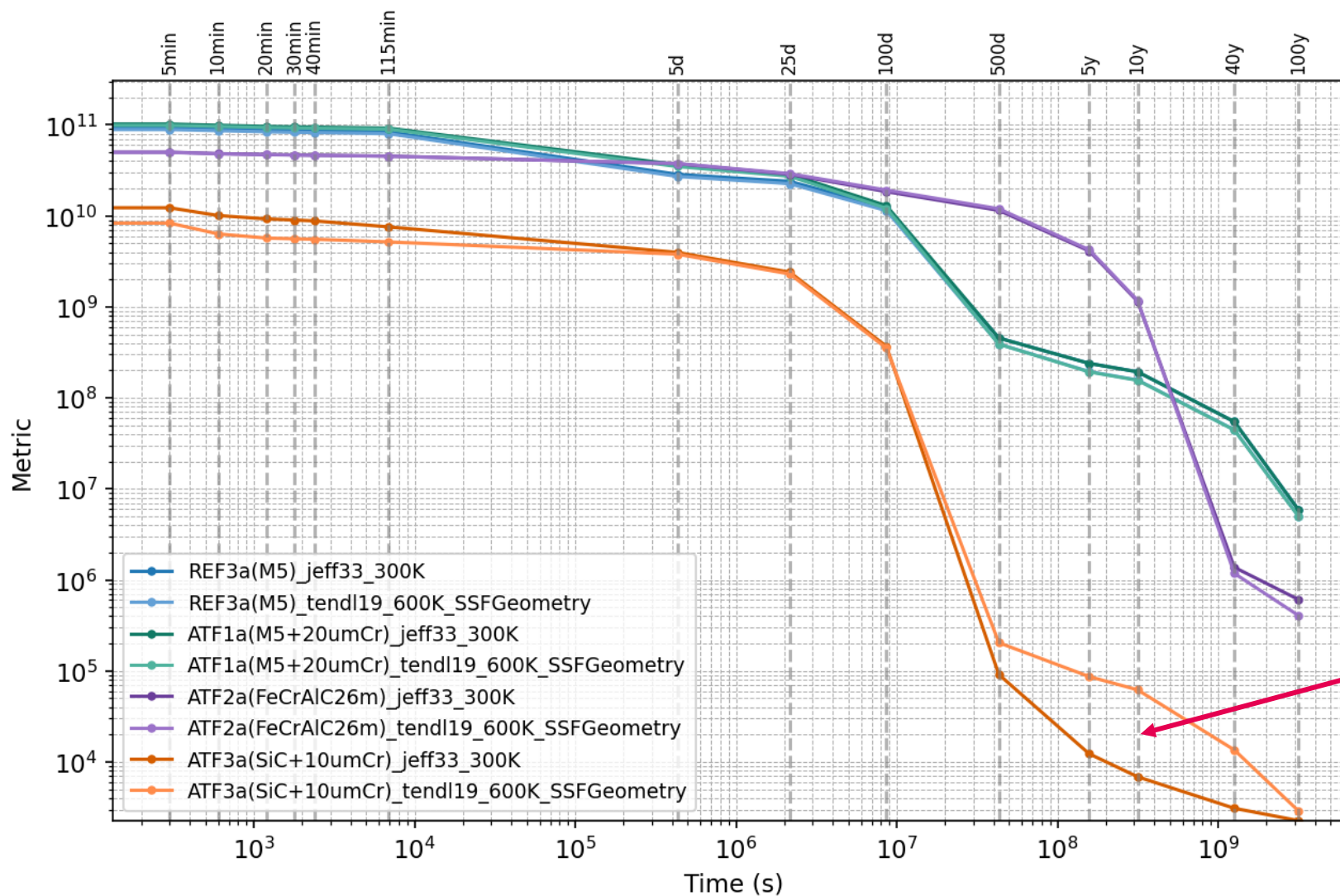
- Similar order and evolution as for activity
- M5 shifted upwards (higher MeV/second) compared to FeCrAl
- SiC shifted upwards (Cr51 gamma lines)





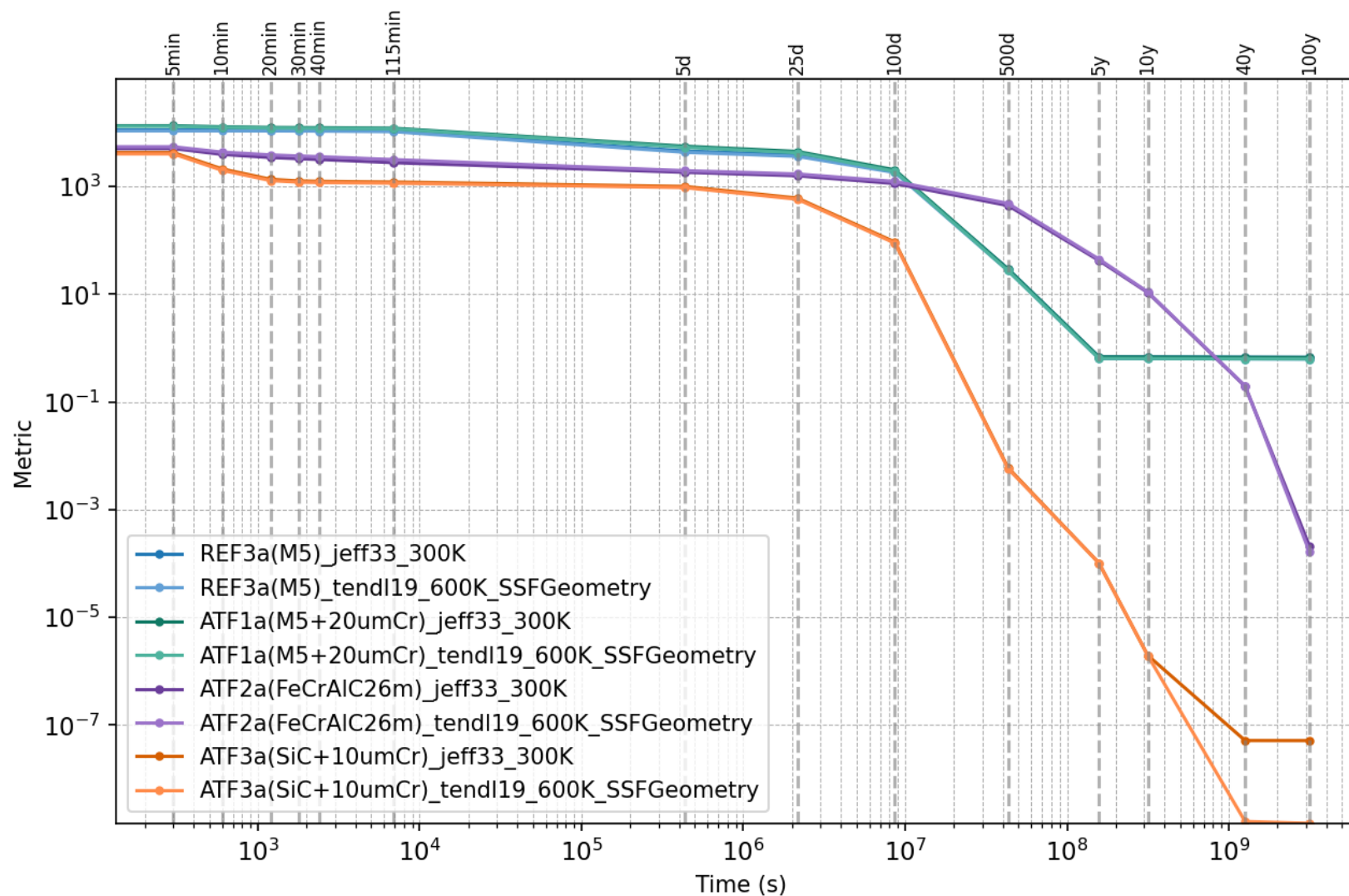


# Bq/cm (activity): Library > +300K > +SSFGeometry

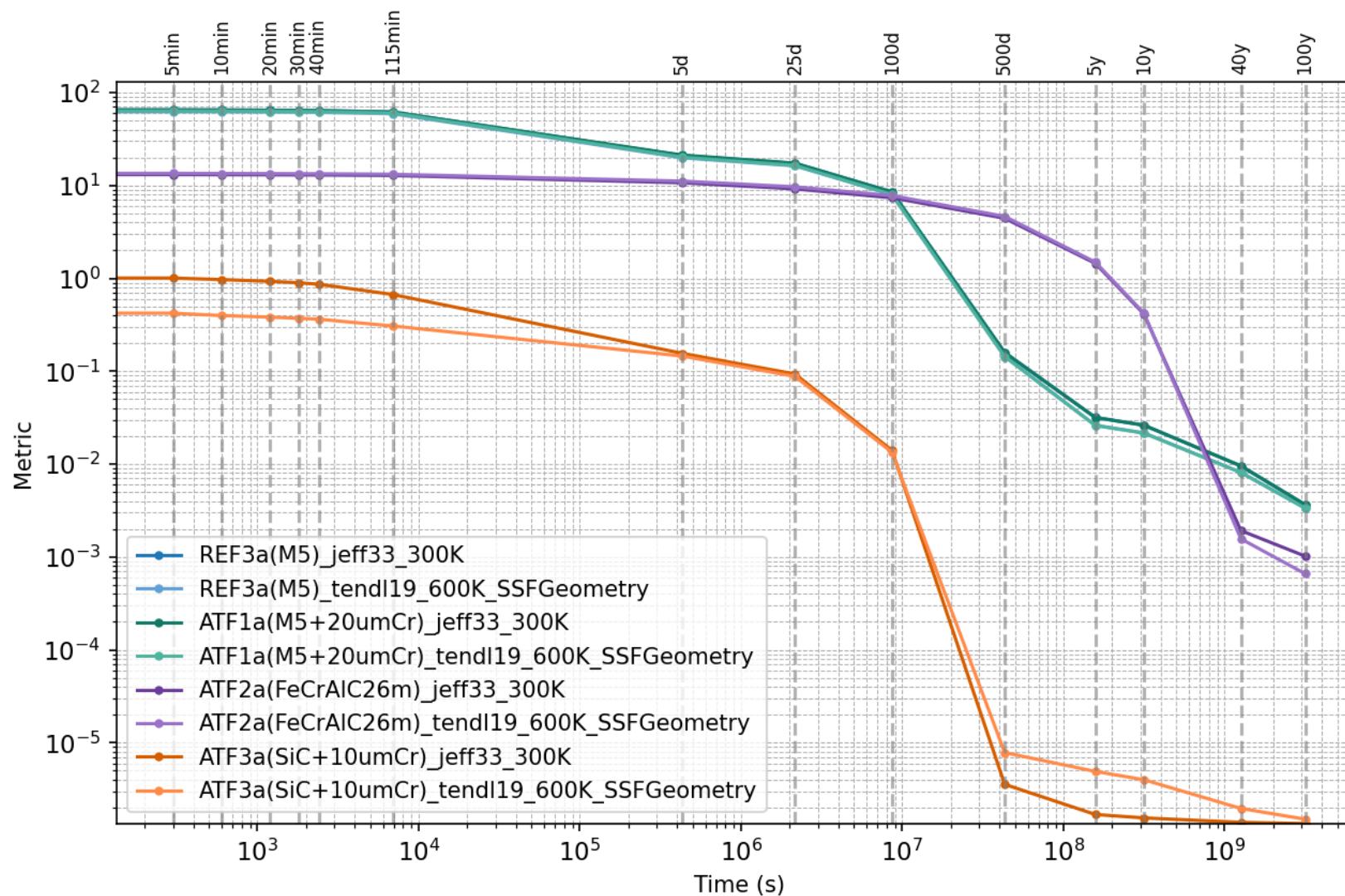




# Sv/h.cm (contact dose rate semi-infinite slab)



# Sv/kg.cm (ingestion)





**Dong-Hwa Lee**

KAERI

## **Simulation of Cr-coated Zry-4 cladding tube ballooning and burst behavior using MERCURY**

Nuclear fuel is inserted into the reactor core to generate thermal energy and transfer the resulting heat to the coolant. Throughout operation, the fuel must remain free from mechanical failure under normal operating conditions, and its thermo-mechanical behavior must stay within regulatory safety limits during accident scenarios.

To support the assessment of nuclear fuel performance under both normal and accident conditions, a variety of finite difference method (FDM) based analysis codes - such as FRAPCON [1], FRAPTRAN [2], and ROPER [3] - have been developed. More recently, to enable higher-fidelity simulations, finite element method (FEM) based performance analysis codes capable of modeling mesh deformation and heterogeneous material behavior have been introduced. Representative FEM-based codes include BISON [4], developed at the Idaho National Laboratory (INL), and MERCURY [5–7], developed by the Korea Atomic Energy Research Institute (KAERI).

MERCURY (Multi-dimensional Entire fuel Rod Code for Understanding Reaction Yield behaviors) V1.0 was developed in accordance with KAERI's software quality assurance (SQA) procedures, and its verification was completed through a series of numerical benchmarks [8]. As part of the validation effort - intended to evaluate the code's ability to reproduce relevant physical phenomena - the MERCURY code was applied to the Zry-4 DIMAT experiment. The DIMAT (Deformation In-situ Measurement Apparatus by image-analysis Technique) experiment reproduces the high-temperature expansion and rupture behavior of nuclear fuel cladding under Loss-of-Coolant Accident (LOCA) conditions, which represent a one of the key reactor Design-Basis-Accidents (DBAs). The deformation response of Zry-4 cladding, including ballooning and burst behavior, was characterized using in-situ imaging techniques [9–10].

In this study, the MERCURY code was used to simulate the DIMAT experiment, and the resulting predictions were compared with experimental measurements to assess the code's predictive capability. Additionally, the MERCURY code was employed to simulate the ballooning and burst behavior of Cr-coated Zry-4 cladding tubes, providing further insight into its applicability to advanced cladding concepts.

### **References**

- [1] Geelhood, K. J., et al. FRAPCON-4.0: A Computer Code for the Calculation of Steady-State, Thermal-Mechanical Behavior of Oxide Fuel Rods for High Burnup, PNNL-19418, Vol.1 Rev.2, 2015.
- [2] Geelhood, K. J., et al. FRAPTRAN-2.0: A Computer Code for the Transient Analysis of Oxide Fuel Rods, PNNL-19400, Vol.1 Rev2, 2016.

## 30<sup>th</sup> International QUENCH Workshop

- [3] Choi, J. M., et al. A Fuel Rod Performance Analysis and Design Code—ROPER. In: Korean Nuclear Society Spring Meeting, 2009.
- [4] J. D. Hales et al. BISON Theory Manual The Equations Behind Nuclear Fuel Analysis. Idaho National Laboratory. Idaho Falls, Idaho, Oct. 2014.
- [5] Kim, Hyochan, et al. Development of MERCURY for simulation of multidimensional fuel behavior for LOCA condition. Nuclear Engineering and Design, 2020, 369: 110853.
- [6] Lee, Sung-Uk, et al. Validation of MERCURY code under LOCA condition with Out-of-pile and In-pile tests. Nuclear Engineering and Design, 2022, 392: 111775.
- [7] Kim, Hyochan, et al., MERCURY V1.0 Theory Manual, KAERI/TR-10442/2024, 2024.
- [8] Lee, DongHwa, et al. Verification of FEM based thermo-mechanical solving system for fuel performance code and its results, KAERI/TR-9835, 2023.
- [9] Choi, K.H. et al. Development of Strain Measurement Method by Image Analysis for Cladding Deformation, KAERI/TR-7930, 2019.
- [10] Choi, K.H. et al. Measurement and Evaluation of High-temperature Deformation of Fuel Cladding using image analysis technique, KAERI/TR-8338, 2020.

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# Simulation of Cr-coated Zry-4 cladding tube ballooning and burst behavior using **MERCURY**

*December 17, 2025*

*Dong-Hwa Lee*

*LWR fuel technology research division, KAERI*



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**KAERI**

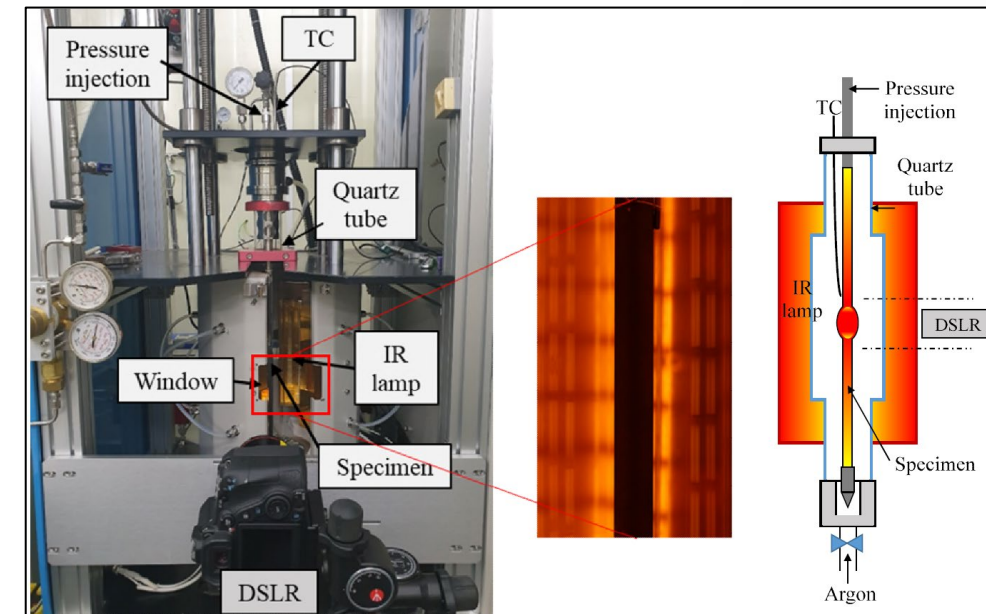
Korea Atomic Energy Research Institute

- 01 Introduction of DIMAT experiment**
- 02 Introduction of MERCURY code**
- 03 Simulation of DIMAT experiment**
- 04 Simulation of Cr-coated Zr-4 cladding tube**
- 05 Conclusion and future work**

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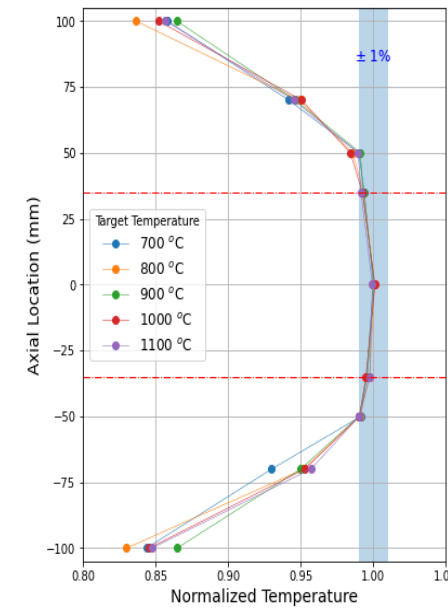
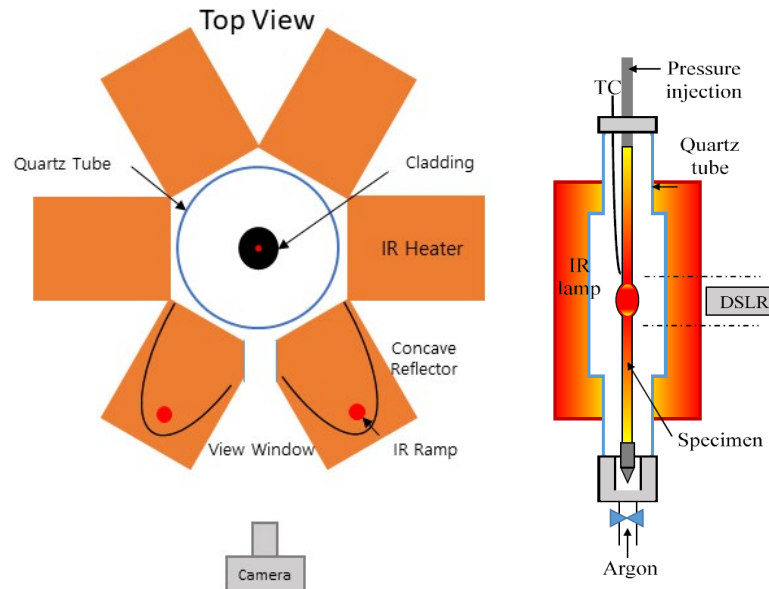
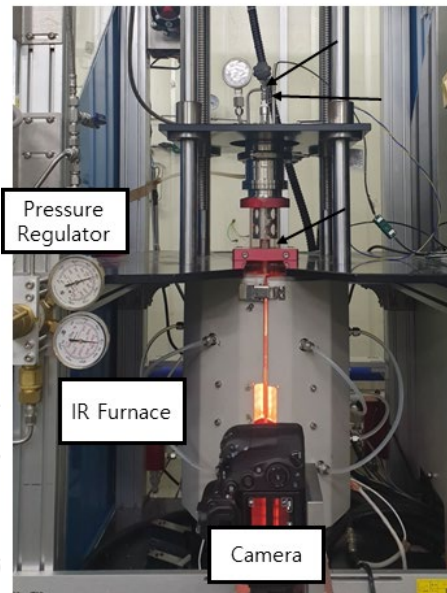
# Introduction of DIMAT experiment

- **DIMAT (Deformation In-situ Measurement Apparatus by Image-analysis Technique)**
- **KAERI's real-time measurement system for high-temperature cladding deformation**
- **Consists of an IR furnace for heating rate control, an internal pressure controller, and a camera for imaging**
- **Ar gas injection via the top to create internal rod pressure**
- **Ar gas injection via the furnace bottom for specimen inerting**
- **6 IR lamps arranged outside the quartz tube for heating**



## ■ Axial temperature gradient

- Due to IR furnace structure, 1% axial temperature gradient exist in +50cm ~ -50cm



## ■ Zircaloy-4 cladding tube

- Outer radius and its thickness are 9.5mm, 0.57mm
- Residual stress has been removed at 753K for 3.5 hour

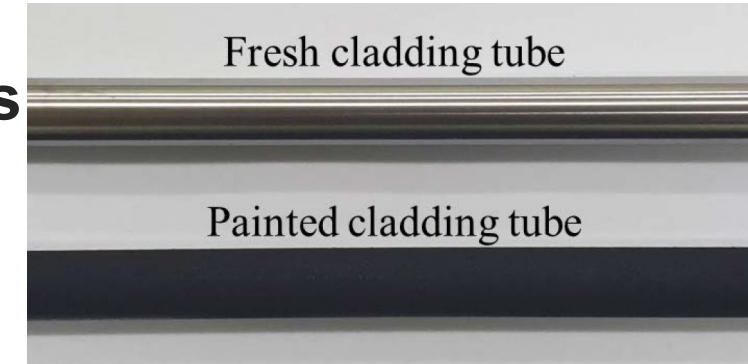


# Introduction of DIMAT experiment

## Measurement of deformation behavior through image processing

### Painted cladding tubes are used to eliminate reflections

- 1 pixel = 21~22 $\mu$ m, uncertainty : 5 pixel



### Post processing of images taken by camera

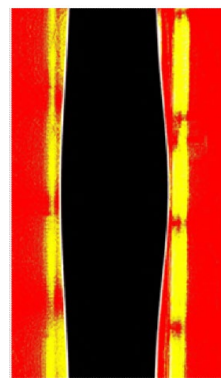
- Canon EOS 90D camera with EF 100mm F2.8L Macro IS USM with a close-up lens



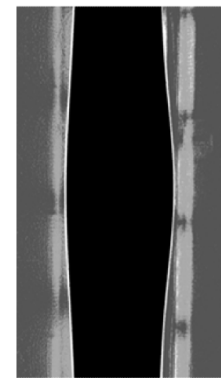
Resolution adjustment



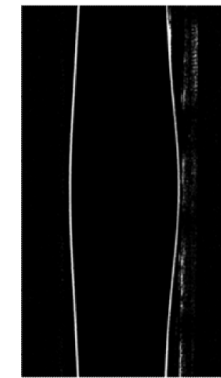
Clarity adjustment



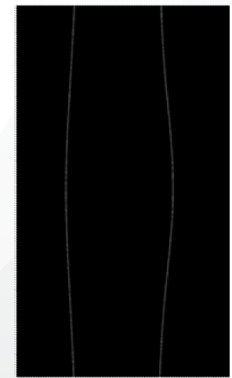
Color contrast adjustment



Black & white conversion



Contour extraction



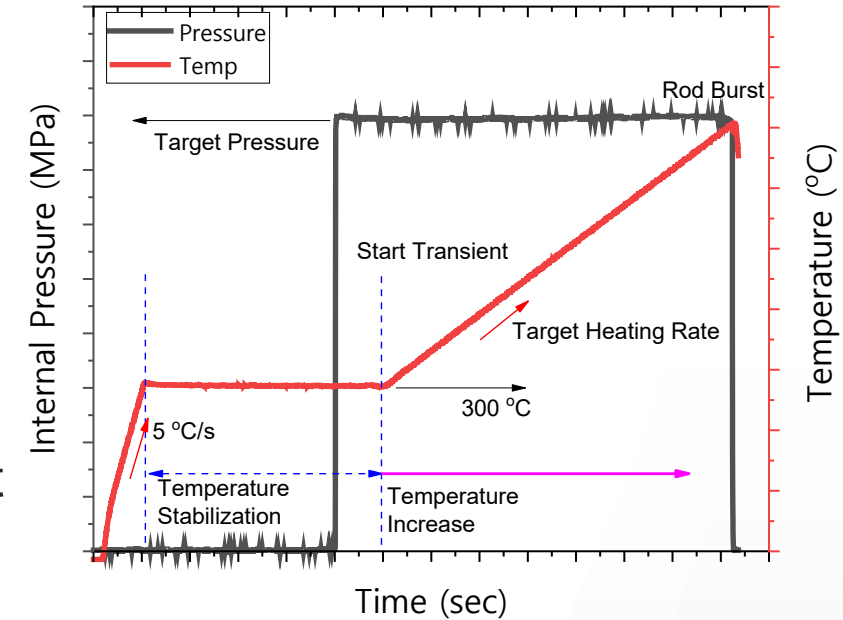
Final image

# Introduction of DIMAT experiment

## High temperature deformation experiment

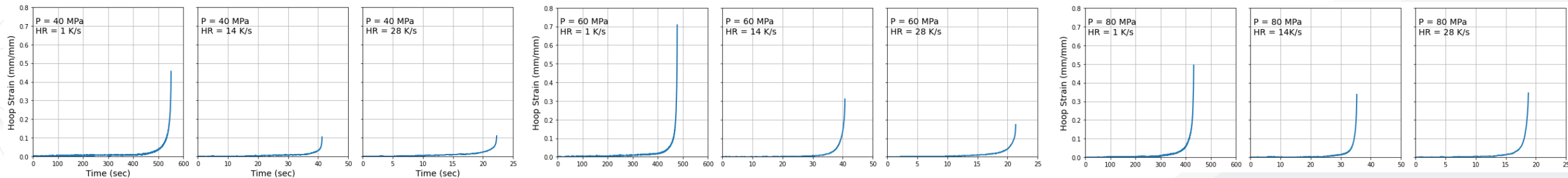
### Tube burst experiment in transient condition

- Step 1. Heating from room temperature to 300°C
- Step 2. Iso-thermal condition for 300s for stabilization
- Step 3. Inject Ar gas to create internal gas pressure
- Step 4. 60s later, increase temperature at constant speed until burst



### Experiment matrix

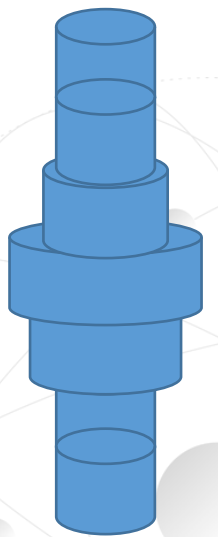
- 3 kinds of heating rates (1 K/s, 14 K/s, 28 K/s), 3 kinds of internal pressure (40 bar, 60 bar, 80 bar)
- 9 experiment conditions in total



## MERCURY (Multi-dimensional Entire fuel Rod Code for Understanding Reaction Yield behavior)

### FEM based nuclear fuel performance code

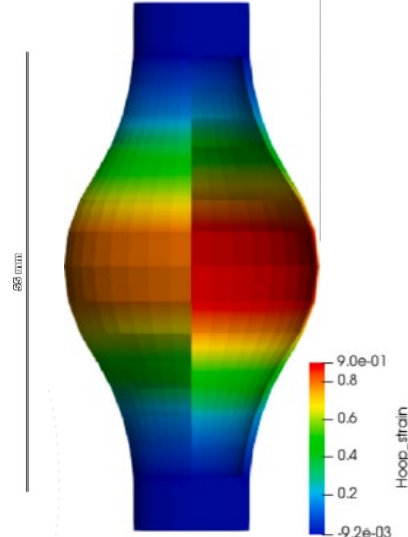
- Thermal/Mechanical coupling analysis of multi-material
- Including large deformation, creeping, etc...



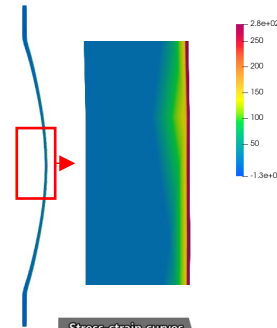
Ballooning analysis using FEM



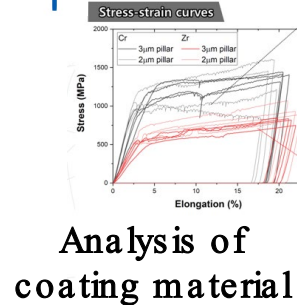
Ballooning/Burst experiment



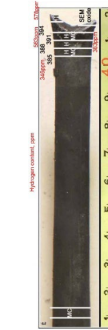
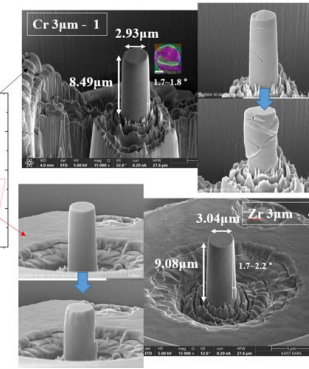
Ballooning analysis using FEM



Stress distribution of ATF



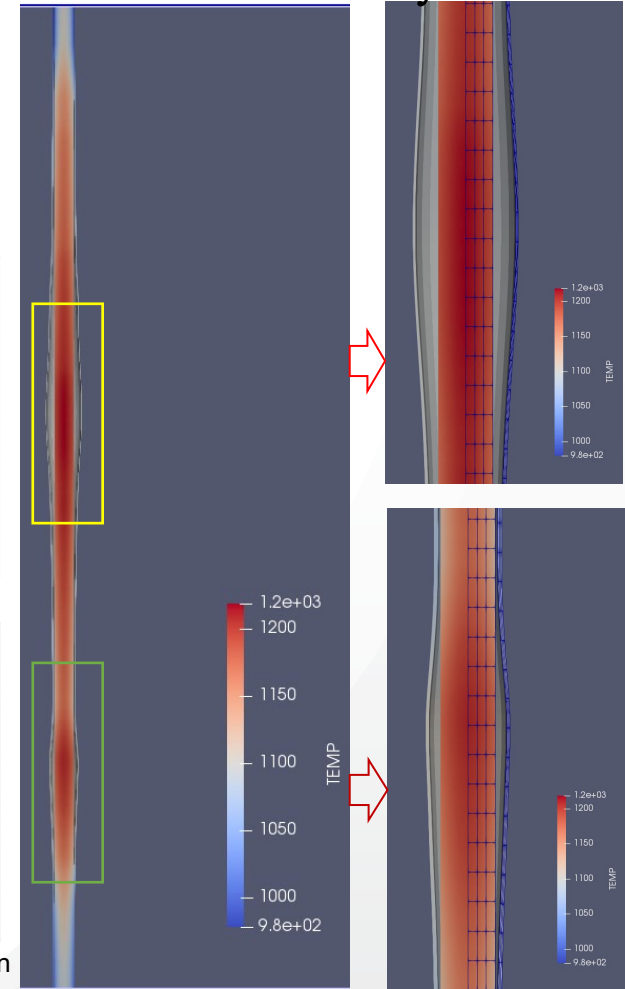
Analysis of coating material



Specimen image

HRP IFA650.9 analysis result

Double ballooning

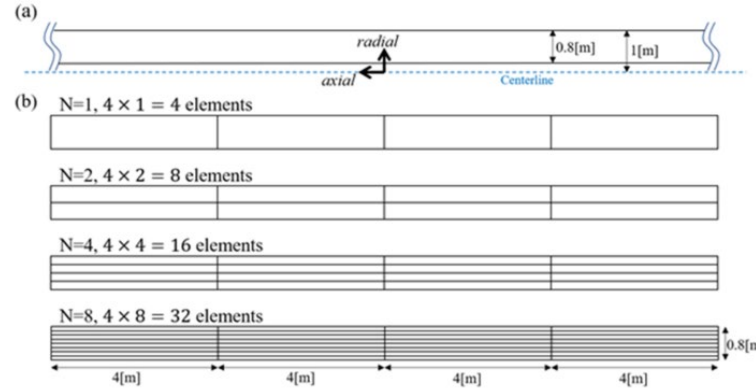


## Code Verification of MERCURY

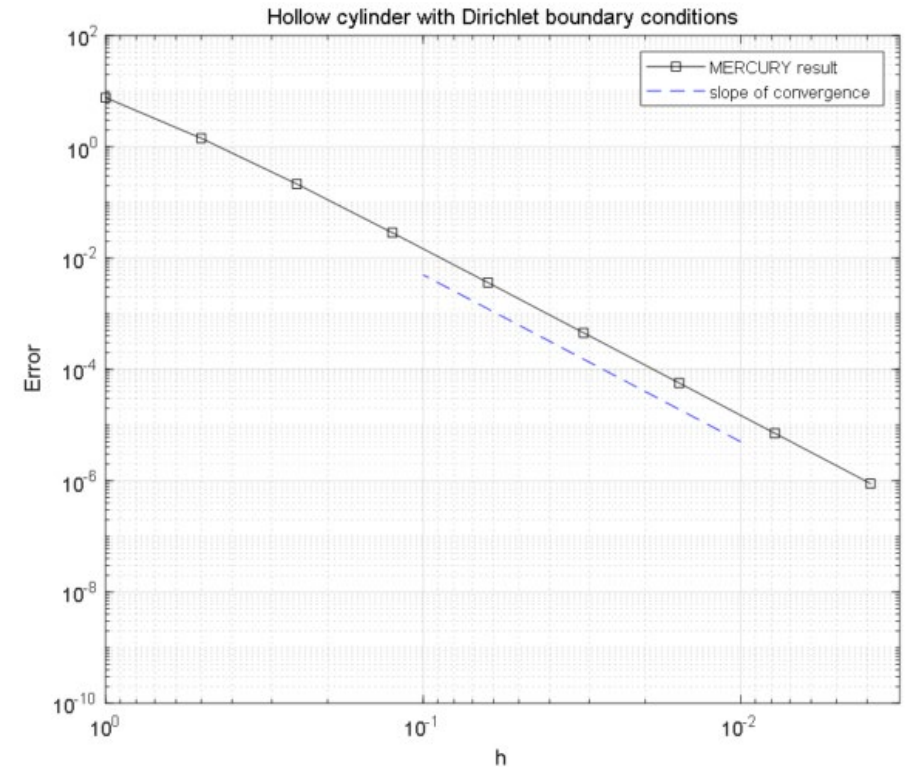
For code Verification, we used Method of Manufactured Solutions (MMS) and checked the simulation results converges to analytic result

Reference	Transient	Steady State	Coordinate System			Dimension						Properties and External Sources					Boundary Conditions		
			Cartesian	Cylindrical	Spherical	$x_1$	$x_2$	$x_3$	$k_c$	$k(T)$	$q'''$	$q'''(\bar{x})$	$c_c$	$\alpha(T)$	Dirichlet	Neumann	Convective		
<b>Method of Exact Solutions</b>																			
3.1	[26]	✓	✓		✓			✓		✓						✓			
3.2	[26]	✓	✓		✓			✓		✓						✓			
3.3	[27]	✓	✓		✓			✓		✓						✓			
3.4	[28]	✓	✓		✓	✓		✓		✓						✓			
3.5	[26]	✓	✓		✓			✓		✓						✓			
3.6	[26]	✓	✓		✓			✓		✓						✓			
3.7	[28]	✓	✓		✓			✓		✓						✓			
3.8	[29]	✓	✓		✓			✓		✓						✓	✓		
3.9	[29]	✓	✓		✓			✓		✓						✓	✓		
3.10	[28]	✓	✓		✓		✓			✓						✓			
3.11	[29, 30]	✓	✓		✓			✓		✓						✓			
3.12	[26]	✓	✓		✓			✓		✓						✓			
3.13	[26]	✓	✓		✓			✓		✓						✓			
3.14	[29, 31]	✓	✓		✓			✓		✓						✓			
3.15	[29, 32]	✓	✓		✓			✓		✓						✓			
3.16	[29]	✓	✓		✓			✓		✓						✓	✓		
<b>Method of Manufactured Solutions</b>																			
3.17		✓	✓		✓			✓		✓						✓	✓		
3.18		✓	✓		✓			✓		✓						✓	✓		
3.19	[1]	✓	✓		✓			✓		✓						✓	✓		

Verification of BISON using analytic and manufactured solutions, CASL-U-2020-1939-000



N	온도 오차
1	7.64374E+00
2	1.42421E+00
4	2.14758E-01
8	2.85282E-02
16	3.62220E-03
32	4.54508E-04
64	5.68671E-05
128	7.11006E-06
256	8.88810E-07

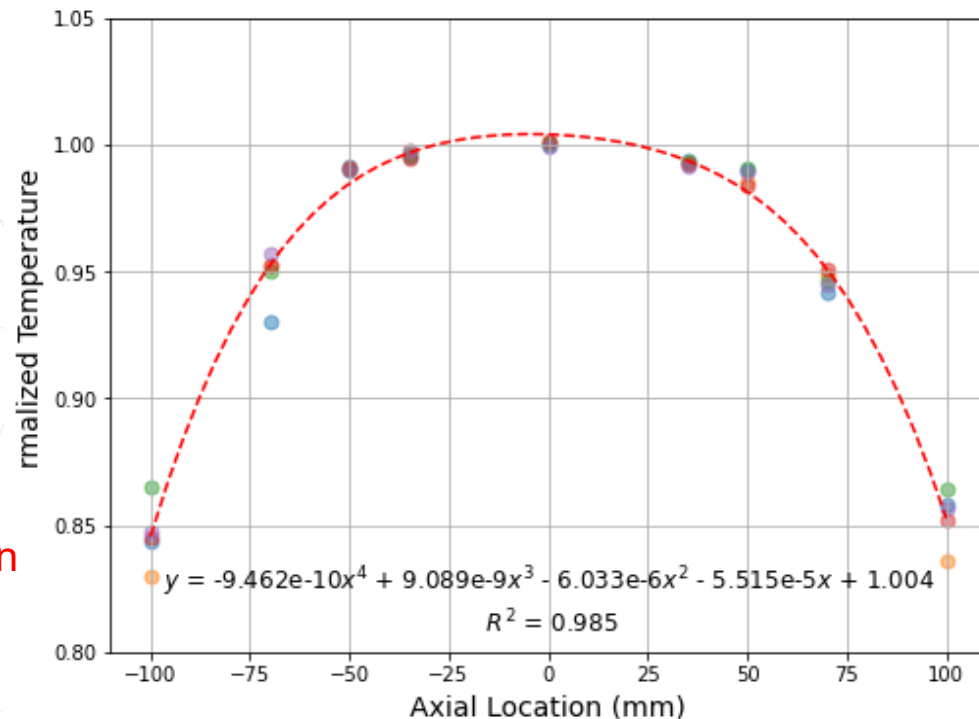


$$u(r) = \frac{u_o \ln(r_i) - u_i \ln(r_o)}{\ln(r_i/r_o)} + \frac{u_i - u_o}{\ln(r_i/r_o)} \ln(r)$$

## MERCURY code input

### Axial temperature gradient input

- The +100mm ~ -100mm section is divided into 10mm units
- Using temperature gradient correlation measured experimentally
- 573K, 1573K, 14573K, 28593K are chosen as peak temperature

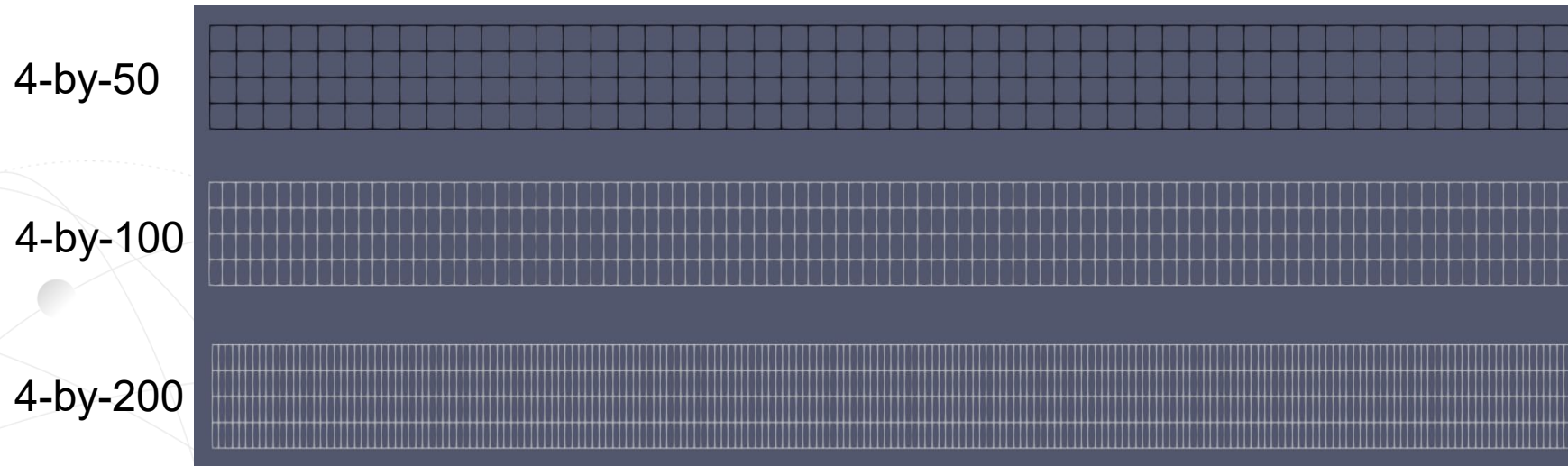


HEIGHT[MM]	573K	1573K	14573K	28593K
-100	484.4577	1329.934	12321.12	24157.79
-90	510.7665	1402.157	12990.23	25469.69
-80	530.822	1457.213	13500.29	26469.77
-70	545.7613	1498.224	13880.24	27214.73
-60	556.5917	1527.956	14155.69	27754.79
-50	564.1902	1548.815	14348.94	28133.69
-40	569.3037	1562.853	14478.99	28388.68
-30	572.549	1571.762	14561.53	28550.51
-20	574.4128	1576.879	14608.93	28643.45
-10	575.2517	1579.181	14630.27	28685.28
0	575.292	1579.292	14631.29	28687.29
10	574.6301	1577.475	14614.46	28654.29
20	573.2321	1573.637	14578.9	28584.58
30	570.9342	1567.329	14520.46	28469.99
40	567.4423	1557.743	14431.65	28295.86
50	562.3321	1543.714	14301.69	28041.04
60	555.0494	1523.722	14116.47	27677.88
70	544.9099	1495.887	13858.59	27172.27
80	531.0988	1457.973	13507.34	26483.57
90	512.6716	1407.387	13038.68	25564.69
100	488.5536	1341.178	12425.29	24362.03

## Mesh inputs

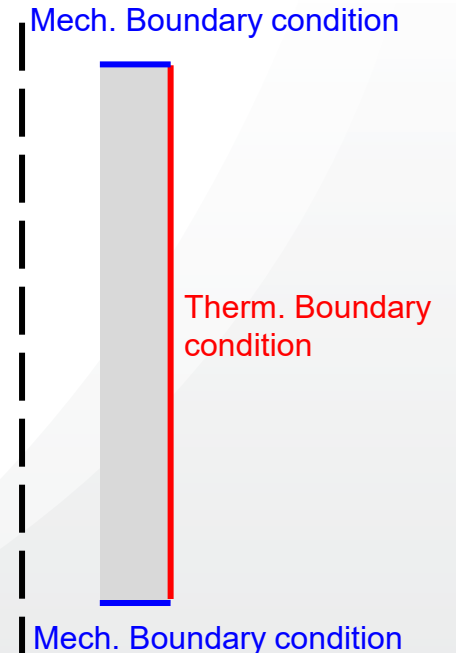
### Investigation on Mesh Dependency

- Cladding tube has 200mm in its length, 8.36mm in its inner diameter, 0.57mm on its thickness
- Mesh Dependency is investigated using 4 and 50/100/200 number of 8-node elements



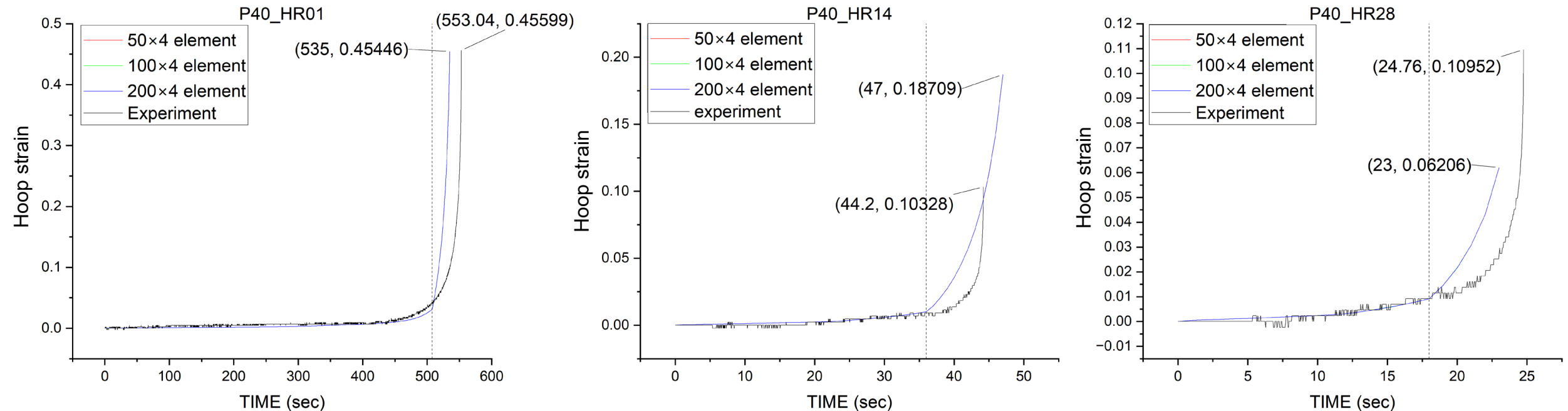
### Boundary conditions

- Thermal boundary conditions on outer surface of cladding tube
- Mechanical boundary conditions on upper and lower cladding tube



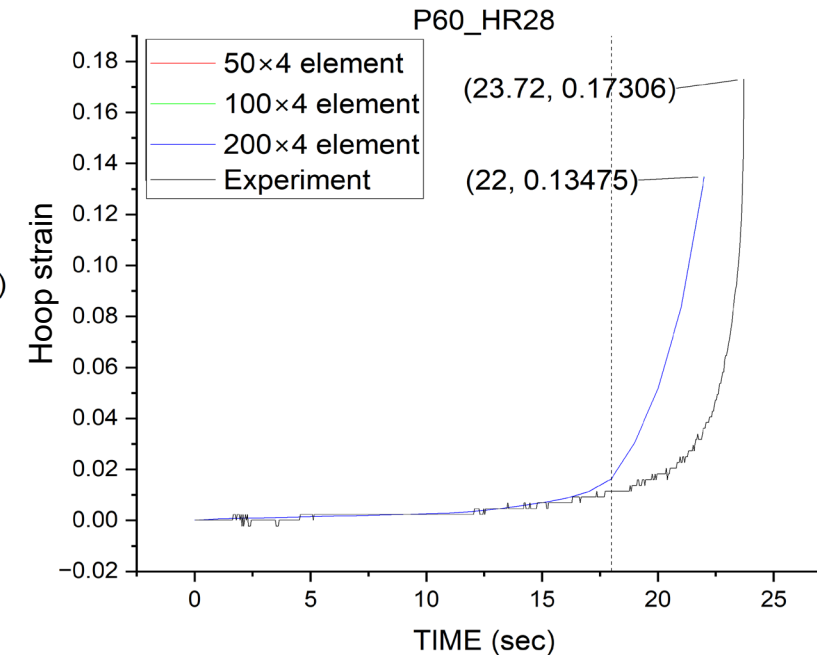
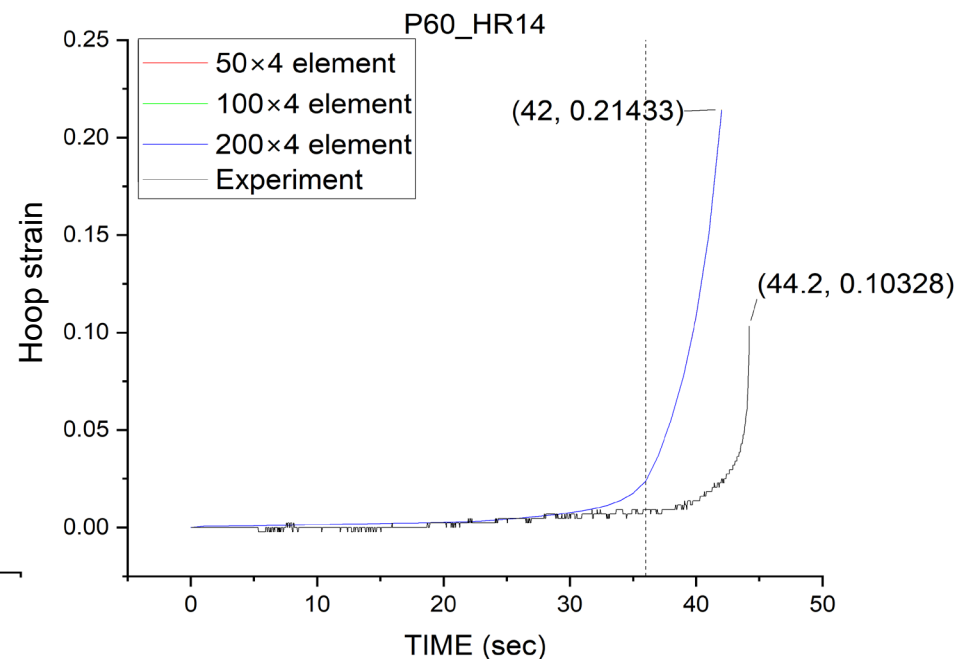
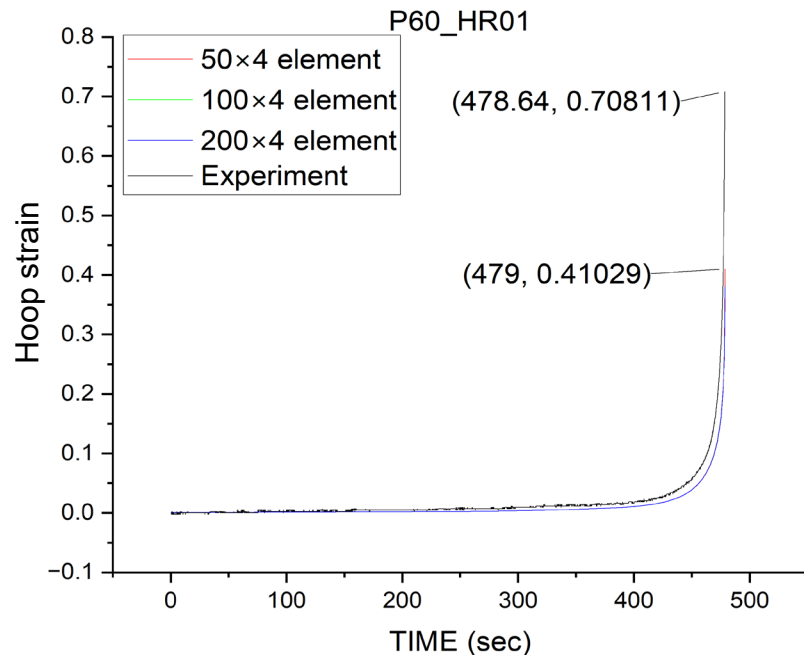
## Results of 40 bar internal gas pressure

- Ballooning and burst occurred at the center of cladding tube
- No effect on Mesh Dependency
- Sudden change observed at 1085.1K, where creep coefficient of Zry-4 change from  $\alpha$  phase to  $\alpha + \beta$  phase



## Results of 60 bar internal gas pressure

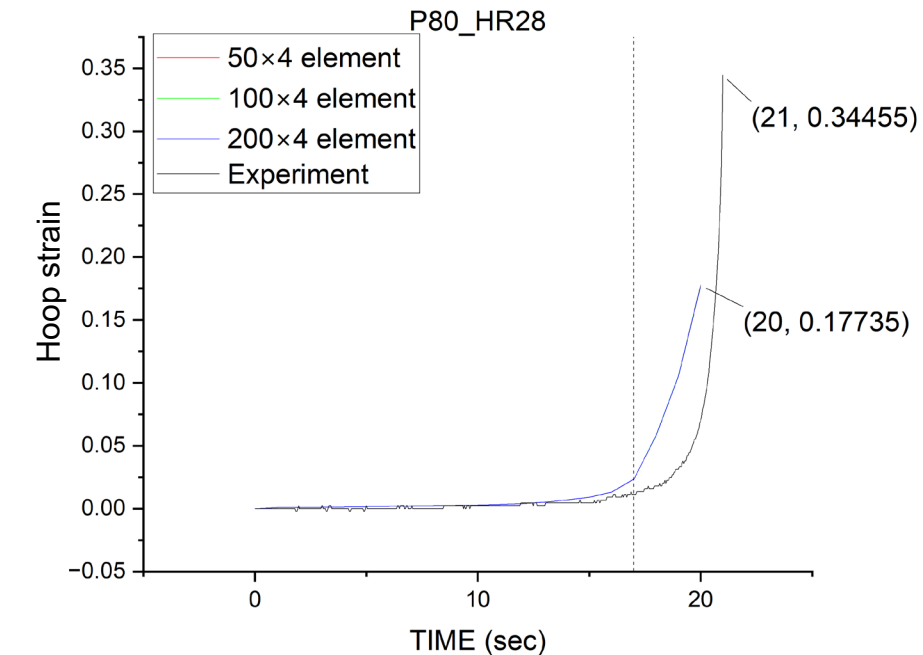
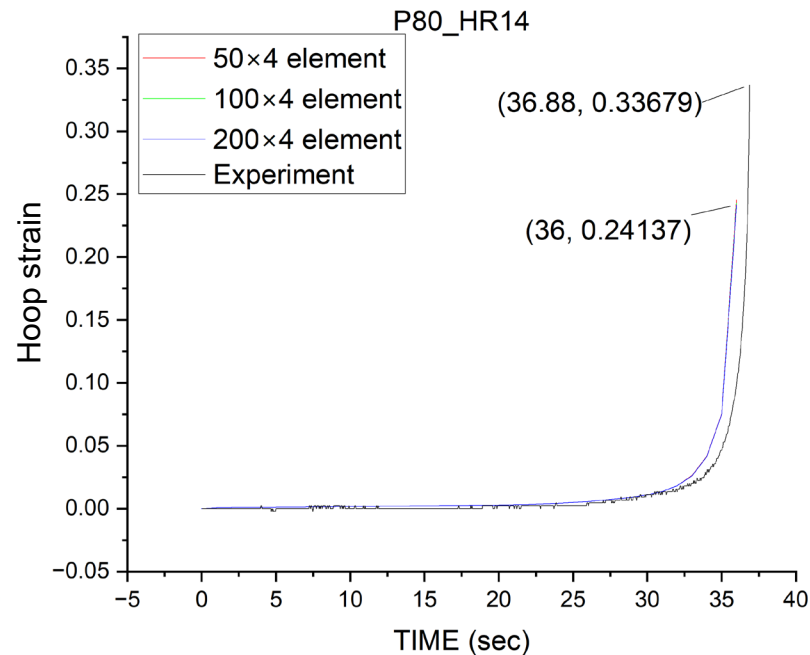
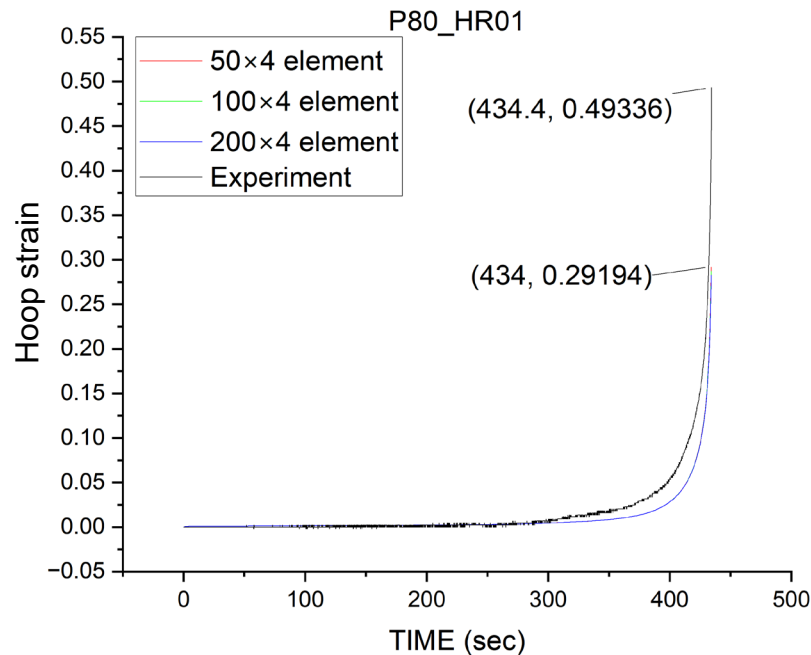
- Ballooning and burst occurred at the center of cladding tube
- No effect on Mesh Dependency
- Sudden change observed at 1085.1K, where creep coefficient of Zry-4 change from  $\alpha$  phase to  $\alpha + \beta$  phase





## Results of 80 bar internal gas pressure

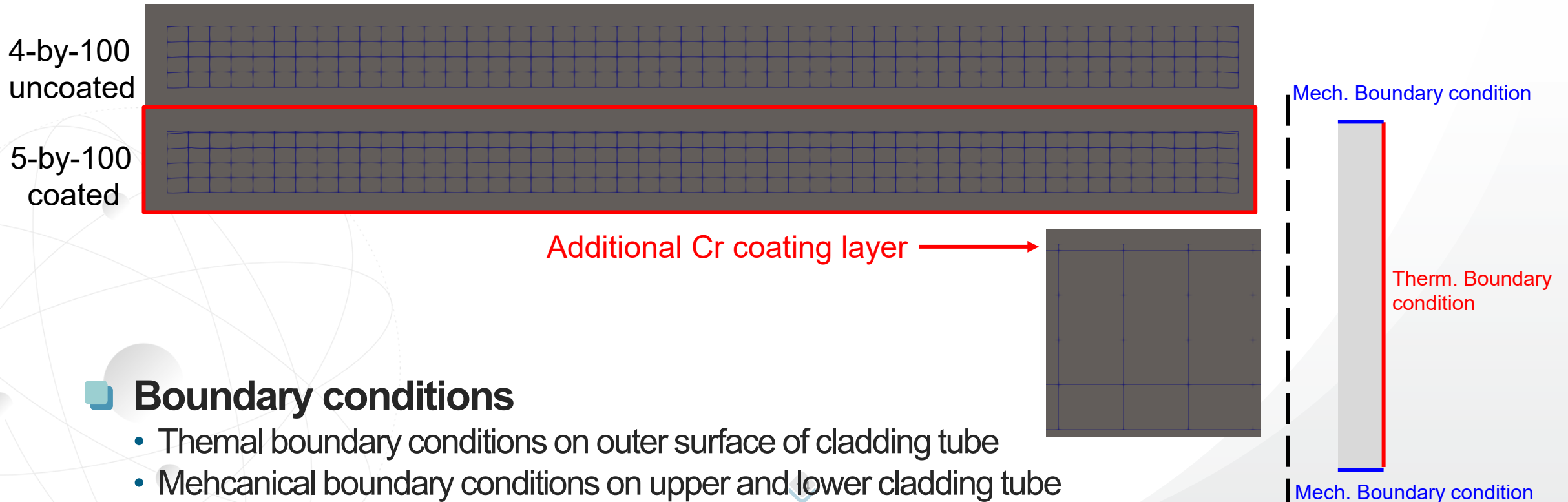
- Ballooning and burst occurred at the center of cladding tube
- No effect on Mesh Dependency
- Sudden change observed at 1085.1K, where creep coefficient of Zry-4 change from  $\alpha$  phase to  $\alpha + \beta$  phase



## Mesh inputs

### Cr-coated Zr-4 cladding tube

- Cladding tube has 200mm in its length, 8.36mm in its inner diameter, 0.55mm on its thickness, 0.02mm of Cr coating layer
- Same creep coefficients used for both Zry-4 and Cr coating



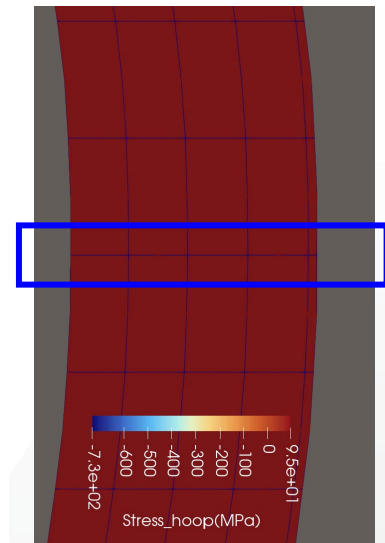
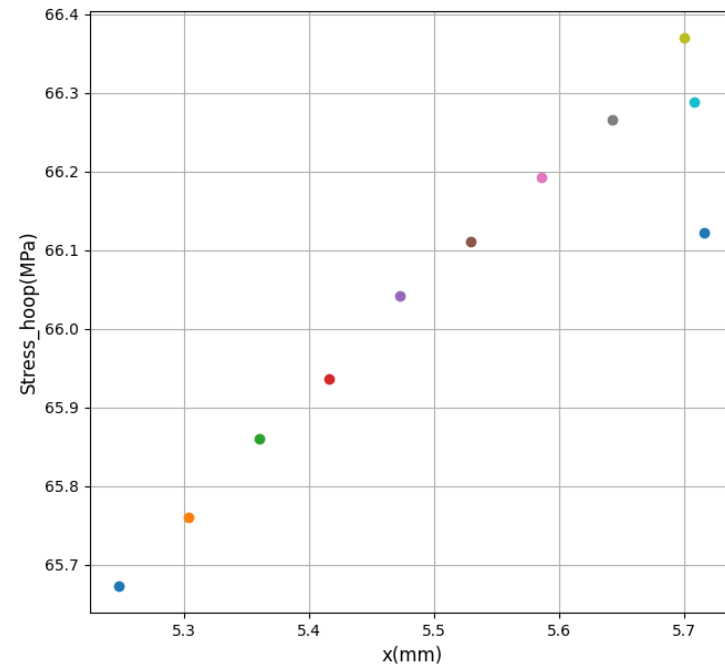
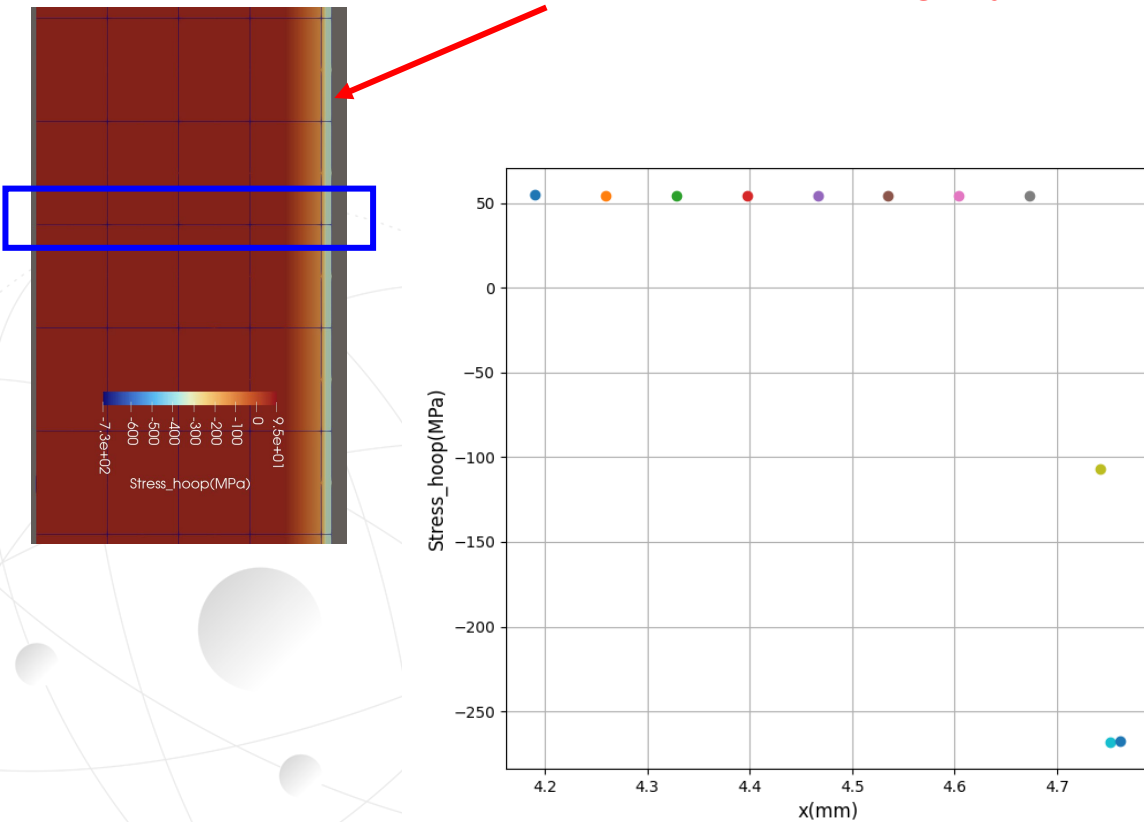
### Boundary conditions

- Thermal boundary conditions on outer surface of cladding tube
- Mechanical boundary conditions on upper and lower cladding tube

## Hoop stress distribution along radial direction

### Hoop stress distribution change after deformation

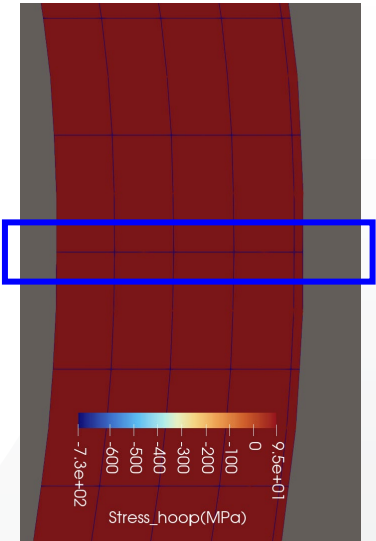
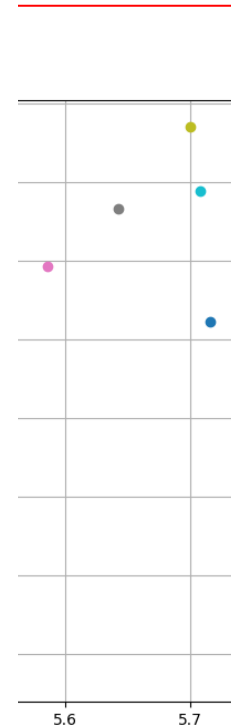
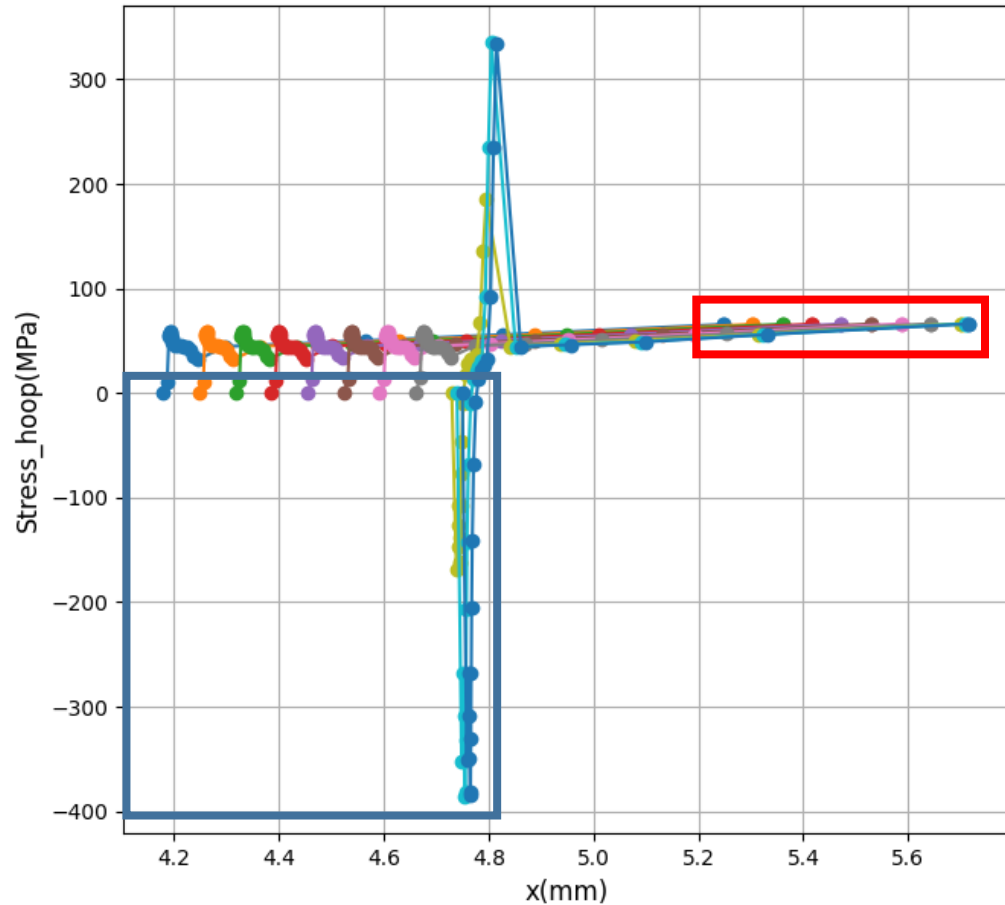
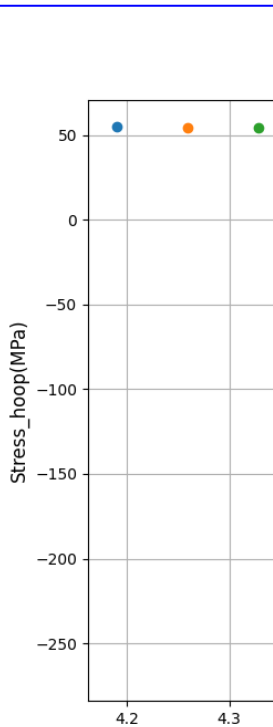
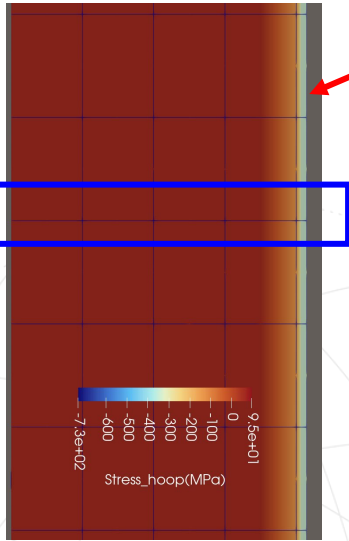
Additional Cr coating layer



## Hoop stress distribution along radial direction

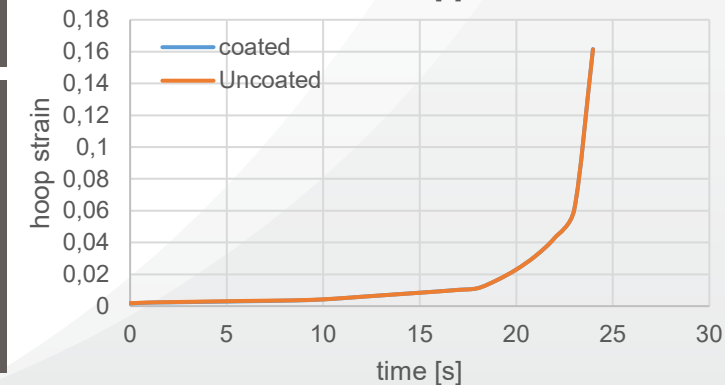
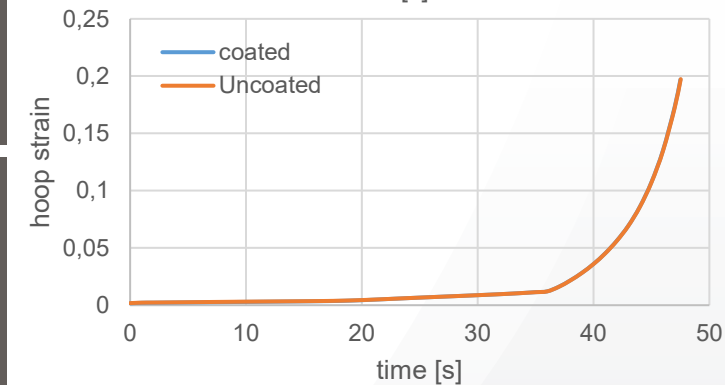
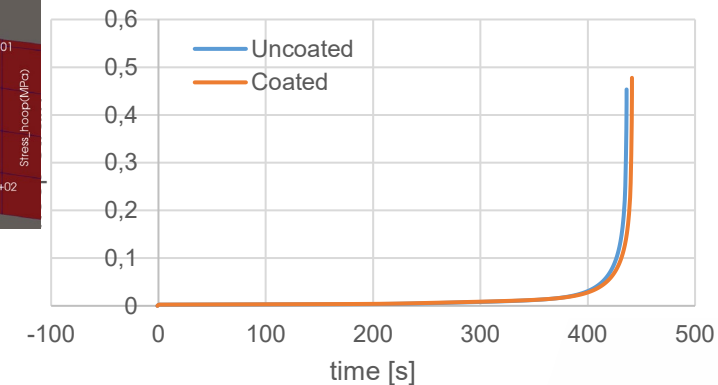
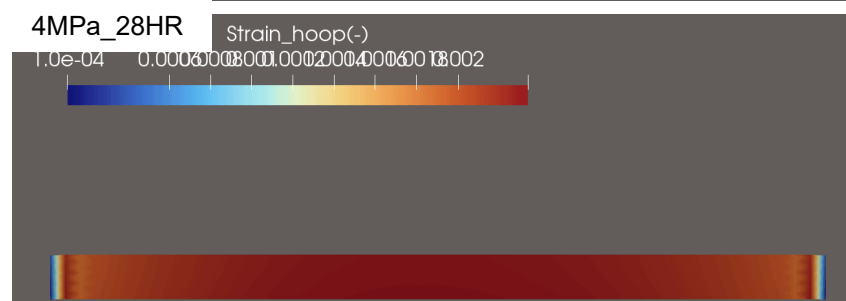
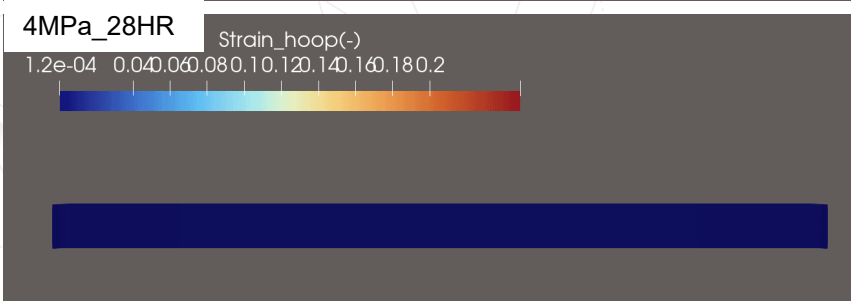
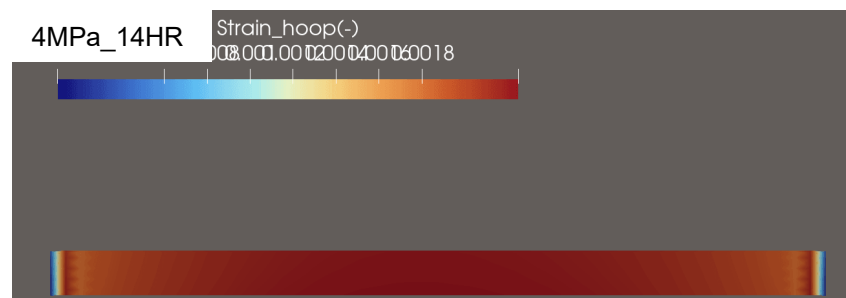
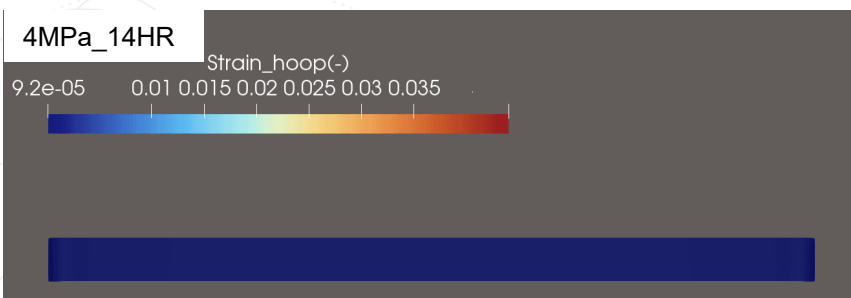
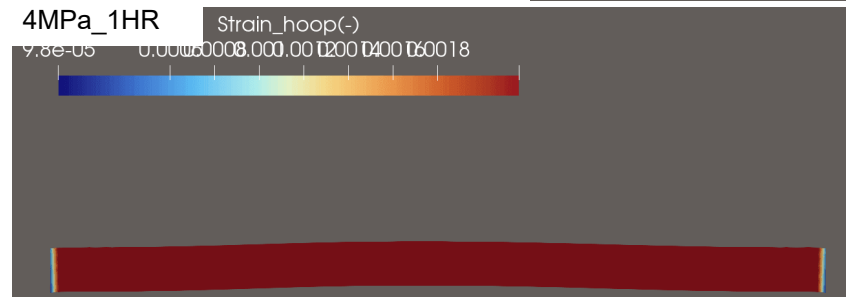
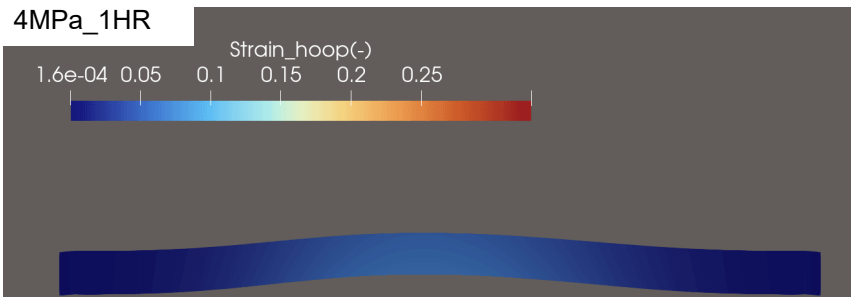
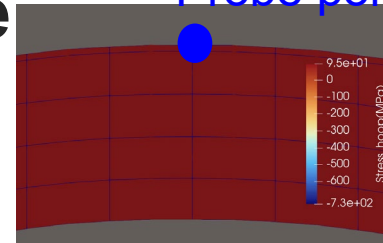
### Hoop stress dist

Additional



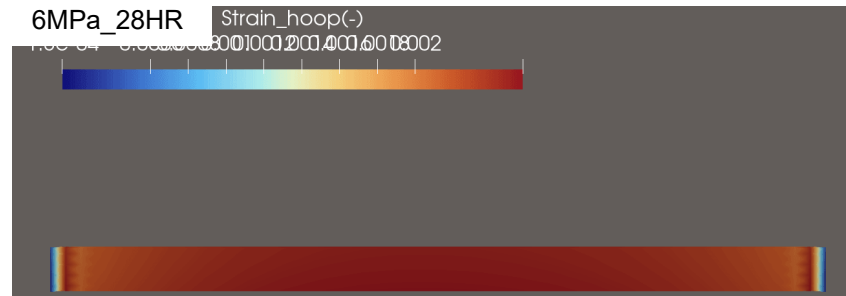
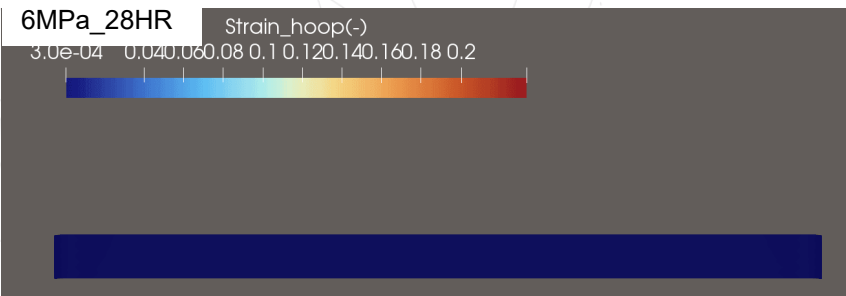
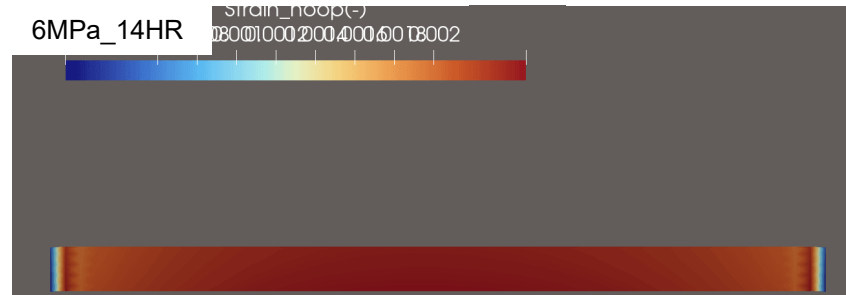
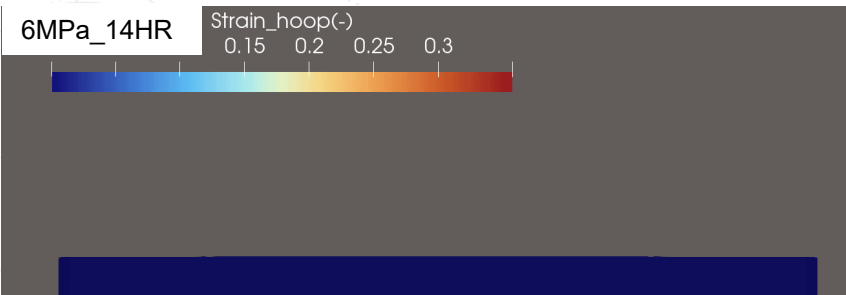
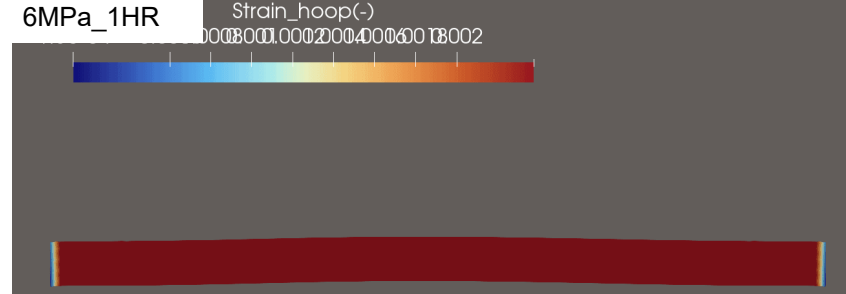
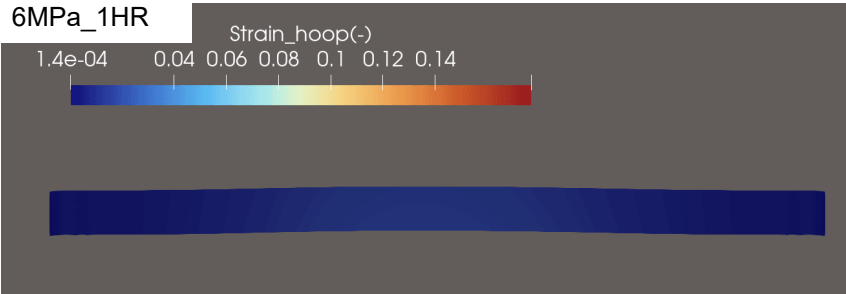
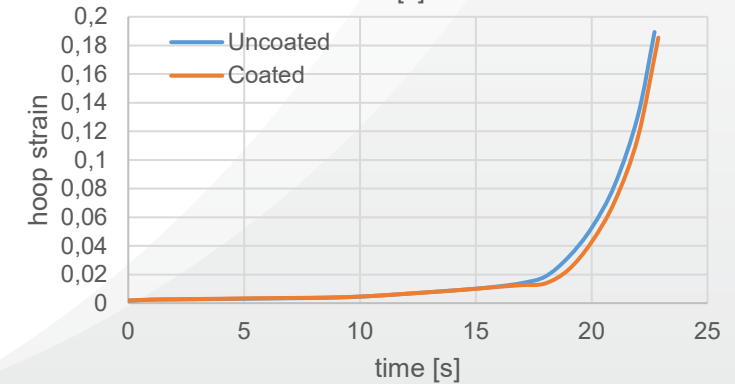
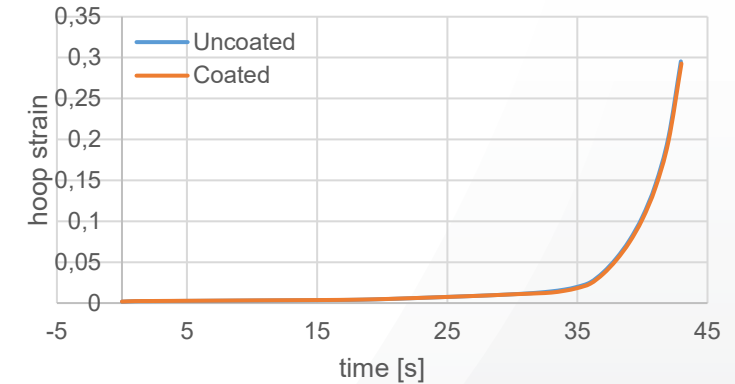
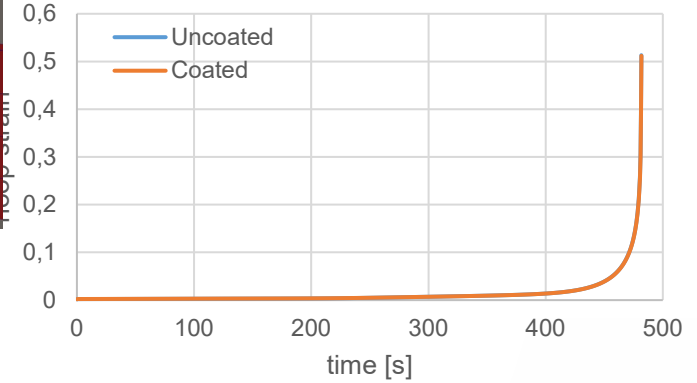
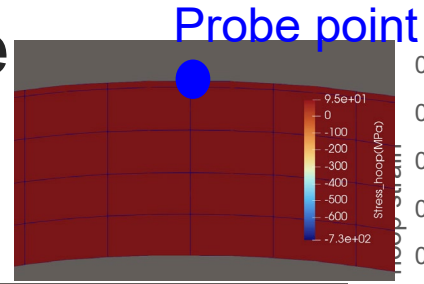
 Results of 40 bar internal gas pressure

Probe point



# Simulation of Cr-coated Zr-4 cladding tube

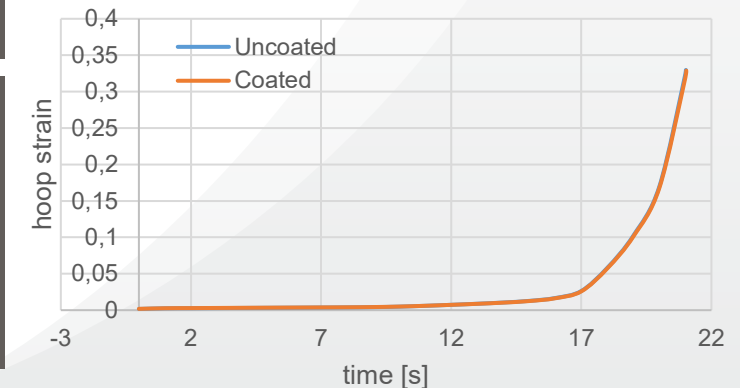
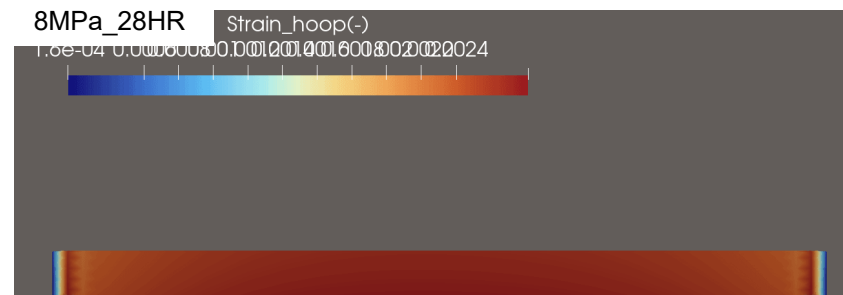
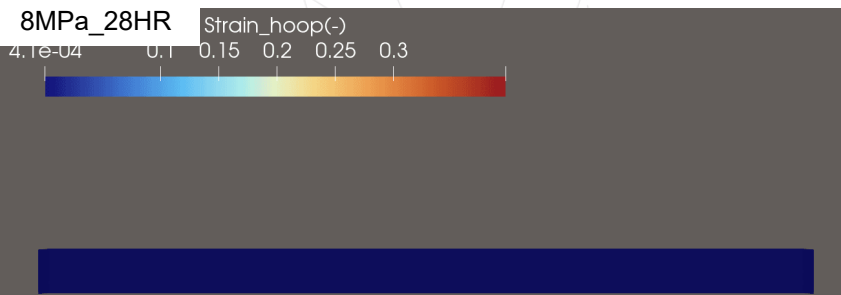
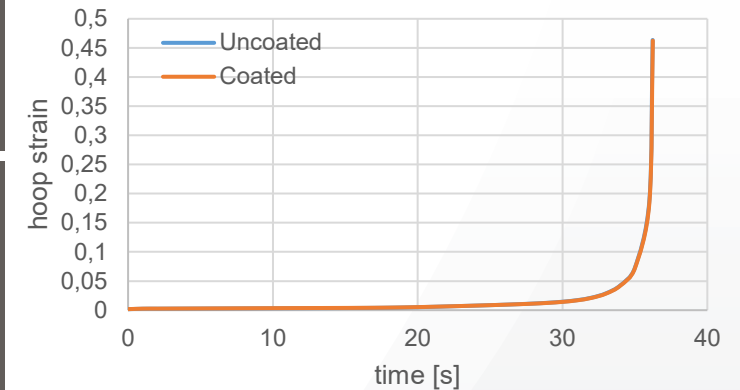
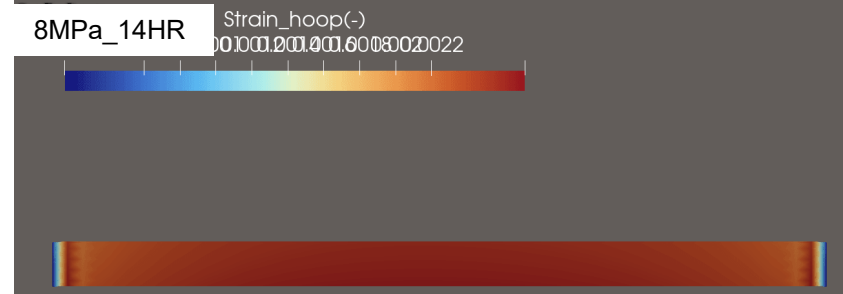
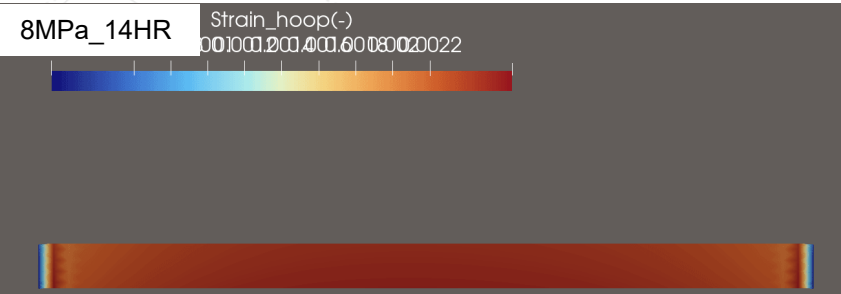
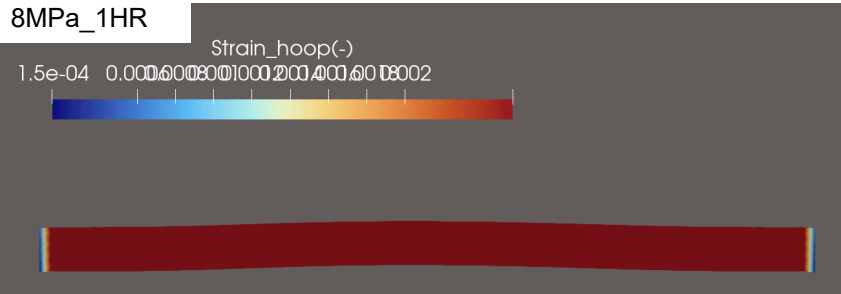
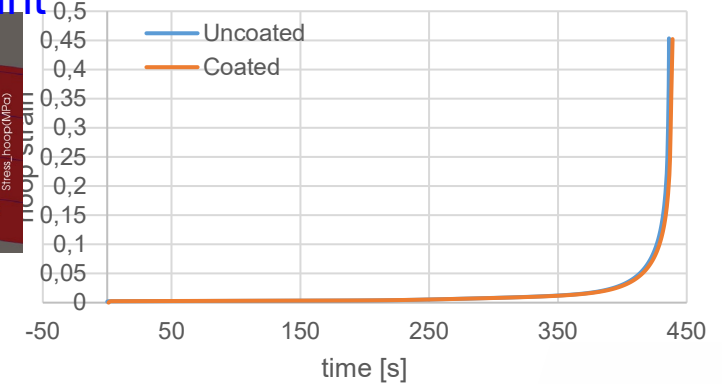
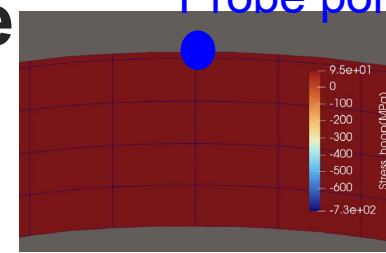
## Results of 60 bar internal gas pressure



# Simulation of Cr-coated Zr-4 cladding tube

## Results of 80 bar internal gas pressure

Probe point



## Conclusion

- A real-time measurement system, DIMAT, was established to monitor high-temperature cladding deformation during experiments
- A FEM-based nuclear fuel performance code, MERCURY, was developed and employed to analyze the DIMAT experiment
- The grid size had only a minimal effect on the rupture time and strain change.
- A sudden change was observed due to the input of the discontinuous creep property coefficient of Zry-4.
- The lower the heating rate and the higher the internal pressure, the more consistent the experimental and analytical results were.

	40 bar	60 bar	80 bar
1K/s	o	o	o
14K/s	x	x	o
28K/s	x	x	x

- Burst simulation was conducted using Cr coated Zry-4 cladding tube
- Hoop stress gradient was observed along axial direction
- We aim to develop a continuous phase transition model by applying a temperature-dependent function to the creep coefficients of Zry-4 and Cr-coating



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on **peoples trust**



# THANK YOU FOR YOUR ATTENTION

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Korea Atomic Energy  
Research Institute



**Gregor T. Stahlberg**

RUB

## **Simulating Cr-Coating Behavior with AC<sup>2</sup>: From QUENCH Analysis towards Integral Plant Application**

The integration of Advanced Technology Fuel (ATF) concepts, particularly Chromium (Cr) coated claddings, into safety analyses requires advanced simulation capabilities that go beyond standard Zircaloy models. The primary objective of this work is to present a dedicated modeling approach for the oxidation behavior of Cr-coated core components under severe accident conditions.

This model has been developed and implemented exclusively within an internal development branch (PSS v2025) at Plant Simulation and Safety Group (PSS) at Ruhr-Universität Bochum (RUB). While built upon the AC<sup>2</sup> code package provided by GRS gGmbH, the specific Cr-oxidation logic (Option 27) is an in-house extension and not yet part of the official code distribution. The model logic accounts for the delayed oxidation onset and the critical transition phase once the protective coating fails.

The assessment strategy presented in this work is twofold. The model development and basic validation are grounded in the analysis of the QUENCH-ATF experimental series. However, as the detailed results are subject to data restrictions, this work focuses on an exemplary application by re-investigating the large-scale bundle experiment QUENCH-15. Although the original experiment utilized uncoated claddings, it serves as a thermal-hydraulic reference case to analyze the sensitivity of the new model under hypothetical, beyond-design-basis conditions. Special attention is paid to the delayed hydrogen escalation and the steep increase in oxidation rates following the postulated coating failure at elevated temperatures.

Scaling up to integral plant behavior, the second phase of the analysis applies the model to a generic integral Pressurized Water Reactor (iPWR) type SMR. This application investigates the behavior and potential safety margins gained through the coating. The results highlight the non-linear dependency of safety gains on the assumed failure criteria and identify key areas for future code development regarding the transition from protective Cr-oxidation to rapid Zirconium degradation.

### Acknowledgement

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Responsibility for the content lies with the authors.

The results were obtained using in-house versions of the GRS software package AC<sup>2</sup> 2023 and AC<sup>2</sup> 2025.



# Simulating Cr-Coating Behavior with AC<sup>2</sup>

## From QUENCH Analysis towards Integral Plant Application

**Gregor T. Stahlberg, Marco K. Koch**

30th International QUENCH-Workshop | Karlsruhe, Germany | December, 2025

# AGENDA

- Introduction

  - Motivation, Current Status

- Modeling

  - Oxidation Correlation

- Results

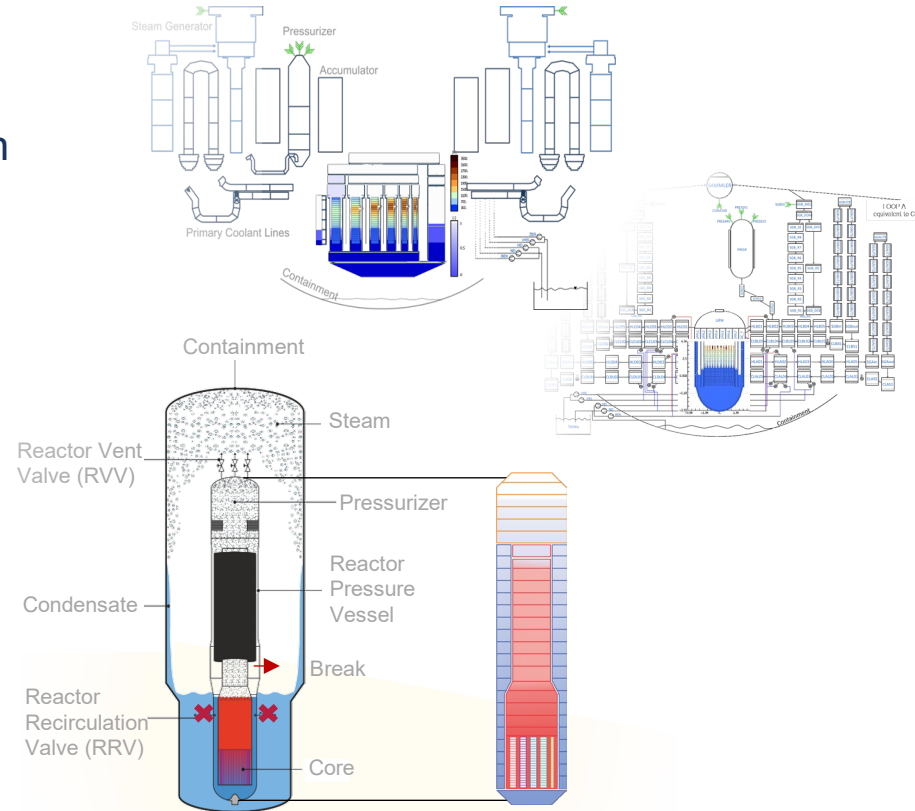
  - QUENCH-Facility, Plant Application

- Conclusion



# MOTIVATION AND OBJECTIVE

- An unmitigated accident can lead to exposure of fuel elements, heat release due to oxidation and fuel damage
  - Evaluation of simulation model(s) of iPWR (and full-scale PWR)
  - Investigations into the progression of the accident, the safety features and the influence of advanced fuel concepts
  - Analyzing possible increased time margins due to improved accident behavior → **ATF**



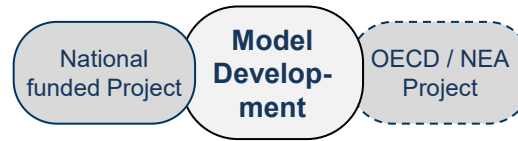
# MOTIVATION AND OBJECTIVE

## Current Options within AC<sup>2</sup>

### AC<sup>2</sup> 2023.4 Release

- Opt. 1-3
  - Different correlations for Zircaloy
- Opt. 20-22
  - Different approaches for FeCrAl oxidation (user defined)
- Opt. 23-26
  - Different correlations for Steel

- This work utilizes the PSS v2025 development branch, which extends the capabilities of AC<sup>2</sup> by a dedicated option for oxidation of Cr-coated claddings – a feature currently unique to this in-house version.



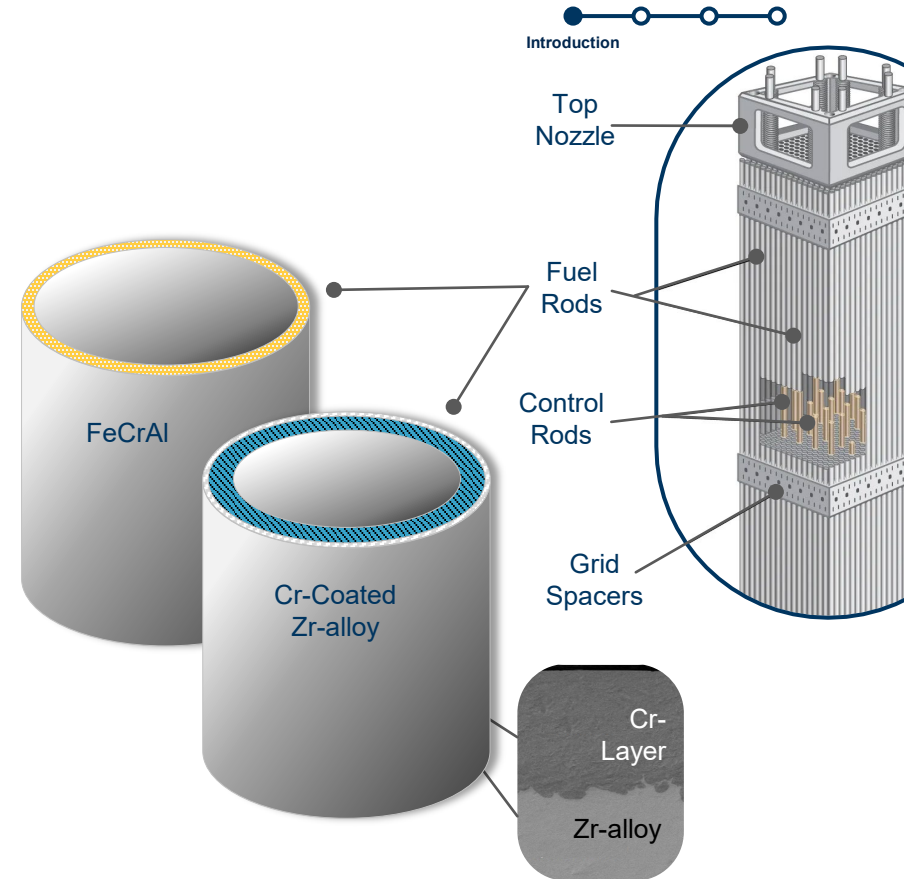
### AC<sup>2</sup> PSS Development (v2025 branch)

- **Opt. 27** - New Model for Cr-Oxidation
  - Validation: QUENCH-ATF-1 & -ATF-2, prospectively ATF-3 & CODEX
- *Opt. 28*
  - *Testing of new correlations for FeCrAl (EU-Project SASPAM-SA) based on publications by KIT*

# MOTIVATION AND OBJECTIVE

## ATF Concepts

- Analysis of technologies that specifically target improved accident behavior and/or favor higher burnup for longer operation
- Reduce potential hydrogen and heat release, that must be removed by cooling systems (i.e. ECCS) in the event of incidents or accidents → coping time?
- 🎯 Development of preliminary model for oxidation of **Cr-coated claddings** available as new option for AC<sup>2</sup> at RUB PSS (ongoing development)



**HOW TO MODEL ATF BEHAVIOR?**



# ADVANCED TECHNOLOGY FUEL

## Cr-Coated Zr-alloy

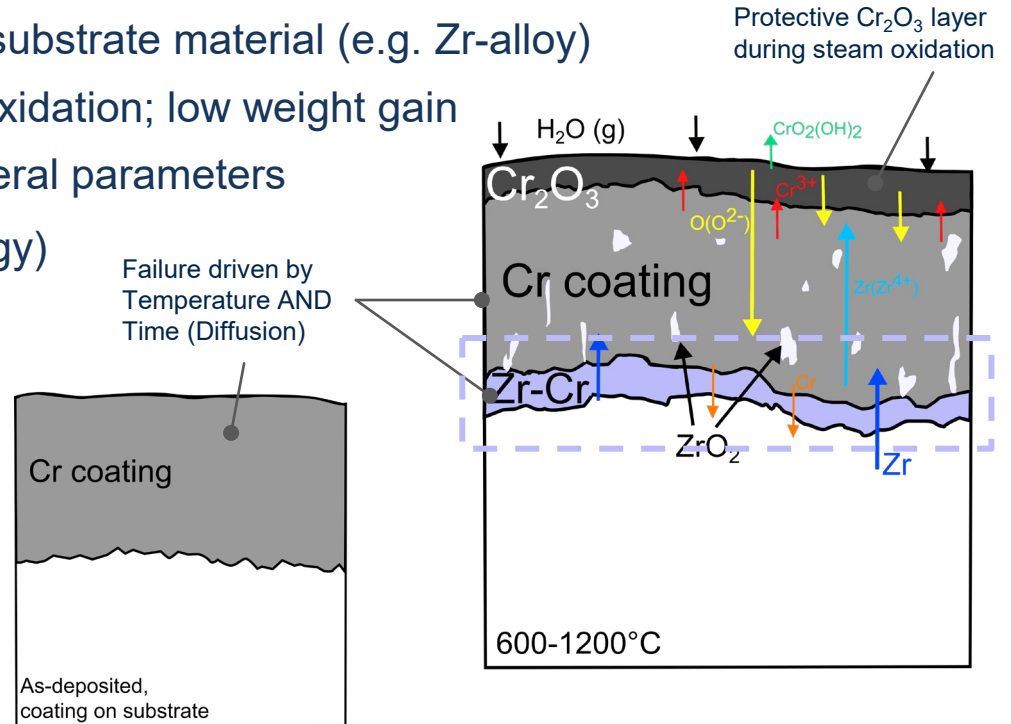
- Coating as diffusion barrier, protecting substrate material (e.g. Zr-alloy)
- Protective  $\text{Cr}_2\text{O}_3$  scale prevents rapid oxidation; low weight gain
- Corrosion resistance influenced by several parameters

↗ Microstructure (deposition technology)

↗ Applied uniform layer thickness

↗ Degradation mechanisms

↗ **Transient Boundary Conditions**

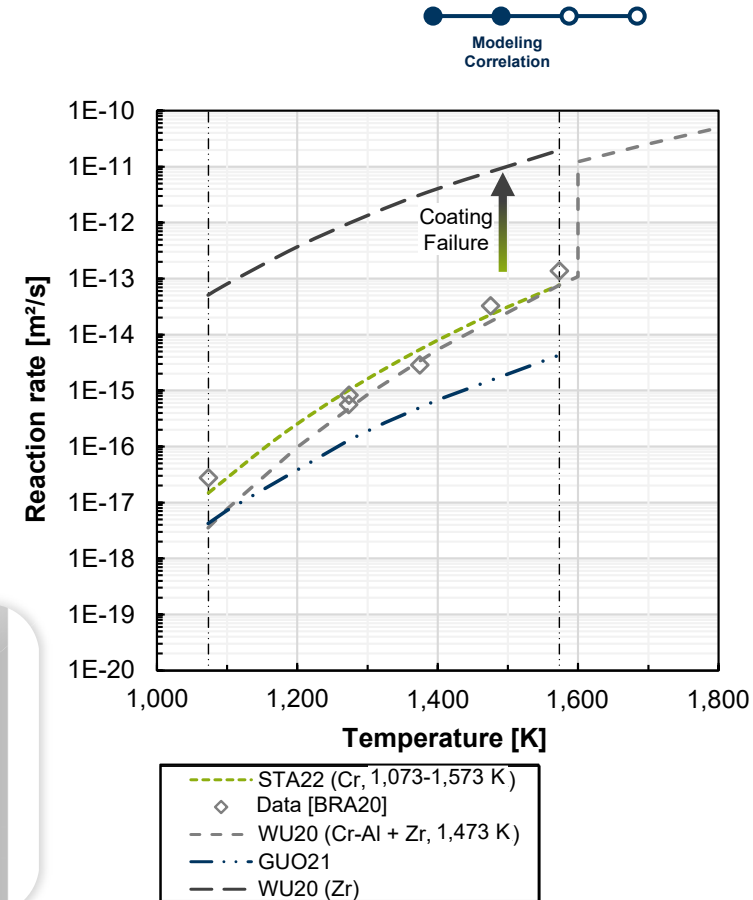
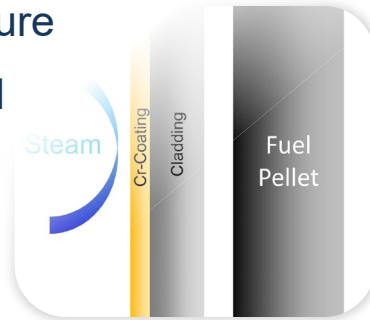


adapted from J. Liu et al. 2021

# MODELING

## Current correlation under development

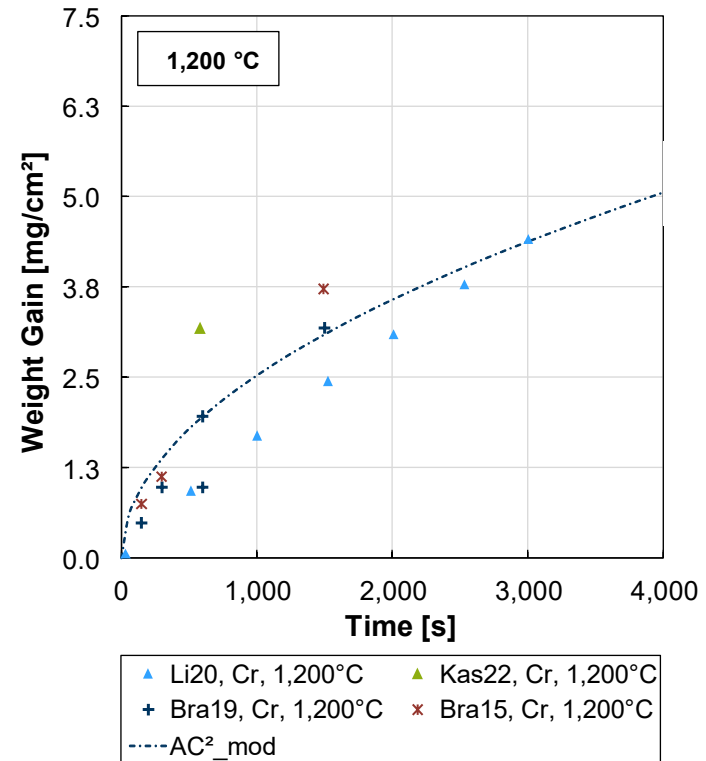
- Implemented correlation based on Brachet et al. (2020), representing the current state-of-the-art for Cr-coating behavior
  - Adapted for code-specific Weight Gain
  - Parametric thermal threshold ( $T_{fail}$ ) to investigate sensitivity of coping time; Transition from Cr  $\rightarrow$  Zr
  - Explicit switch of reaction enthalpy from Cr-oxidation to Zr-oxidation upon failure
  - Inner oxidation currently assumed negligible to focus on primary outer coating failure mechanisms



# VERIFICATION

## Weight Gain at 1,200°C

- Calculated mass gain curve shows good agreement at 1,200°C
  - Calculated mass gain tends to be slightly overestimated; most data are captured adequately (few outliers)
  - Coating failure seems to occur for some isothermal tests around ~5,000 s, despite lower than eutectic temperature
  - *Different experimental settings and different deposition technologies may lead to different failure behavior*

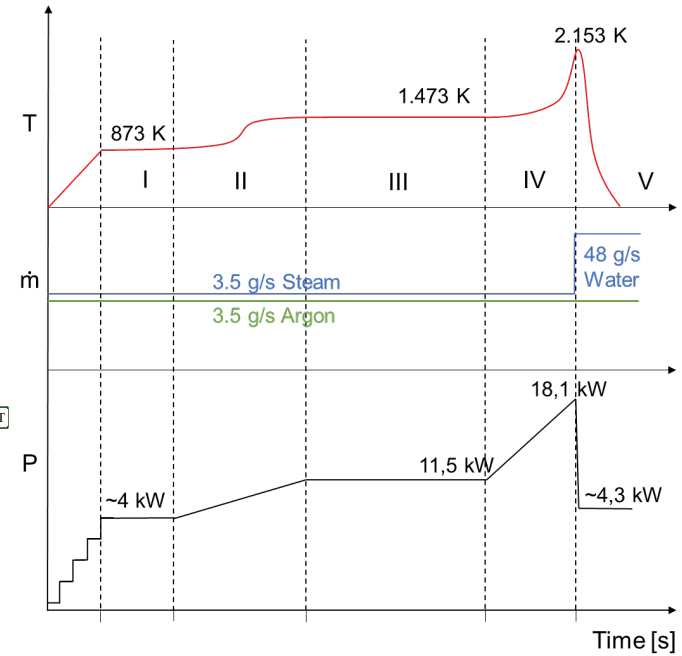
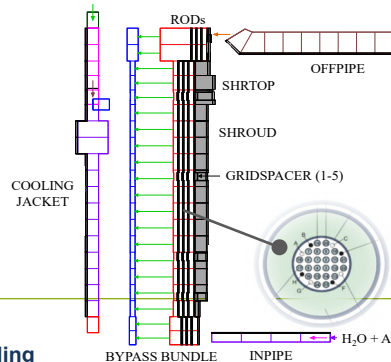


# APPLICATION TO QUENCH-FACILITY

# MODELING

## Cr-Oxidation applied to QUENCH-15 simulation model

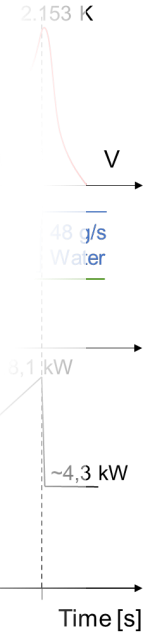
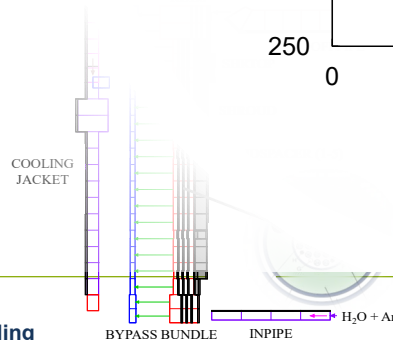
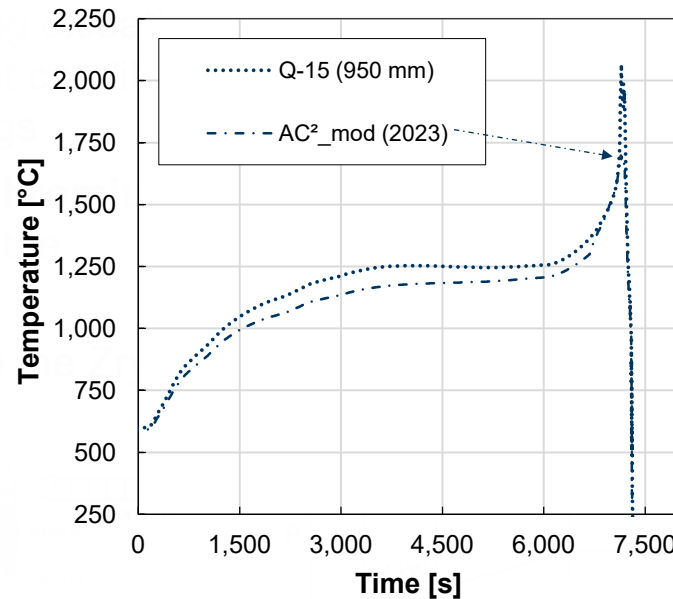
- QUENCH-15 investigates ZIRLO™ cladding oxidation and reflood behavior under severe accident conditions (up to 2,150 K) using originally Zry claddings
- Adapted as **hypothetical scenario with Chromium oxidation**, as a reference case to analyze the sensitivity of the new model
- For spacer grids and above threshold ( $T_{fail}$ ) the Zry oxidation for all components is active



# MODELING

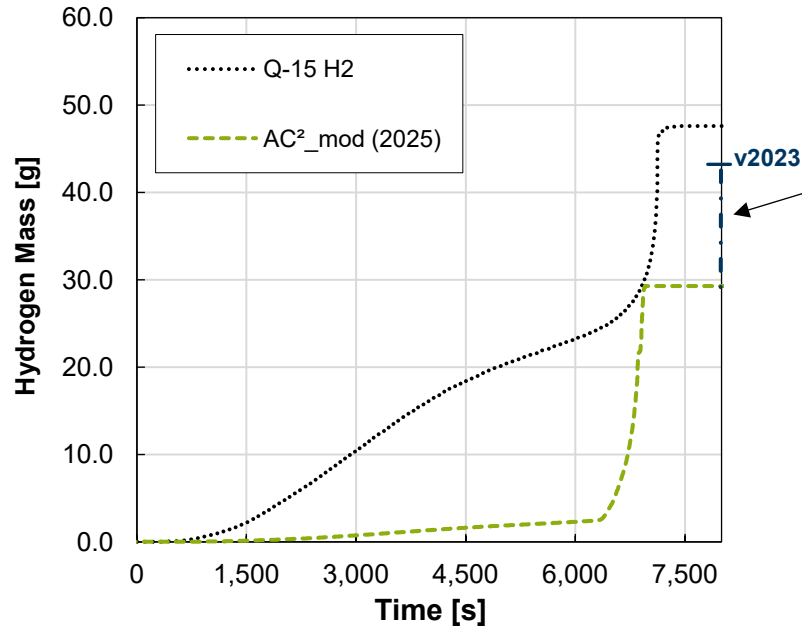
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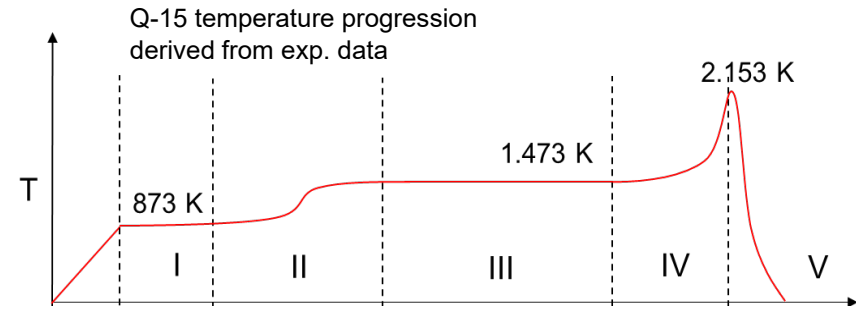


# RESULTS

## Preliminary: in-house AC<sup>2</sup> development branch (v2025)

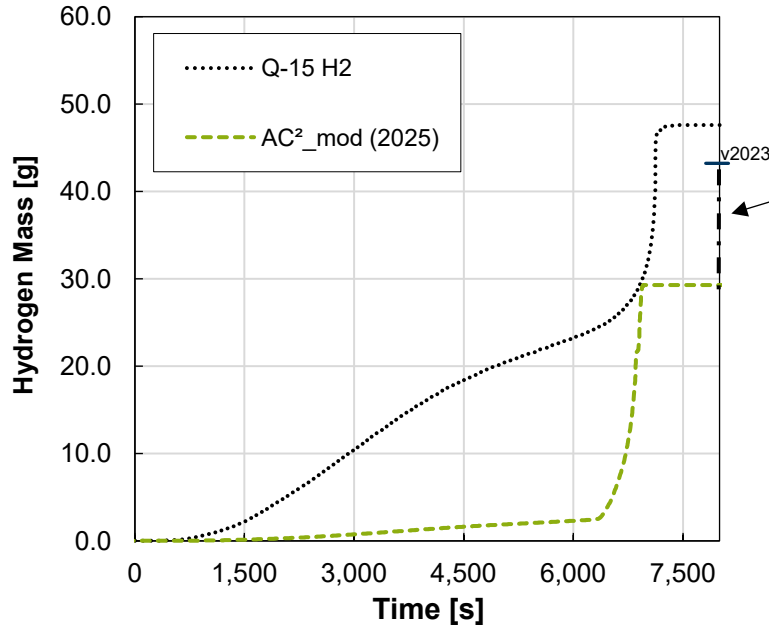


- The update to current AC<sup>2</sup> code branch (2025) resulted in some deviations (H<sub>2</sub>) compared to previous in-house version
- This is likely due to changes in underlying code but also changes to the model itself
- *Current analyses focus on understanding the changes of the transient progression*

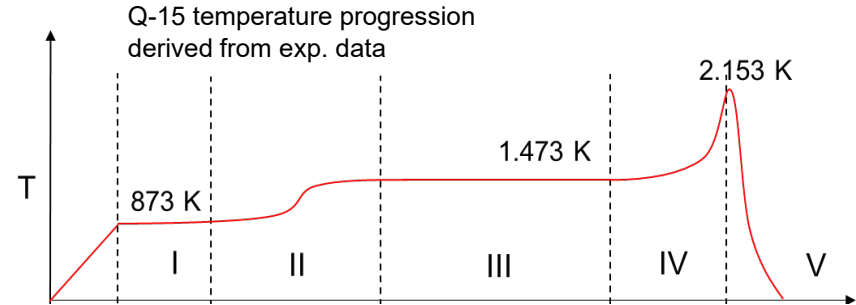


# RESULTS

## Preliminary: in-house AC<sup>2</sup> development branch (v2025)



- The Cr-coated simulation [---] effectively delays onset of H<sub>2</sub> generation compared to the uncoated Q-15 experiment [····]
- Post Cr-coating failure (~6,500s): significant H<sub>2</sub> generation with steep slope as underlying Zry is oxidized



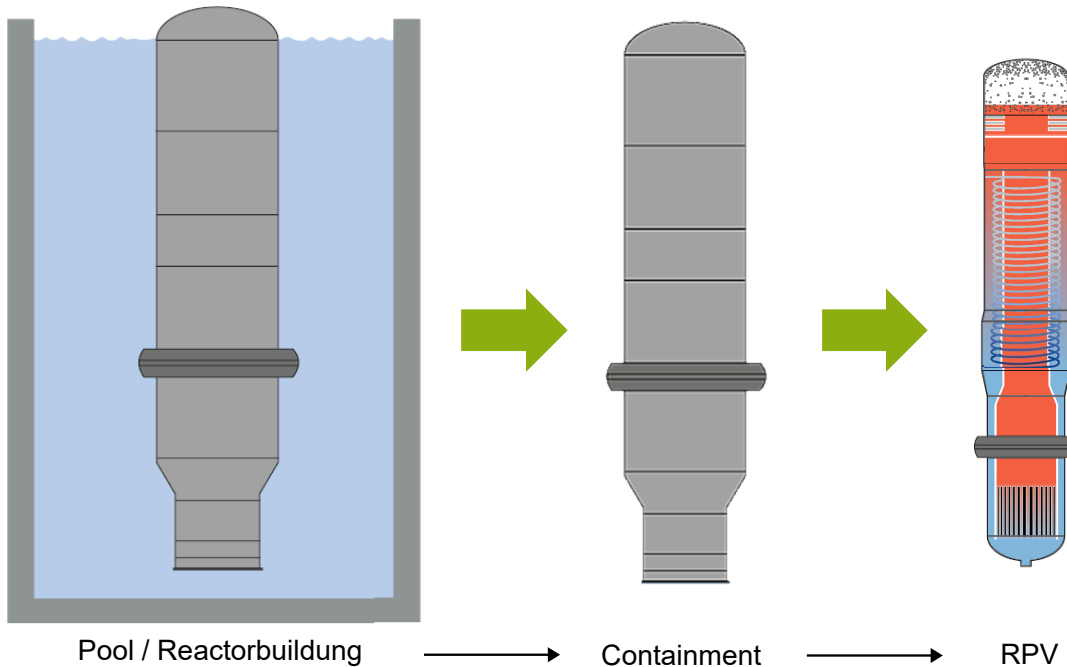


# PLANT APPLICATION - OUTLOOK

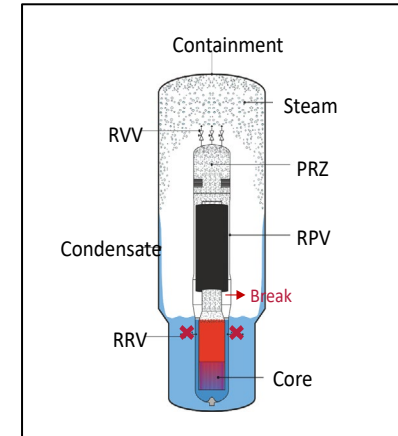
# MODELING

## Plant Modeling using AC<sup>2</sup> TFD module

- Simulation model of a generic integral PWR modelled with AC<sup>2</sup> based on public information



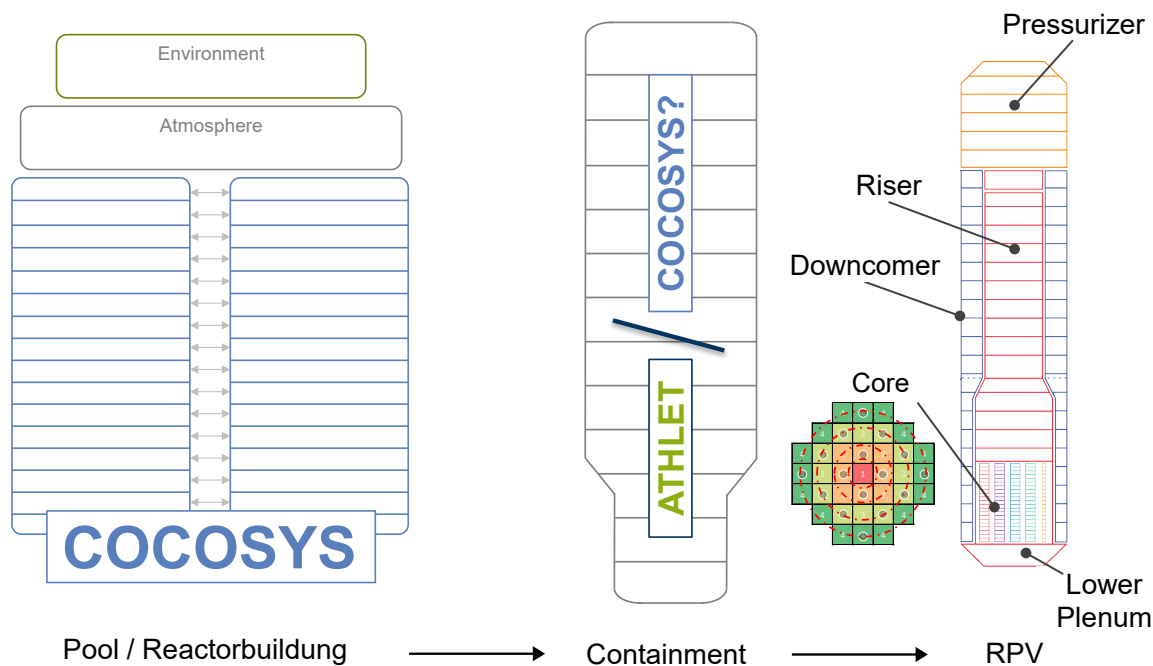
- During postulated SA (e.g.)
- Steam release in containment
  - **No** recirculation (blocked RRV)
  - **Break** ~ 3.5 m above top of active fuel



# MODELING

## Plant Modeling using AC<sup>2</sup> TFD module

- Simulation model of a generic integral PWR modelled with AC<sup>2</sup> based on public information



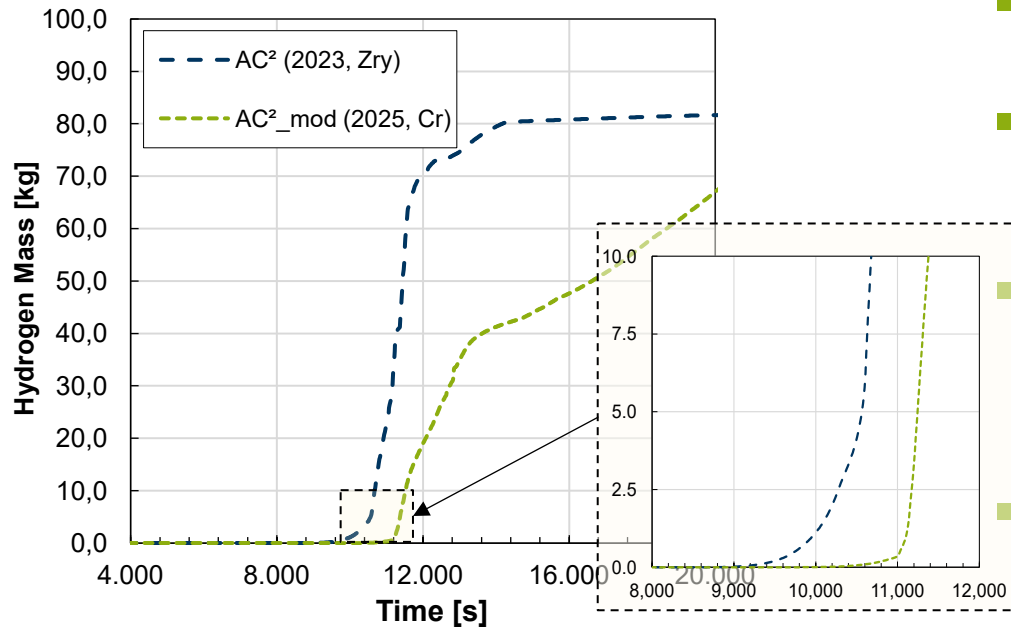
### AC<sup>2</sup> modules

- ECOREMOD – Core
- OREST/FIPISO – Inventory
- AIDA – Late Phase
- FIPREM – FP release
- SAFT – FP behavior

# RESULTS

## Plant Calculation: Investigating impact of Cr-coating on H<sub>2</sub> release

### ■ Preliminary results with new option for Cr-coating



- The Cr-coating model successfully delays onset of the early Zry escalation
- The post-failure rate (green) is observed to be even steeper than the Zry-oxidation (blue)
- This aligns with the hypothesis that failure at these temperatures leads to a more intense oxidation, which the model successfully captures
- This highlights a key modeling challenge: ensuring correct transition from Cr- to Zry-oxidation logic

# MODELING PERSPECTIVES

## Robustness and Limitations

### ■ Impact of Failure Temperature ( $T_{fail}$ ):

- Current model utilizes a parametric thermal threshold to trigger loss of protective effect
- The timing of this loss dictates the onset of the H<sub>2</sub> escalation
- Sensitivity Check: A variation in  $T_{fail}$  results in a notable shift of the escalation onset
- Determination of failure limits is relevant to reduce uncertainties in predicting hydrogen source term

### ■ Physical Limitations

- Current approach approximates transition using interpolation to capture gradual degradation
- Interdiffusion; formation of intermetallic layers reduces the effective protective scale (time-at-temperature)
- Potential for failure below eutectic temperature if exposure time is sufficiently long
- Investigation of diffusion-based degradation models to be assessed

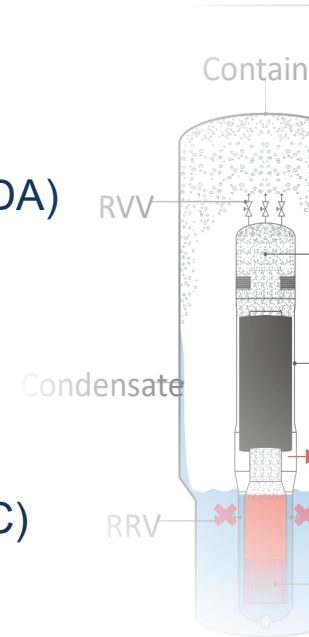
# CONCLUSION

## ■ Application to QUENCH facility and preliminary plant application

- Model demonstration based on public reference data (QUENCH-15)
- Model confirmation based on proprietary data (QUENCH-ATF-1/-2, under NDA)
- Plant application shows plausible behavior, indicates hypothetically slight gain in coping time

## ■ High-Temperature Modeling Challenges

- Numerically smooth transition to Zircaloy oxidation required (approx. 1,300°C)
- Highly sensitive to kind of interpolation function and interval size
- Potential of diffusion-based approaches for time-dependent failure limits to be assessed in future investigations



RUB

Thank you for your attention!

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# REFERENCES

[Bou19] Bourdon, Gauthier; Ševecek, Martin; Krejčí, Jakub; Cvrček, Ladislav: HIGH-TEMPERATURE STEAM AND AIR OXIDATION OF CHROMIUM-COATED OPTIMIZED ZIRLO™. Acta Polytechnica CTU Proceedings, 24, 2019. DOI: 10.14311/APP.2019.24.0001.

[Bra15] Brachet, Jean-Christophe; Le Saux, Matthieu; Le Flem, Marion; Urvoy, Stephane; Rouesne, Elodie; Guilbert, Thomas; Cobac, C.; Lahogue, F.; Rousselot, J. L.; Tupin, Marc; Billaud, Pierre; Hossepied, Charles; Monsifrot, Eric: On-going studies at CEA on chromium coated zirconium based nuclear fuel claddings for enhanced accident tolerant LWRS fuel, cea-02492582, Top Fuel 2015 - Reactor Fuel Performance Meeting, Zurich, Switzerland, 2015.

[Bra18] Brachet, Jean-Christophe; Guilbert, T.; Le Saux, Matthieu; Rousselot, J.; Nony, G.; Toffolon-Masclat, C.; Michau, Alexandre; Schuster, Frederic; Palancher, Herve; Bischoff, Jeremy; Augereau, J.; Pouillier, Edouard: BEHAVIOR OF Cr-COATED M5 CLADDINGS DURING AND AFTER HIGH TEMPERATURE STEAM OXIDATION FROM 800°C UP TO 1500°C - LOSS-OF-COOLANT ACCIDENT & DESIGN EXTENSION CONDITIONS, Top Fuel 2018 - Reactor Fuel Performance, Prague, Czech Republic, 2018.

[Bra19] Brachet, Jean-Christophe; Idarraga-Trujillo, Isabel; Le Flem, Marion; Le Saux, Matthieu; Vandenberghe, Valérie; Urvoy, Stephane; Rouesne, Elodie; Guilbert, Thomas; Toffolon-Masclat, Caroline; Tupin, Marc; Phalippou, Christian; Lomello, Fernando; Schuster, Frédéric; Billard, Alain; Velisa, Gihan; Ducros, Cédric; Sanchette, Frédéric: Early studies on Cr-Coated Zircaloy-4 as enhanced accident tolerant nuclear fuel claddings for light water reactors. Journal of Nuclear Materials, 517, S. 268–285, 2019. DOI: 10.1016/j.jnucmat.2019.02.018.

[Bra20] Brachet, Jean-Christophe; Rouesne, Elodie; Ribis, Joël; Guilbert, Thomas; Urvoy, Stéphane; Nony, Guillaume; Toffolon-Masclat, Caroline; Le Saux, Matthieu; Chaabane, Nihed; Palancher, Hervé; David, Amandine; Bischoff, Jérémy; Augereau, Julien; Pouillier, Edouard: High temperature steam oxidation of chromium-coated zirconium-based alloys: Kinetics and process. Corrosion Science, 167, 2020. DOI: 10.1016/j.corsci.2020.108537.

[Gre19] Gremme, Florian: Analyse des Einflusses anlageninterner Notfallmaßnahmen auf die Kernkühlbarkeit bei auslegungsüberschreitenden Störfällen in Druckwasserreaktoren. PhD thesis. Ruhr-University Bochum. Plant Simulation and Safety (PSS). Shaker-Verlag. Bochum. Germany. 2019. ISBN 978-3-8440-6516-9.

[Kas22] Kashkarov, E. B.; Sidelev, D. V.; Pushilina, N. S.; Yang, J.; Tang, C.; Steinbrueck, M.: Influence of coating parameters on oxidation behavior of Cr-coated zirconium alloy for accident tolerant fuel claddings. Corrosion Science, 203, S. 110359, 2022. DOI: 10.1016/j.corsci.2022.110359.

[Kim15] Kim, Hyun-Gil; Kim, Il-Hyun; Jung, Yang-Il; Park, Dong-Jun; Park, Jeong-Yong; Koo, Yang-Hyun: Adhesion property and high-temperature oxidation behavior of Cr-coated Zircaloy-4 cladding tube prepared by 3D laser coating. Journal of Nuclear Materials, 465, S. 531–539, 2015. DOI: 10.1016/j.jnucmat.2015.06.030.

# REFERENCES

- [Li20] Li, Guangbin; Liu, Yanhong; Zhang, Yingchun; Li, Huailin; Wang, Xiaojing; Zheng, Mingmin; Li, Yusha: High Temperature Anti-Oxidation Behavior and Mechanical Property of Radio Frequency Magnetron Sputtered Cr Coating. *Metals*, 10, S. 1509, 2020. DOI: 10.3390/met10111509.
- [Liu21] Liu, Junkai; Tang, Chongchong; Steinbrück, Martin; Yang, Jianqiao; Stegmaier, Ulrike; Große, Mirco; Di Yun; Seifert, Hans Jürgen: Transient experiments on oxidation and degradation of Cr-coated Zircaloy in steam up to 1600 °C. *Corrosion Science*, 192, 2021. DOI: 10.1016/j.corsci.2021.109805.
- [Ma21] Ma, Hai-Bin; Yan, Jun; Zhao, Ya-Huan; Liu, Tong; Ren, Qi-Sen; Liao, Ye-Hong; Zuo, Jia-Dong; Liu, Gang; Yao, Mei-Yi: Oxidation behavior of Cr-coated zirconium alloy cladding in high-temperature steam above 1200 °C. *npj Materials Degradation*, 5, 2021. DOI: 10.1038/s41529-021-00155-8.
- [Sha18] Shah, Hemant; Romero, Javier; Xu, Peng; Oelrich, Robert; Walters, Jorie; Wright, Jonathan, Gassmann, William: Westinghouse-Exelon EnCore® Fuel Lead Test Rod (LTR) Program including Coated cladding Development and Advanced Pellets, WAAP-10756, Top Fuel 2018 - Reactor Fuel Performance, Prague, Czech Republic, 2018.
- [Wu20] Wu, Xu; Shirvan, Koroush: System code evaluation of near-term accident tolerant claddings during boiling water reactor short-term and long-term station blackout accidents. *Nuclear engineering and design*, 2020. DOI: 10.1016/j.nucengdes.2019.110362.

# REFERENCES (RUB PSS)

- [Sta22] Stahlberg, Gregor, T., et al.: Preliminary Simulation Results of the Experiments QUENCH-L3HT and QUENCH-ATF-1 Regarding High-Temperature Oxidation Mechanisms Using the System Code AC<sup>2</sup>. 27th International QUENCH Workshop, KIT, Karlsruhe, 2022. <https://doi.org/10.5445/ir/1000152245>
- [Sta23] Stahlberg, Gregor T., et al.: Comparative analyses of the QUENCH experiments L3HT and ATF-1 on high temperature oxidation mechanisms using AC<sup>2</sup>, in Proceedings of NURETH-20 - International Topical Meeting on Nuclear Reactor Thermal Hydraulics, pp. 5450–5461, 2023. <https://doi.org/10.13182/nureth20-39989>
- [Sta23] Stahlberg, Gregor, T., Koch, M. K.: *Development of a preliminary model for Cr-coated Claddings for the System Code Package AC<sup>2</sup>*. 28th International QUENCH Workshop, KIT, Karlsruhe, 2023.
- [Kri24] Krieger, J., Koch, Marco K., Stahlberg, G. T.: *Analyses of a Postulated Severe Accident in a Generic Small Modular Reactor Using AC<sup>2</sup>*. Kerntechnik 2024, Leipzig, 11. Juni 2024.
- [Sta24a] Stahlberg, Gregor T., Koch, M. K.: *Modeling of Oxidation Behavior of Accident Tolerant Fuel by using AC<sup>2</sup>*. 11th European Review Meeting on Severe Accidents Research (ERMSAR 2024, edited by F. Gabrielli, L.E. Herranz, and S. Paci). Stockholm, Sweden, 2024.
- [Sta24b] Stahlberg, Gregor T., Krieger, J., Koch, M. K.: *Analyses of an integral Pressurized Water Reactor during postulated Accident Conditions using the System Code Package AC<sup>2</sup>*. Proceedings of the 14th International Topical Meeting on Nuclear Reactor Thermal-Hydraulics, Operation, and Safety, NUTHOS 2024, S. 1658-1668, 2024. DOI: 10.13182/nuthos14-138 [<https://doi.org/10.13182/nuthos14-138>].
- [Hol24] Hollands, T.M.J., Stahlberg, G., Gabrielli, F., et al.: *Application of AC<sup>2</sup>/Athlet-CD and ASTEC for ATF experiments in the frame of ongoing international projects*. 11th European Review Meeting on Severe Accidents Research (ERMSAR 2024, edited by F. Gabrielli, L.E. Herranz, and S. Paci). Stockholm, Sweden, 2024.
- [Gab24] F. Gabrielli et al.: *Analysis of Postulated Severe Accidents in Generic Integral PWR Small Modular Reactors in the frame of the Horizon Euratom SASPAM-SA Project*. 11th European Review Meeting on Severe Accidents Research (ERMSAR 2024, edited by F. Gabrielli, L.E. Herranz, and S. Paci). Stockholm, Sweden, 2024.



**Stephan Gabriel**

KIT

## **First experiments at the new thermohydraulic facility**

The COSMOS-H facility at KIT is a high-pressure water/steam thermohydraulic test loop capable of up to 17 MPa and 360 °C, reproducing 1:1 conditions of most LWR concepts. It operates with an installed thermal power of 1.8 MW (including 600 kW electrical power for the test section) and uses de-ionised water with precise instrumentation for pressure, temperature and mass-flow control.

Its modular test section features an 80 mm inner-diameter tube up to 3.5 m long, equipped with numerous feedthroughs for heaters, thermocouples (up to 38, 20 currently used) and fiber-optic probes. High-pressure sight glasses and a robotic arm enable optical measurements even when the safety housing is locked, and a trace-heating system with thermal-oil cooling ensures stable two-phase operation.

The first experiment, part of the EU-project OFFERR/COATED, investigated the critical heat flux of a directly heated Zircaloy-4 cladding tube (81 cm heated length) in an annular gap. High-speed recordings identified flow regimes and the onset of nucleate boiling at approximately 12 kW. The state-of-the-art control system rapidly detects boiling crises and reduces power to protect the cladding, allowing repeatable experiments; the dense thermocouple array provides detailed temperature distributions.

Initial results are promising, and future work will extend to chrome-coated cladding tubes and higher pressures while expanding the test track and modular capabilities.

# COSMOS-H

Critical heat flux On Smooth and MOdified Surfaces – High pressure

## First experiments at the new thermohydraulic facility

Stephan Gabriel, Wilson Heiler, Nicolas Wefers

Institute for Thermal Energy Technologies and Safety (ITES)

Dept. Multiphase Flows (MPF)

12/2025



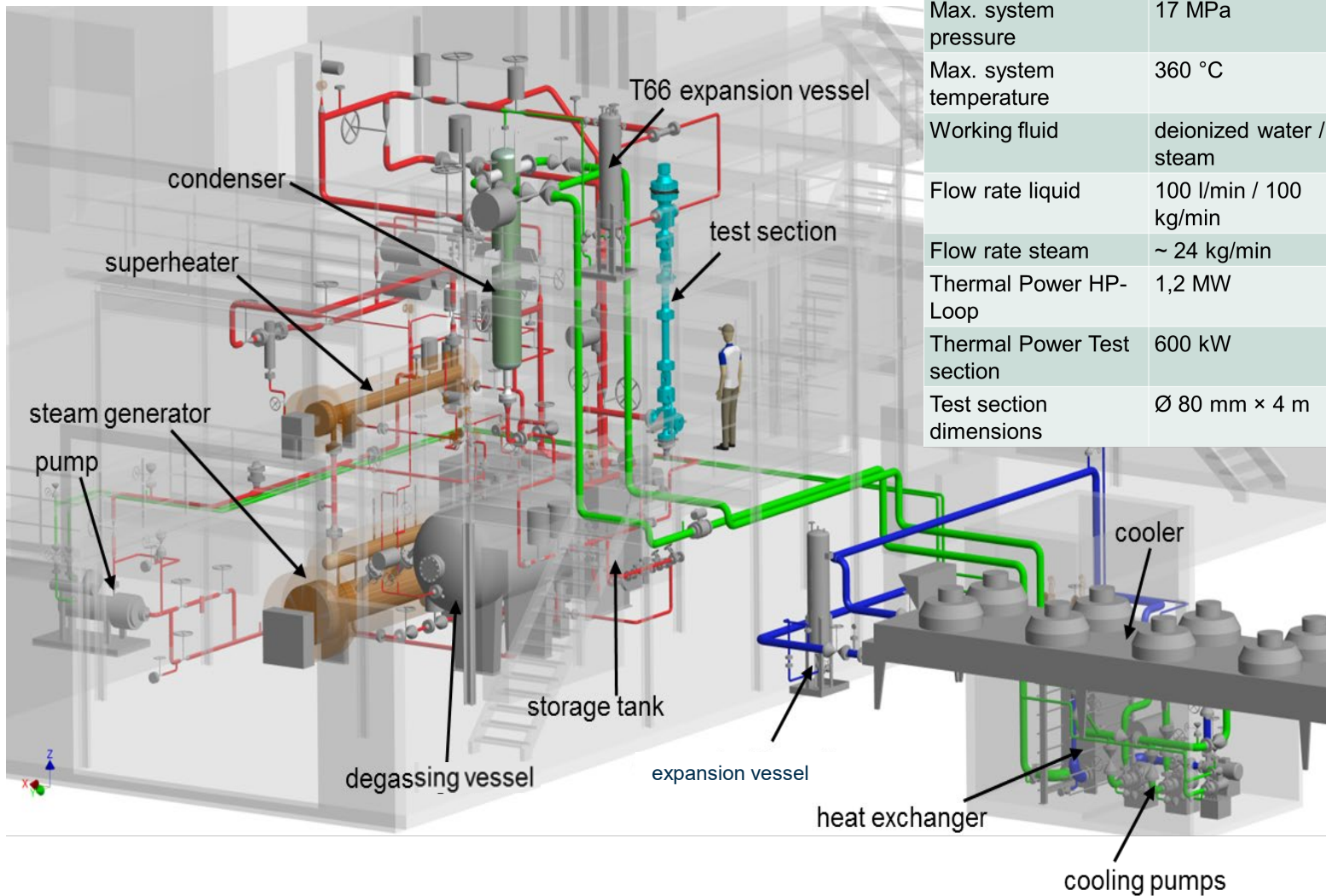
- 1. Facility overview**
- 2. Test section system**
- 3. First experiments**

# Facility overview

- COSMOS-H is a thermohydraulic test facility for water/steam experiments under high pressure conditions up to **17 MPa and 360°C**. **Permits 1:1 conditions to most LWR Concepts**
- The experimental loop has an installed **thermal power of 1.8 MW**. This includes 600 kW of electrical power for the test section.
- The COSMOS-H test loop is operated with **deionized water**. All important experimental boundary conditions - e.g. extensively instrument with pressure, temperature, mass flow - can be precisely measured and controlled.
- COSMOS-H can operate with single tubes and small bundles (3x3 up to 3,5 m length) made of **zirconium alloys**, but also other **ATF materials**.



# Facility overview



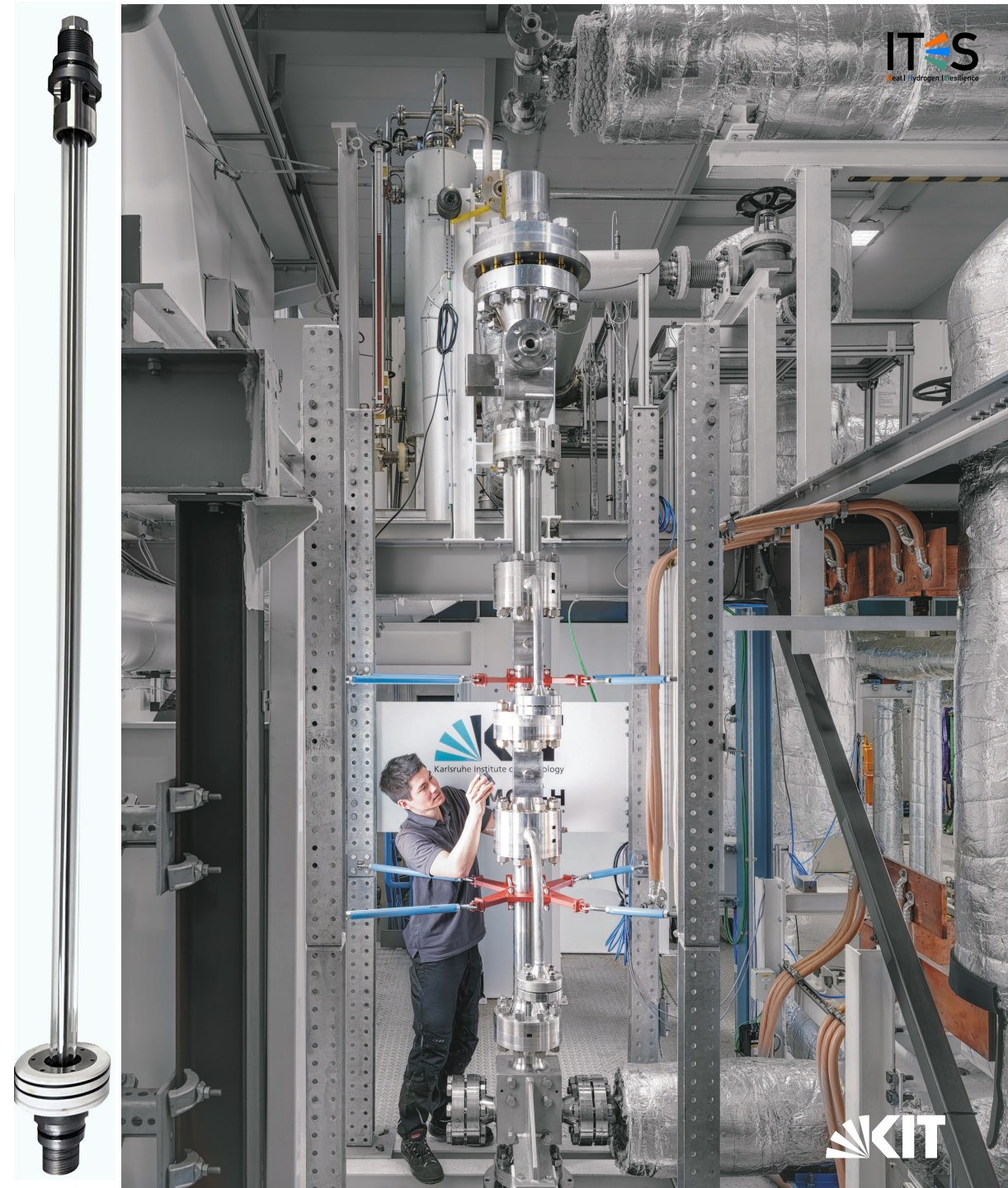
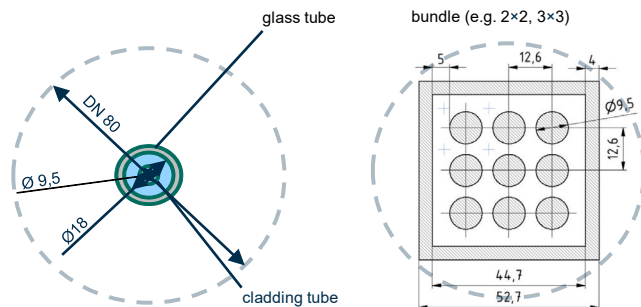
Parameter	Value
Max. system pressure	17 MPa
Max. system temperature	360 °C
Working fluid	deionized water / steam
Flow rate liquid	100 l/min / 100 kg/min
Flow rate steam	~ 24 kg/min
Thermal Power HP-Loop	1,2 MW
Thermal Power Test section	600 kW
Test section dimensions	Ø 80 mm × 4 m

- In addition to the steam generator and steam superheater, COSMOS-H has an extensive trace heating system that allows the thermal boundary conditions to be precisely controlled even for two-phase flows in and around the test section.
- Thermal oil is used as the working medium in the cooling system to ensure constant availability of cooling power for the entire performance spectrum, especially for small cooling loads.
- A comprehensive safety system enables the use of customized measurement equipment such as sight glasses.

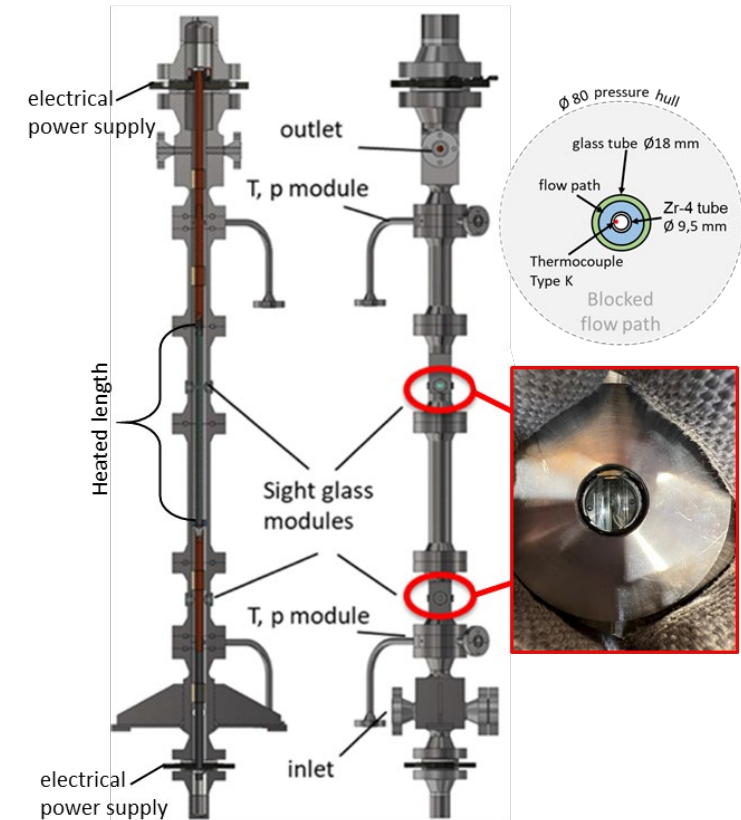
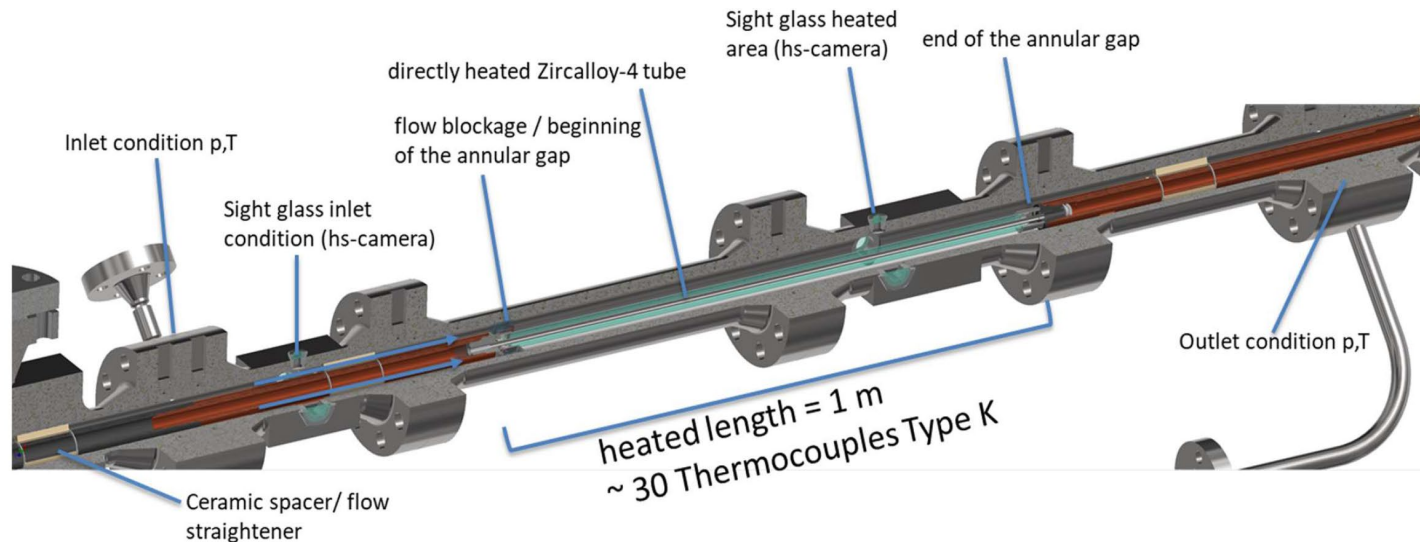


# Test section system

- The modular test section was built for the detailed investigation of boiling flows up to and including the boiling crisis. It has an inner diameter of 80 mm and a length of up to 3,5 m.
- It consists of a modular pressure hull with numerous feedthroughs for the electrical power supply to the heater and for **instrumentation for pressure, thermocouples and fiber probes**.
- The modules can be arranged as required.
- The high-pressure sight glasses developed in-house can also be used for optical measurements. Using a robotic arm, cameras can be moved to the sight glasses even when the safety housing is locked.



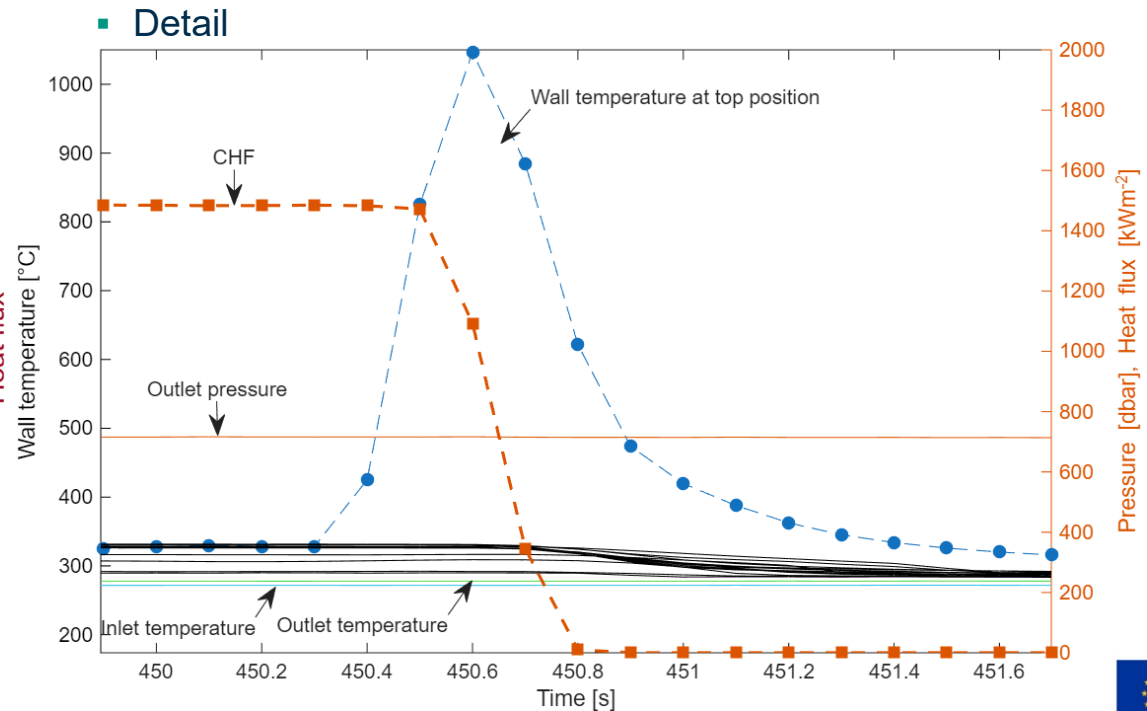
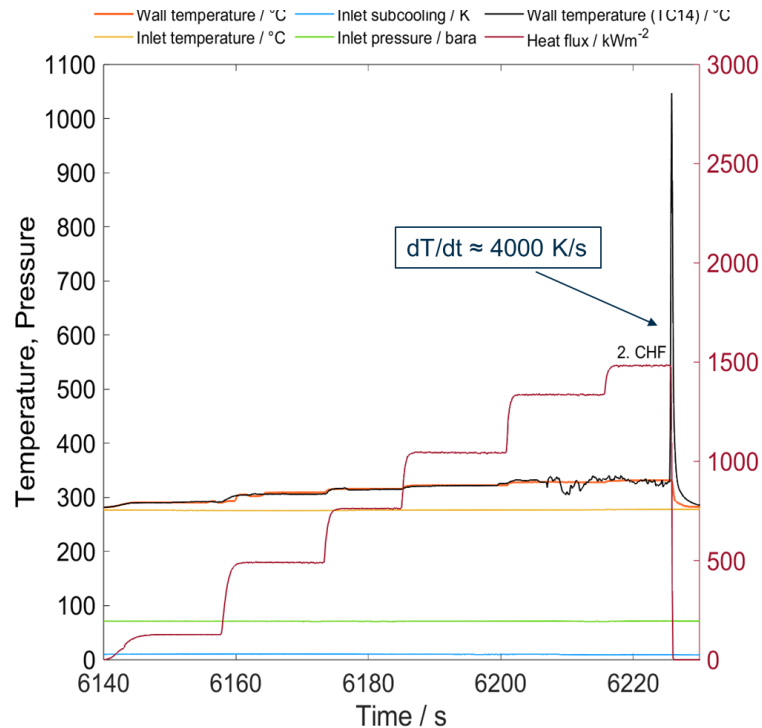
# Test section system



- Directly heated Zircalloy-4 cladding tube, instrumented internally with up to 38 thermocouples. Currently 20 are in use. Heated length 81 cm.
- Pressure sensors before and after the test section, as well as special feedthroughs for glass fibers for void and temperature measurement.
- With the current test section concept, heated lengths of up to 3.5 m and up to 5 tubes in a bundle can be realized. Larger test arrangements are possible, but require a new pressure sleeve for the test section.

# EU-Project OFFERR/COATED

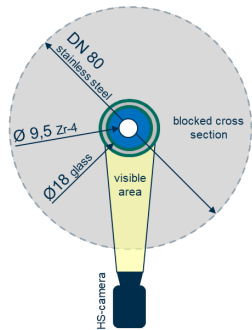
Parameter	COSMOS-H BWR_01
Pressure	7,2 MPa
Temperature	271 °C
Subcooling	16 K
Mass flow rate	4000 kg/m <sup>2</sup> s
Heated length	0,81 m
Heater Material	Zircaloy-4



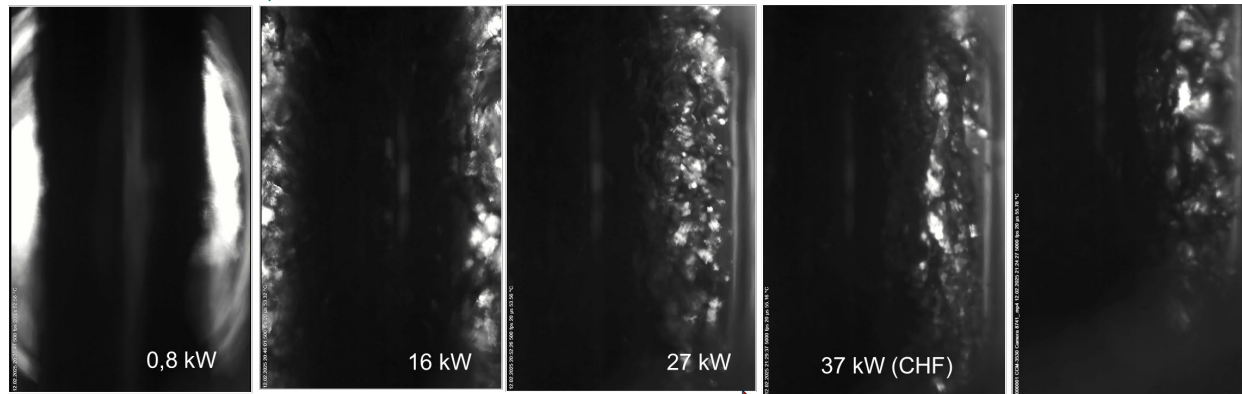
- The main objective of the experiment was to determine the critical heat flux for the Zr-4 cladding tube in the annular gap. This result serves as a reference for later comparison with ATF materials, which will be examined in subsequent experiments.
- Additional data was recorded. Boundary conditions such as temperature, pressure, mass flow, inlet subcooling and temperature distribution at the heater were measured.

# EU-Project OFFERR/COATED

Parameter	COSMOS-H BWR_01
Pressure	7,2 MPa
Temperature	271 °C
Subcooling	16 K
Mass flow rate	4000 kg/m <sup>2</sup> s
Heated length	0,81 m
Heater Material	Zircaloy-4

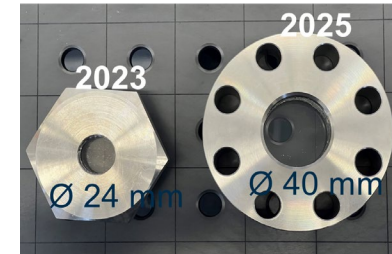
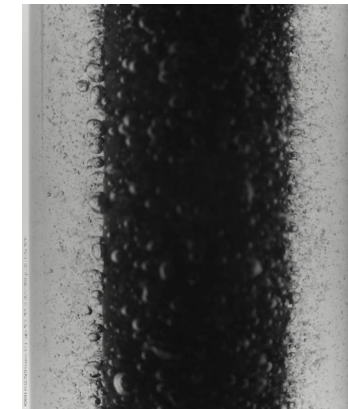


Onset of Nucleate Boiling @ ~12 kW



Increasing heating power

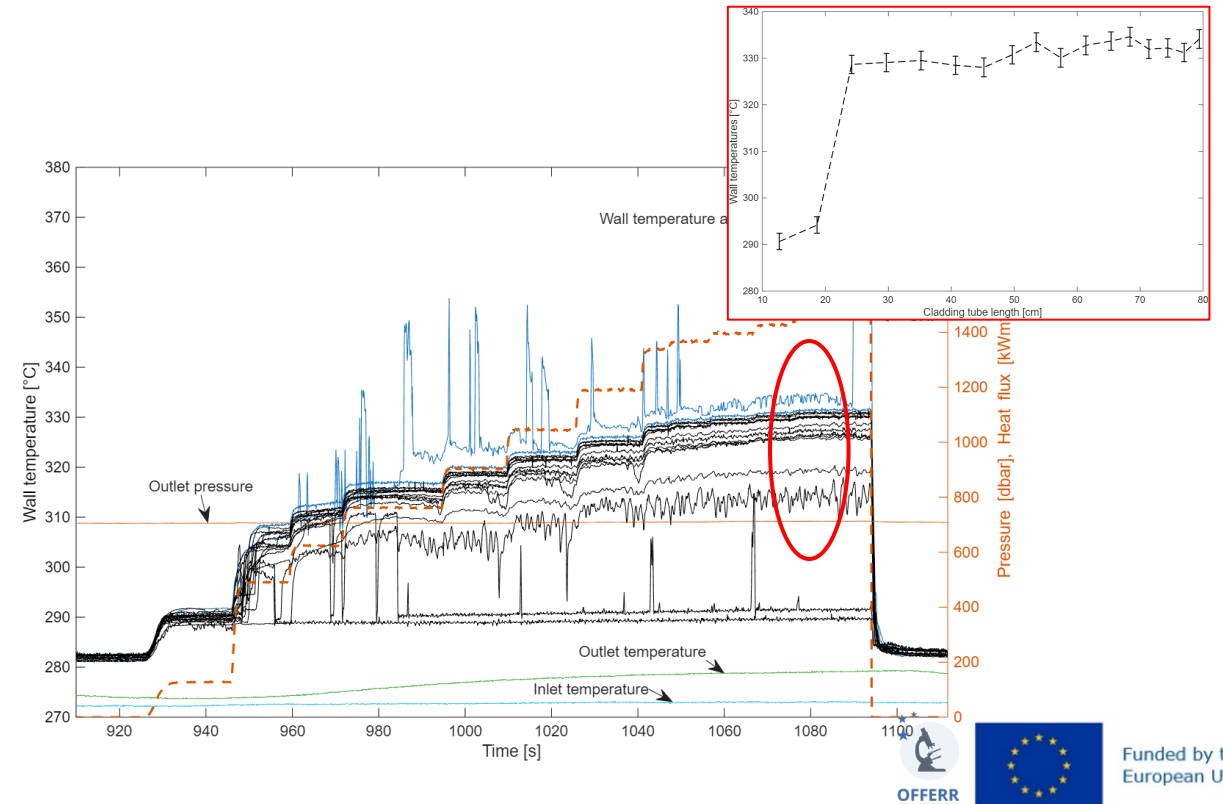
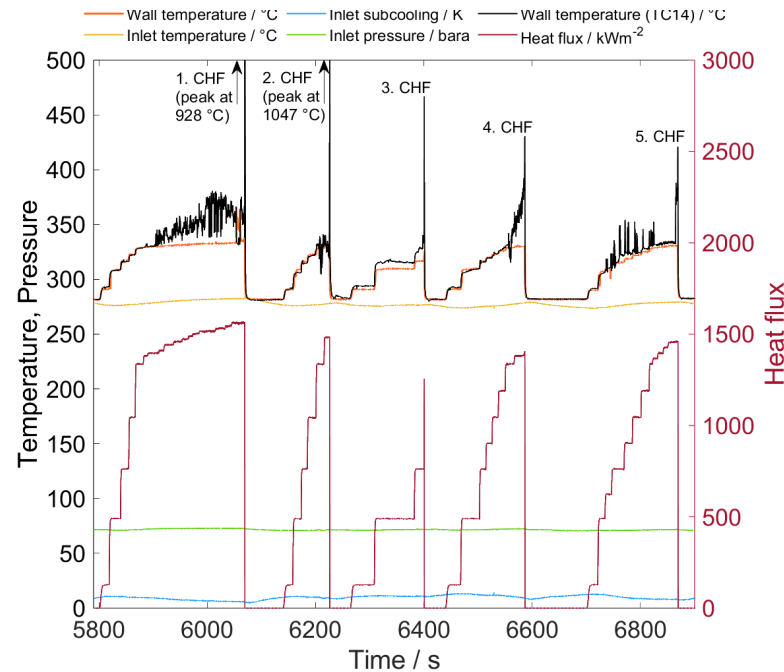
Sequence @ COS-L



- High-speed recordings were used to determine flow regimes and characteristic values such as bubble size or the onset of nucleate boiling.
- Due to the small sight glass of 28 mm, the illumination is not sufficient for high quality images. Therefore the next generation of sight glasses was developed and the imaging technique was improved.

# EU-Project OFFERR/COATED

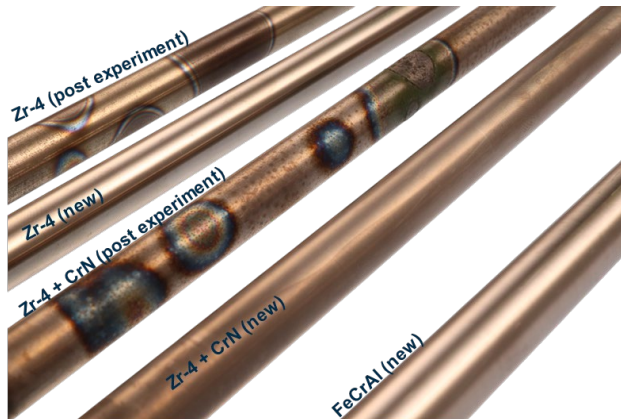
Parameter	COSMOS-H BWR_01
Pressure	7,2 MPa
Temperature	271 °C
Subcooling	16 K
Mass flow rate	4000 kg/m <sup>2</sup> s
Heated length	0,81 m
Heater Material	Zircaloy-4



- The State-of-the-art control system allows to detect the boiling crises very quickly and power to be reduced. The cladding tube remains undamaged. This enables to repeated the experiment.
- The high spacial density of thermocouples makes it possible to narrow down the location of the boiling crisis for each event and to create temperature distributions.

# Summary

- COSMOS-H a new water/steam thermohydraulic facility for experiments on thermohydraulics and materials under high-pressure conditions is now operational.
- Initial experiments are being conducted, and the experimental facility and test track are being expanded and optimized.
- The first experiment with Zircaloy-4 has already yielded useful results, and further experiments with chrome-coated cladding tubes will follow, including at higher pressures.





We look forward to get in contact with you!

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**Tapan K. Sawarn**

BARC

## **Synergistic influence of oxygen, hydrogen and microstructure on thermal shock behavior of PHWR fuel cladding subjected to integral LOCA test**

During a hypothetical loss of coolant accident (LOCA) in a pressurised heavy water reactor (PHWR), fuel cladding temperature may rise up to 1500°C due to coolant positive void coefficient of reactivity. At such a high temperature,  $\beta$ -Zr phase absorbs significant amount of oxygen and hydrogen causing its embrittlement. A novel approach was attempted to study the synergistic effects of oxygen, hydrogen and prior  $\beta$ -Zr layer thickness on the crack initiation and propagation during the thermal shock.

A series of integral LOCA tests were performed on the PHWR cladding. The tests were carried out according to a temperature-time scenario typical for a large break LOCA in PHWRs. The heating cycle simulates the typical power pulse type of transients, which are unique characteristics of the PHWRs. Clad tubes filled with alumina pellets were internally pressurised (7 & 20 bar) and subjected to induction heating in steam environment. It was heated to various oxidation temperatures in the range 1000 - 1500°C (at interval of 100°C), soaked for 12-20s, cooled down to 800°C & then water quenched. The results showed the presence of non-uniform distribution of oxygen, hydrogen and prior  $\beta$ -Zr phase across the clad thickness along the circumference and axial direction of cladding. The presentation discusses the insights generated from the study.





# **Synergistic influence of oxygen, hydrogen and microstructure on thermal shock behavior of PHWR fuel cladding subjected to integral LOCA test**

**Tapan K. Sawarn\*, Shefali Shukla, Suparna Banerjee, P. Nanekar**

**Bhabha Atomic Research Centre, India**

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**30<sup>th</sup> International QUENCH Workshop  
Karlsruhe Institute of Technology (Karlsruhe, Germany),  
Campus North, 16 to 18 December 2025.**

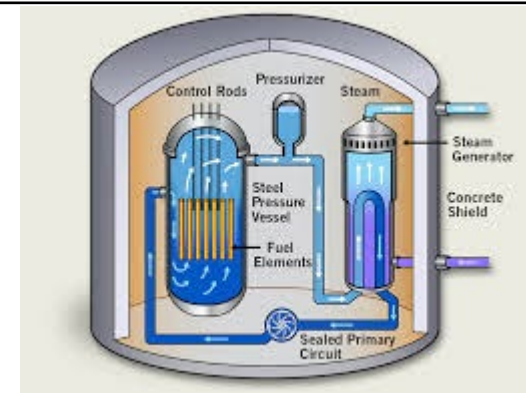
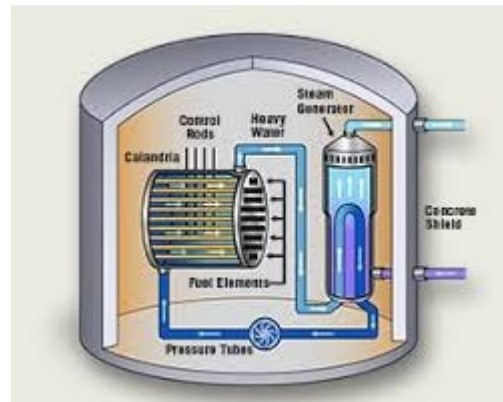
# LOCA transient in PHWRs and LWRs



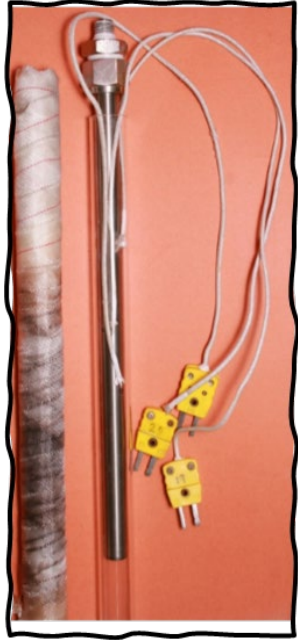
Parameters	PHWRs	LWRs
Coolant void coefficient of reactivity	Positive	Negative
Transient cycle	<ul style="list-style-type: none"><li>Higher and faster rise in cladding temperature during a critical large break LOCA.</li><li>Temperature ramp can be in the range of 53°C/s - 120°C/s for very short duration.</li></ul>	<ul style="list-style-type: none"><li>Temperature rise slowly due to the simultaneous loss of moderation.</li><li>SEH dominate during the first few seconds of the blowdown stage, ramp rate (~100°C/s), followed by a nearly isothermal ramp (~5°C/s) with a DEH.</li></ul>
Peak cladding temperature	1400 -1500°C under critical break condition momentarily with ECCS available	Remain below the regulatory limit of 1204°C, with ECCS available

# LOCA transient in PHWRs and LWRs

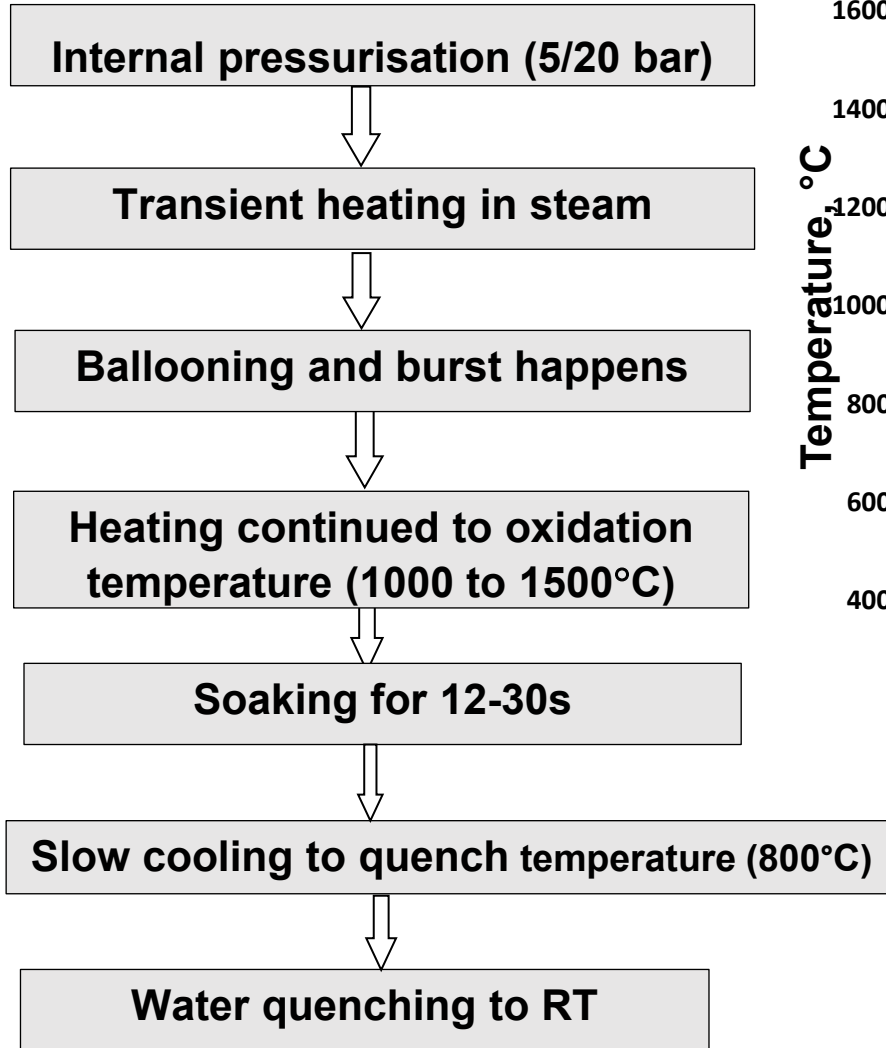
	PHWRs	LWRs
Quenching rate	A higher quenching rate during reflooding, due to horizontal configuration of the fuel channels.	Reflooding involves a relatively low rate of water injection due to vertical core configuration—usually a few cm/s—until the core is completely flooded and quenched.
Accident progression	<ul style="list-style-type: none"> <li>Large heat sink capacity that is inherently available (Moderator, End shield &amp; Calandria vault water).</li> <li>Cause slow progression of accident in case of severe accident.</li> </ul>	<ul style="list-style-type: none"> <li>No such availability of heat sink in case of LWR.</li> <li>Cause fast progression of accident during severe accident.</li> </ul>



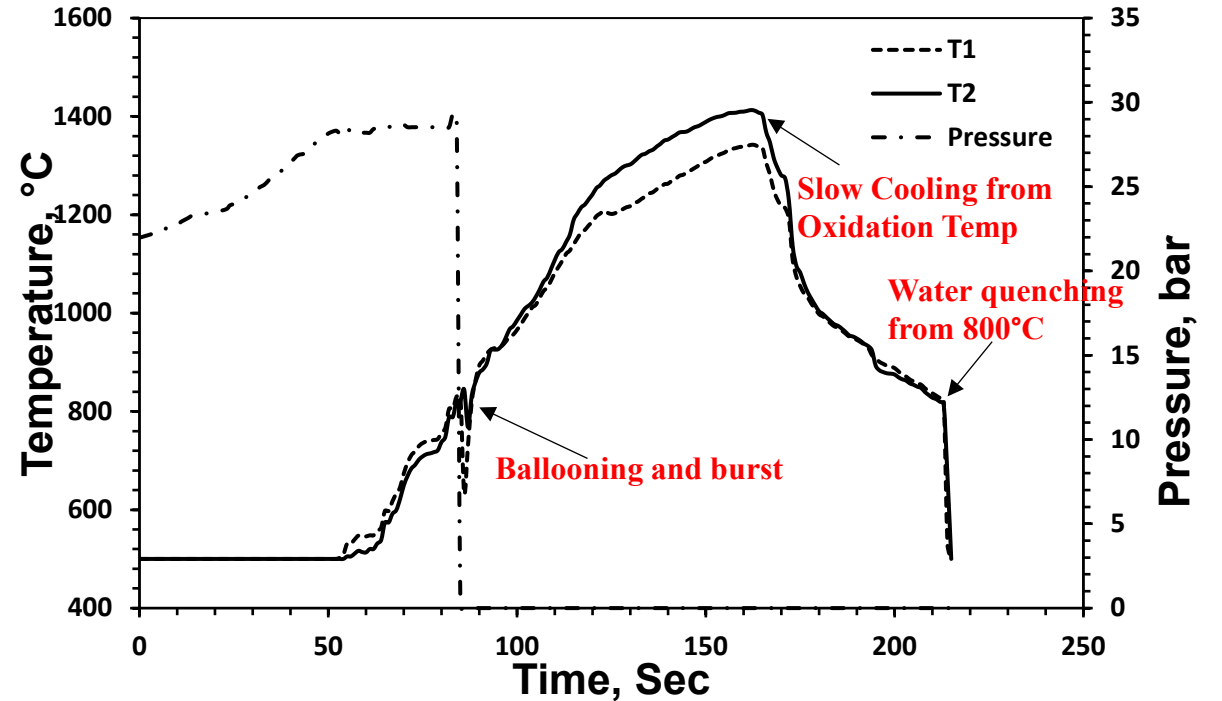
# LOCA Integral Tests



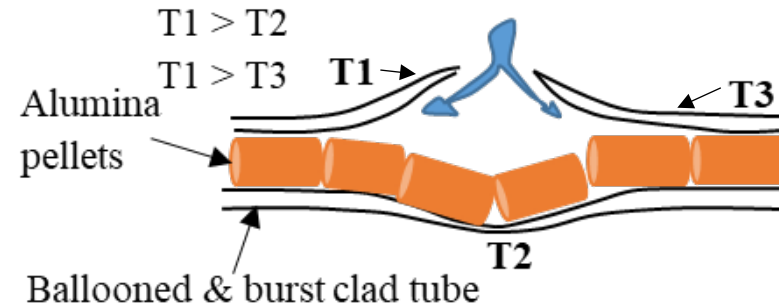
**Test specimen:**  
245 mm long,  
alumina pellets  
filled PHWR  
cladding



**Steps of LOCA Integral Tests**

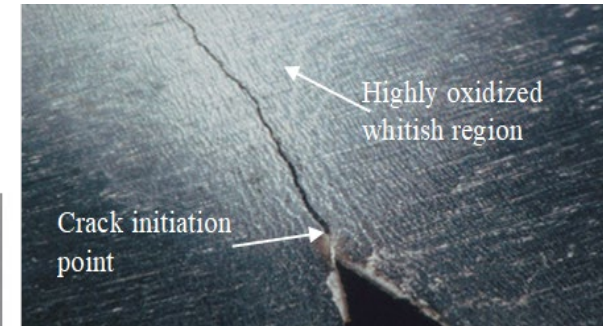
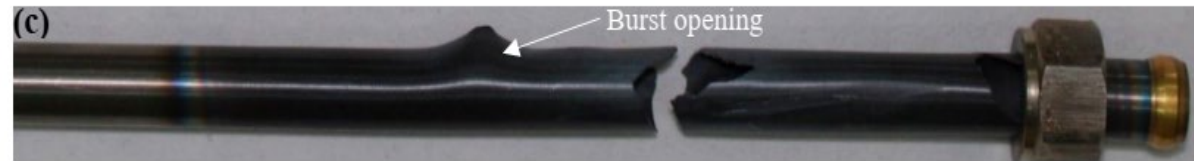
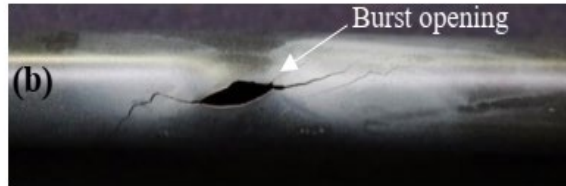


**A typical T-P-t plot**

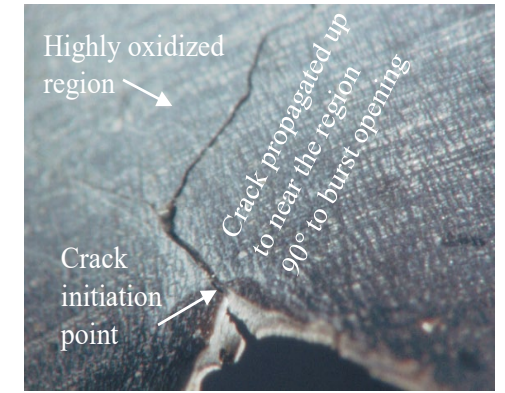


**Establishment of temperature gradient**

# Post-test visual appearance



1250°C-12s, H.R. - 5°C/s



1400°C-12s, H.R. - 10°C/s

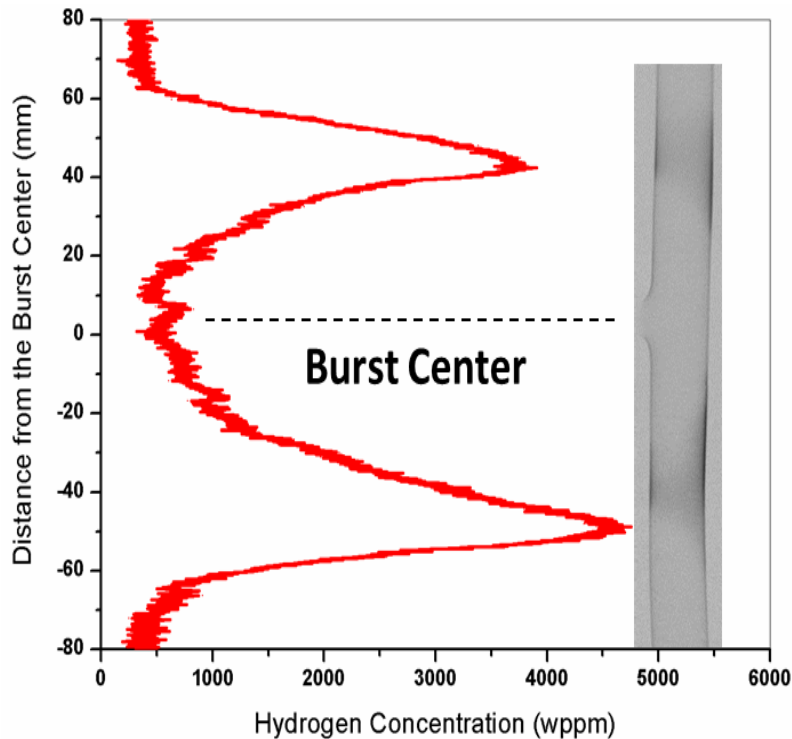
## Response to thermal shock of the ballooned-burst and oxidized cladding:

- i. Survived,
- ii. Cracked ahead of the burst opening tip,
- iii. Disintegrate into two parts during thermal shock or handling away from burst opening, and
- iv. Fragmented into multiple pieces due to severe oxidation at 1500°C.

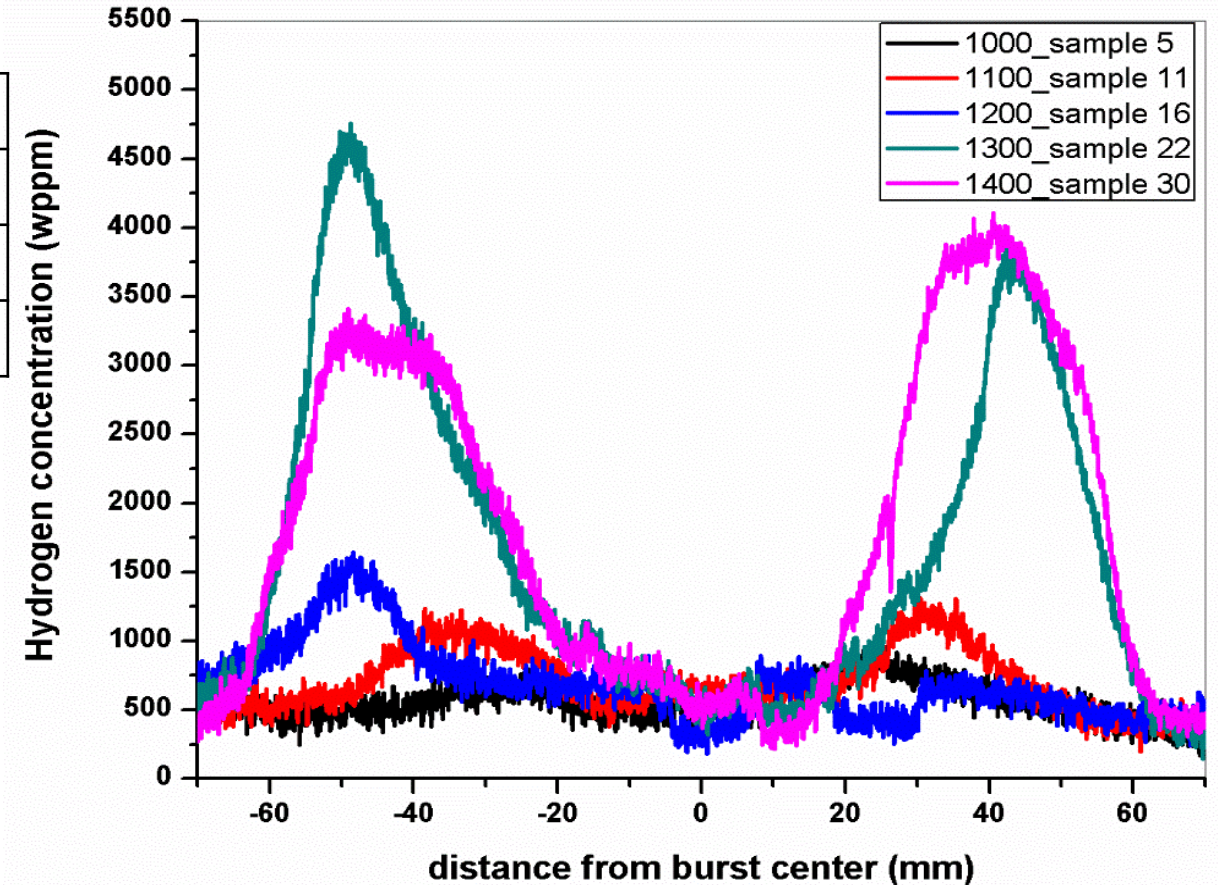
# Axial Hydrogen distribution

## n-radiography & tomography parameters

Scintillator	$^6\text{LiF-ZnS}$
Spatial Resolution	100 $\mu\text{m}$
Radiography	30 images of 30s exposure
Tomography	30s images 900 angles

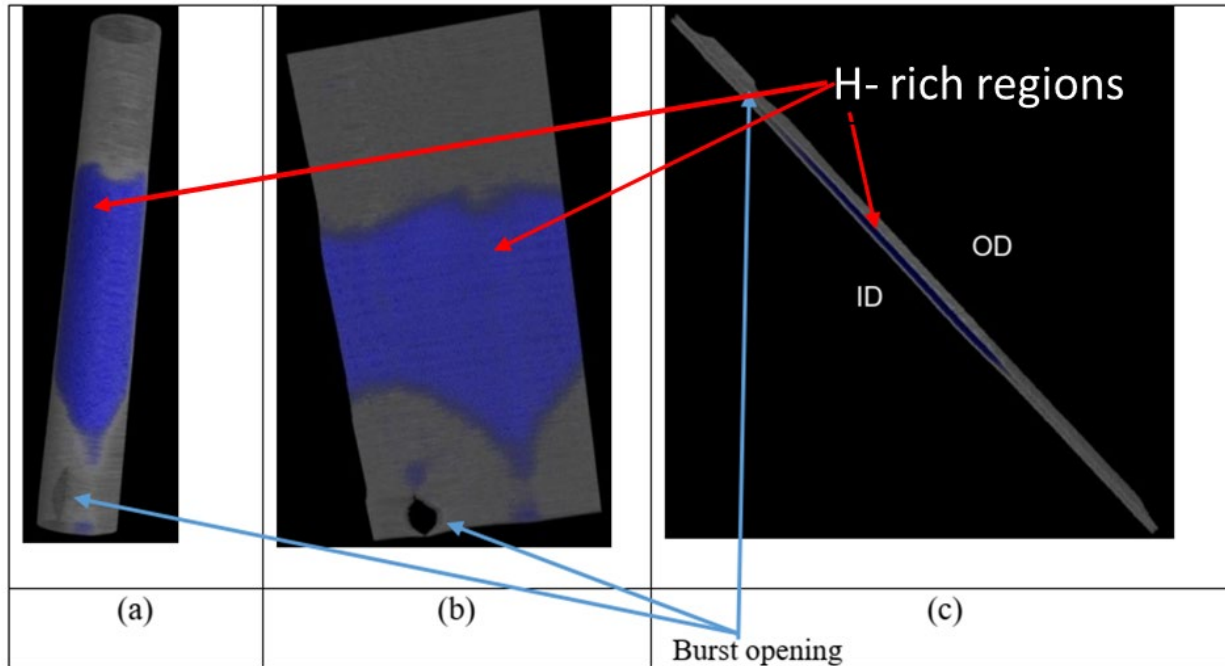


1300°C for 12s



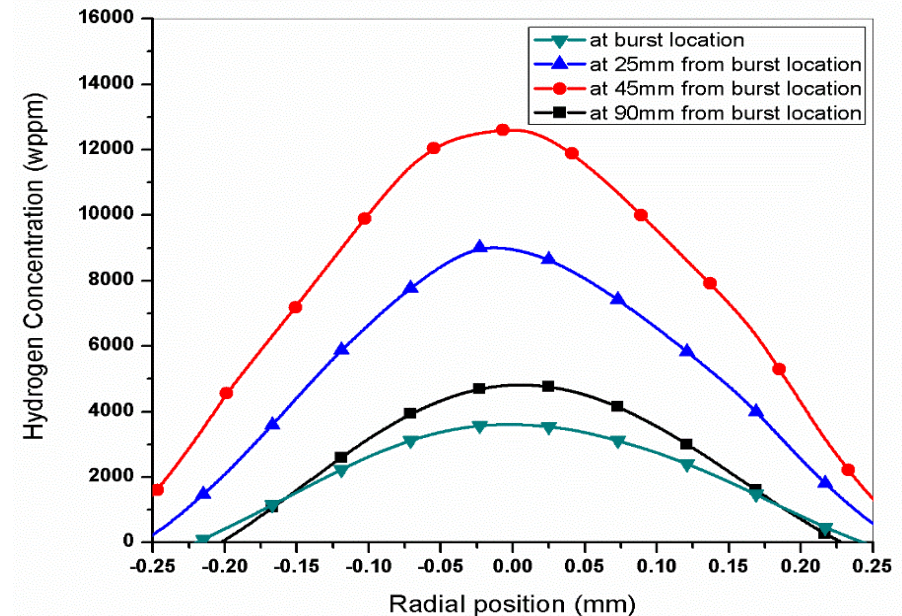
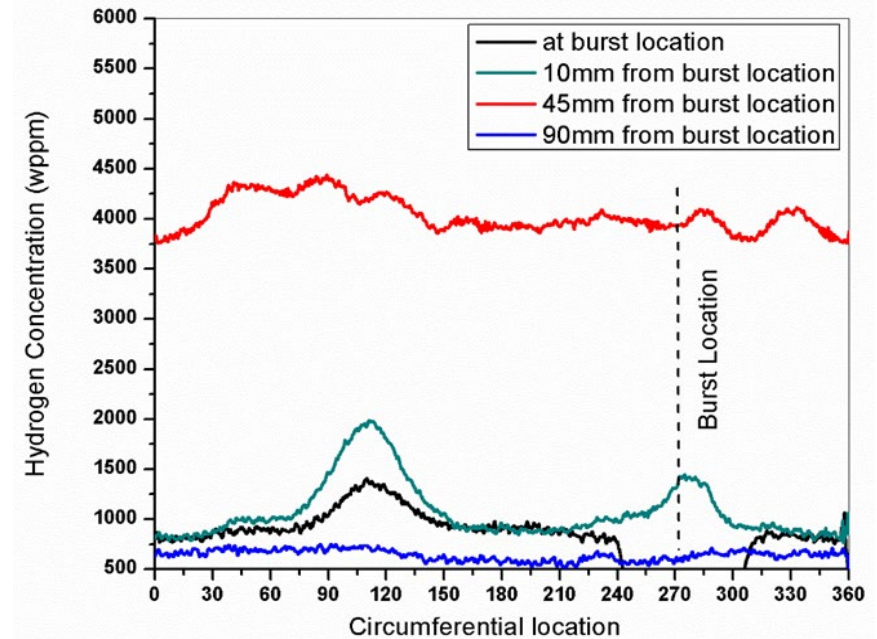
Significantly high hydrogen pick up occurred in the secondary hydriding region (1200 – 4700 wppm), 30 – 50 mm away from the burst opening.

# Circumferential and radial hydrogen distribution

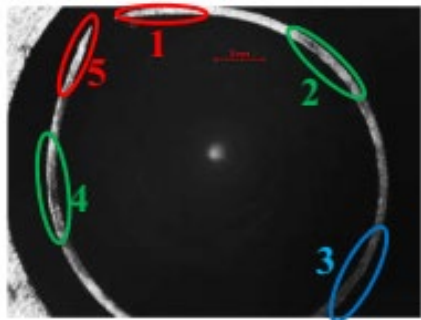


Oxidised at 1250°C for 12s

- Maximum hydrogen was picked up in the region opposite to burst opening.
- Radially maximum hydrogen present in the prior  $\beta$  layer.



# Oxygen distribution along the circumference



Oxygen in the prior  $\beta$  layer of region

- Burst tip : Average of locations 1 & 5 .....(i)
- 90° to burst tip : Average of locations 2 & 4 .....(ii)
- 180° to burst tip: location 3 .....(iii)

Average oxygen in the burst region's prior  $\beta$  layer = Average of i, ii & iii

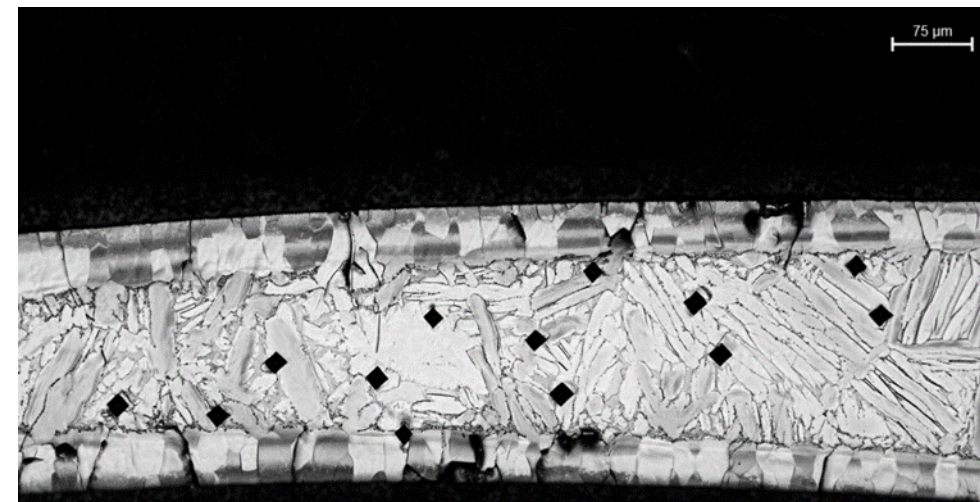


Average oxygen in the region away from the burst opening = Average of locations 1, 2, 3 & 4

Each location spanning over 900 $\mu$ m

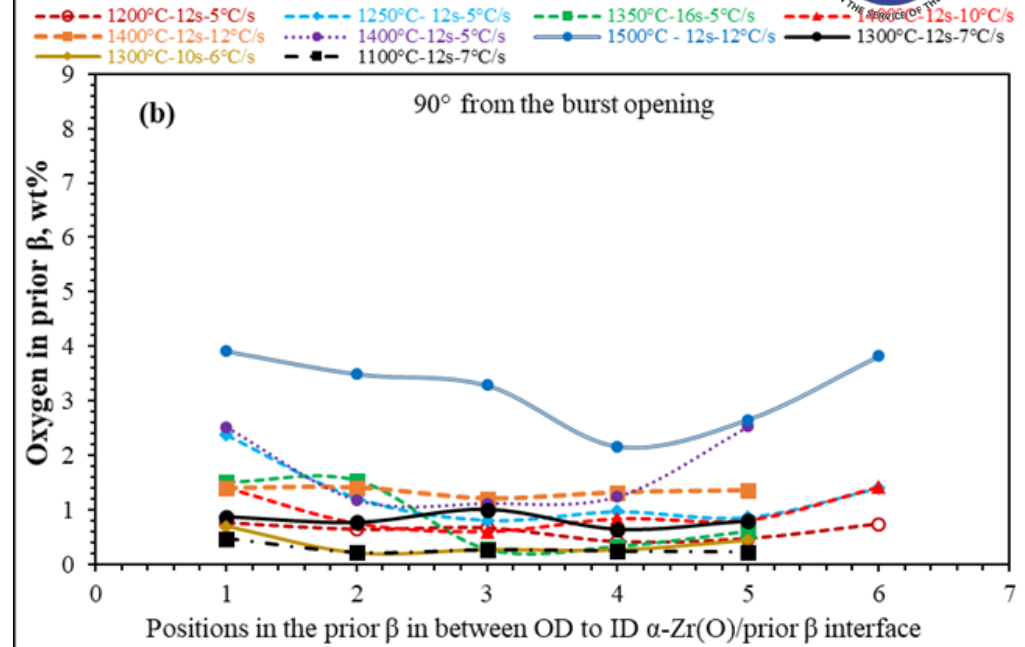
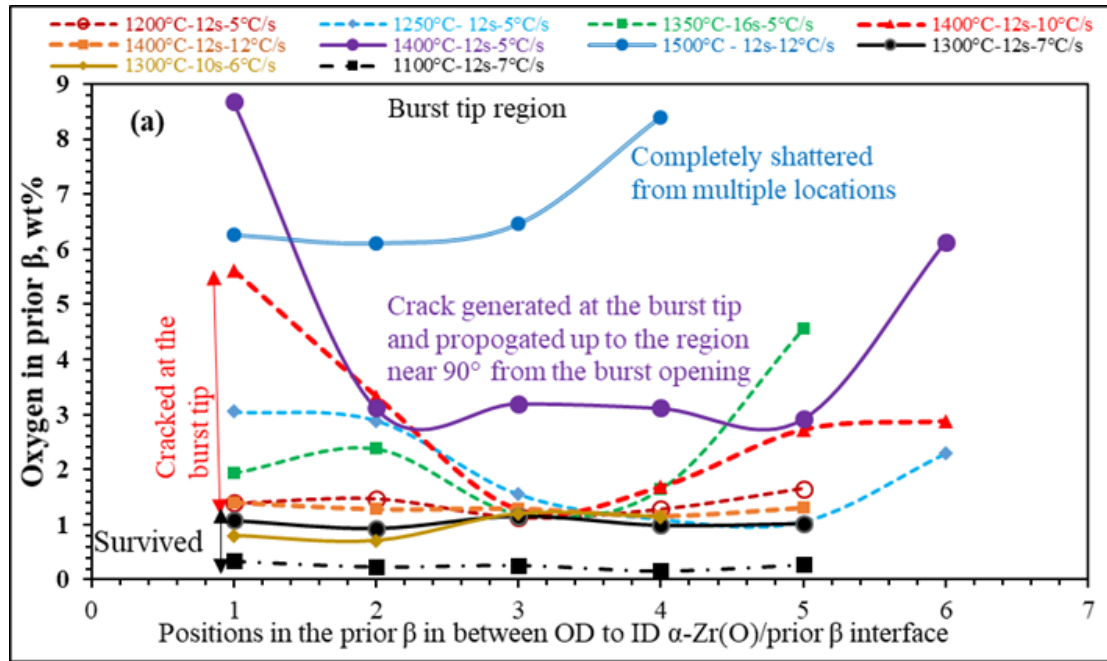
Leistikow correlation used to determine oxygen concentration from Vickers micro-hardness.

Maximum calculated standard error:  $\pm 0.05$  wt.%

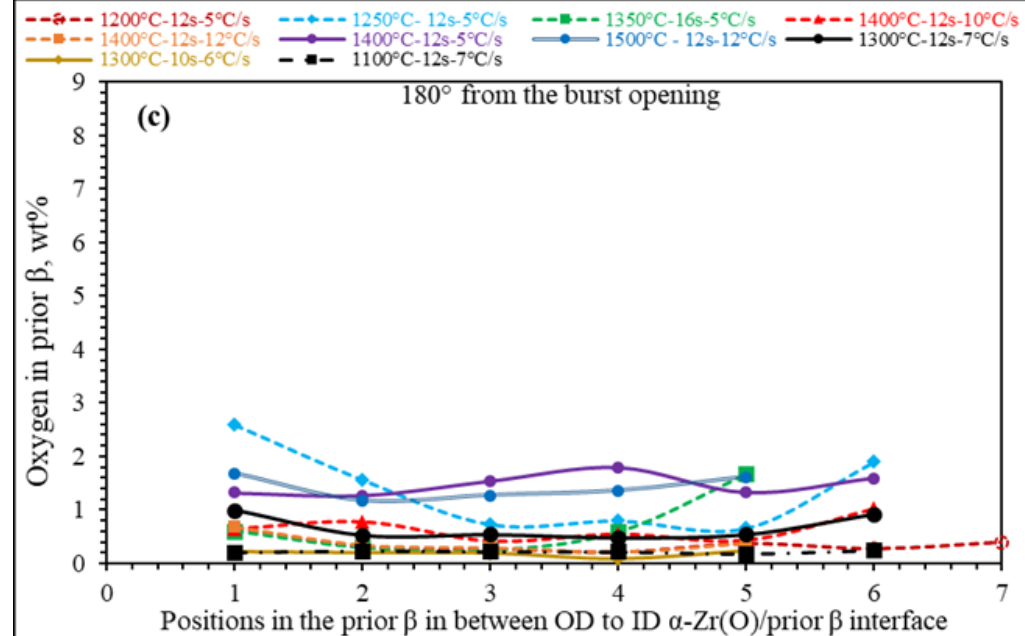




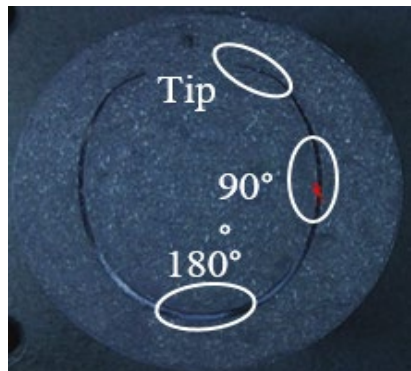
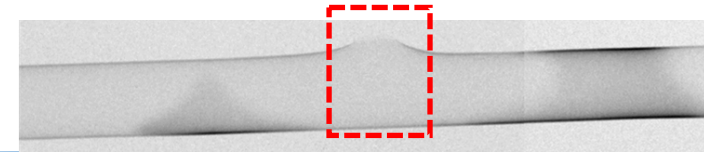
# Oxygen distribution along the circumference



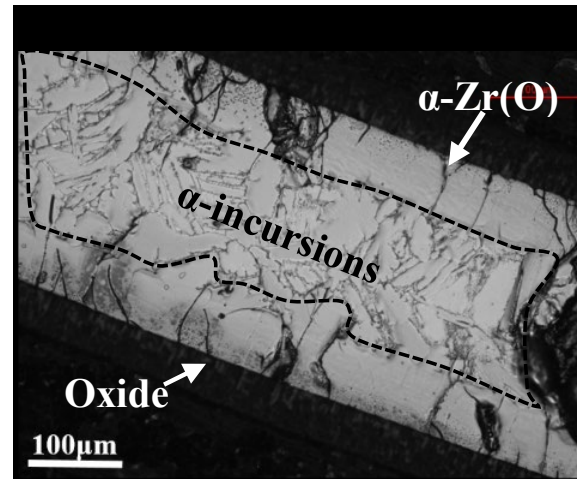
- Oxygen distribution in the prior  $\beta$  layer was non-uniform.
- Maximum non-uniformity & steep concentration gradient was observed in the burst tip region, and
- Non-uniformity progressively decreased in the region circumferentially away from burst tip.



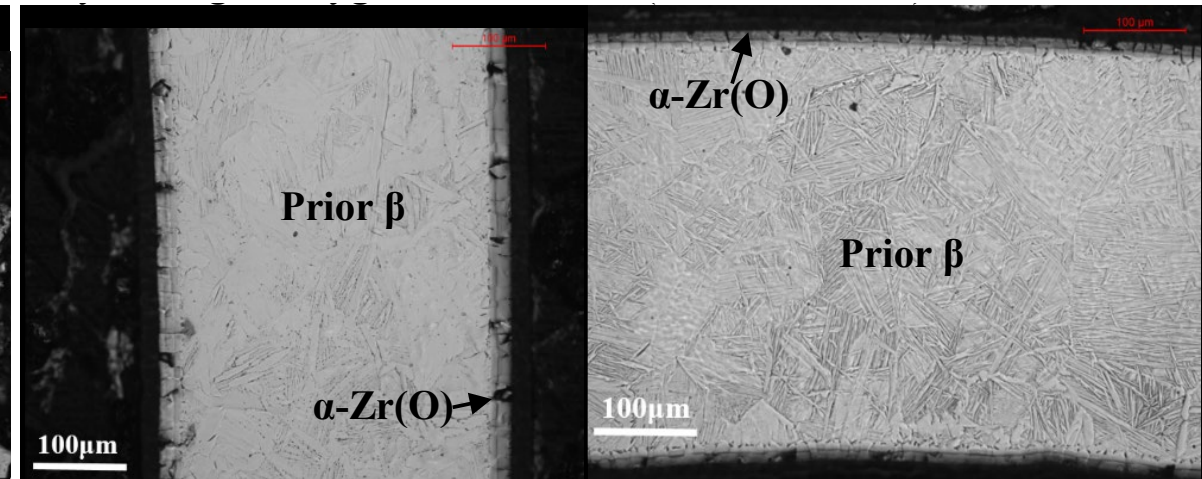
# Microstructure near burst region



9°C/s-1300°C-35s

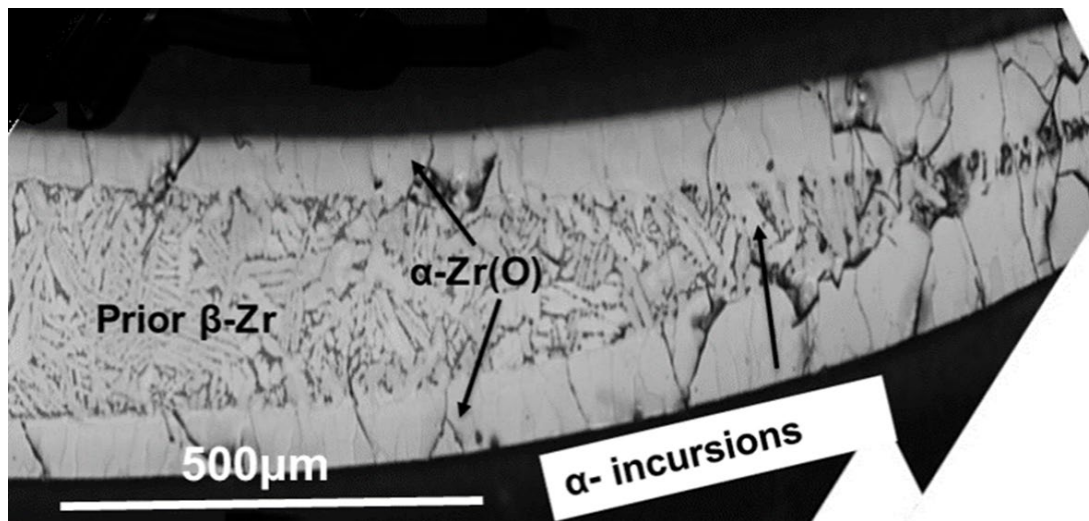


Tip



90°

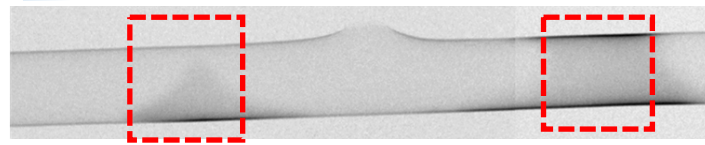
180°



8°C/s-1200°C-12s

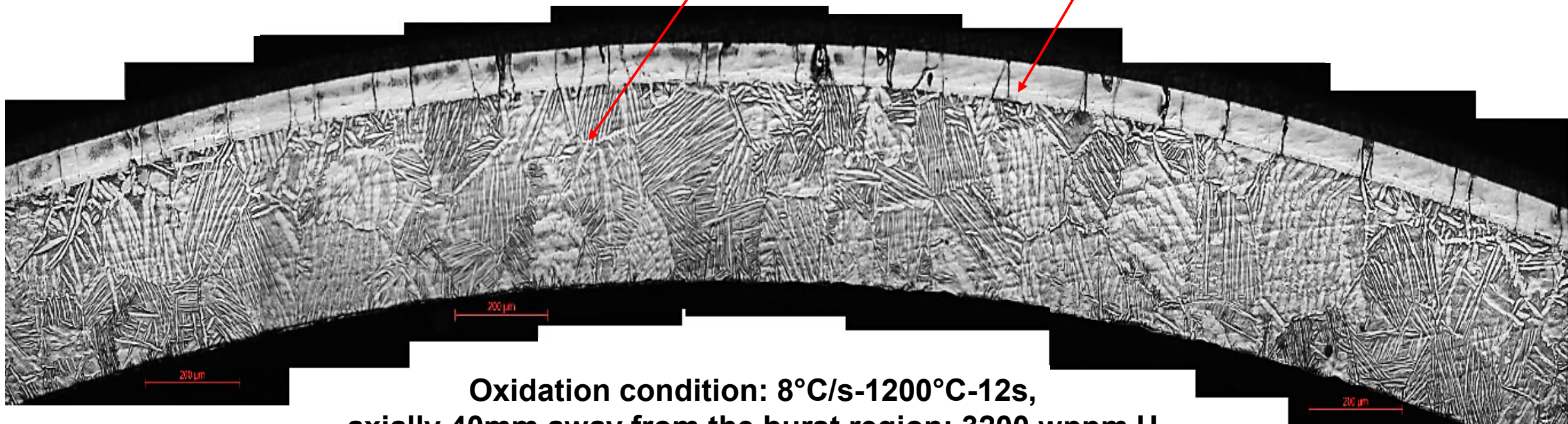
- Heterogeneous microstructure developed around the circumference as a result of azimuthal temperature gradient and localized ballooning deformation.
- $\alpha$ -Zr(O) layer thickness reduced progressively from the burst tip to region opposite to it.
- Maximum oxidation occurred close to the burst tip and minimum opposite to it.

# Microstructure in the secondary hydriding region



Prior  $\beta$ -Zr without  $\alpha$ -Zr (O) incursions/islands

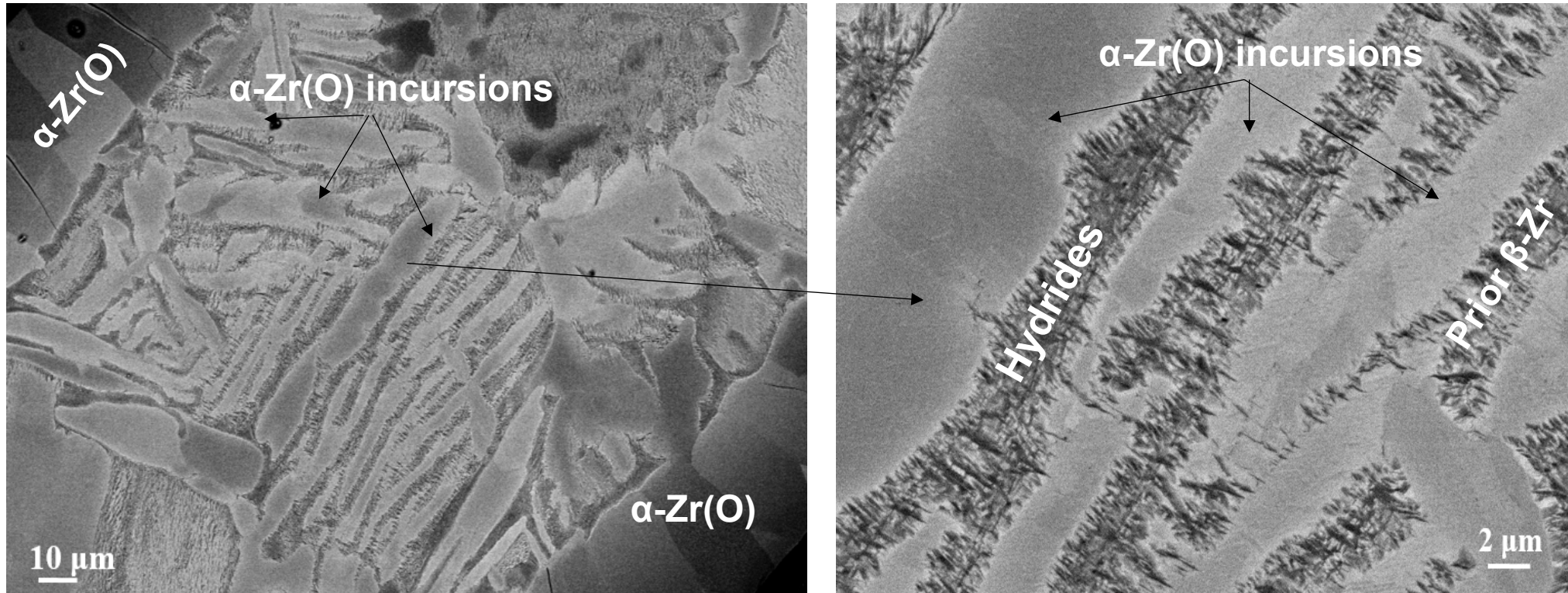
Uniform  $\alpha$ -Zr (O) layer



Oxidation condition:  $8^{\circ}\text{C/s}$ - $1200^{\circ}\text{C}$ - $12\text{s}$ ,  
axially 40mm away from the burst region: 3200 wppm H

- Single sided oxidation occurred.
- No  $\alpha$ -Zr(O) incursions, smooth and regular  $\alpha$ -Zr(O)/prior  $\beta$  interface.
- High hydrogen concentration resulted in relatively thicker prior  $\beta$ -Zr layer.

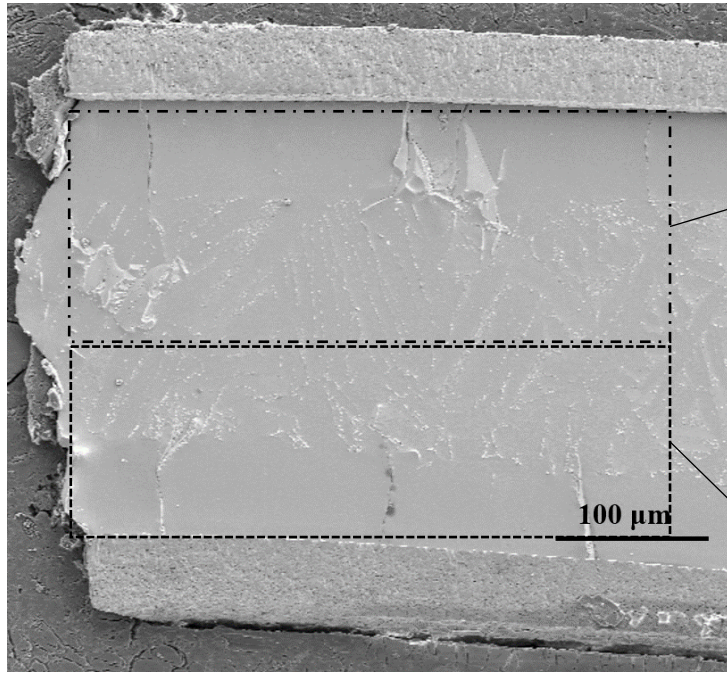
# Hydrides in the burst region



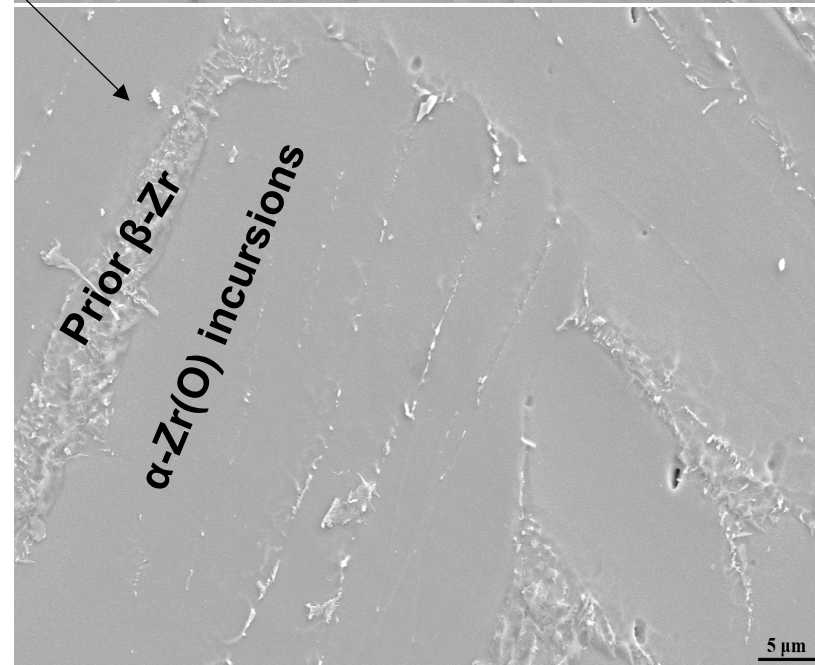
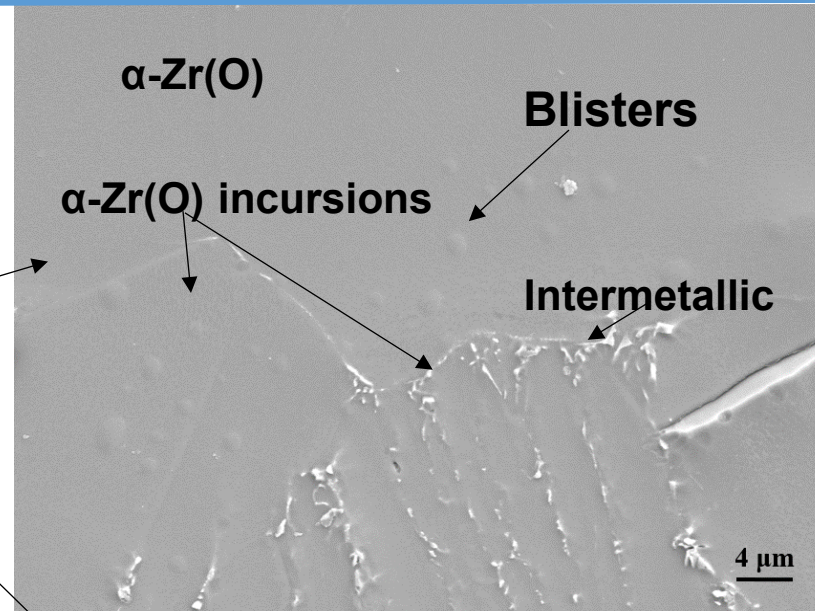
9°C/s-1300°C-35s, O & H in the burst tip region: 1.14 wt.% & 700 wppm respectively

In b/w the  $\alpha$ -Zr(O) intrusions, there were densely packed fine hydrides (<2  $\mu$ m) that took up most of the prior  $\beta$  layer near the burst tip region.

# Hydrides in the burst region



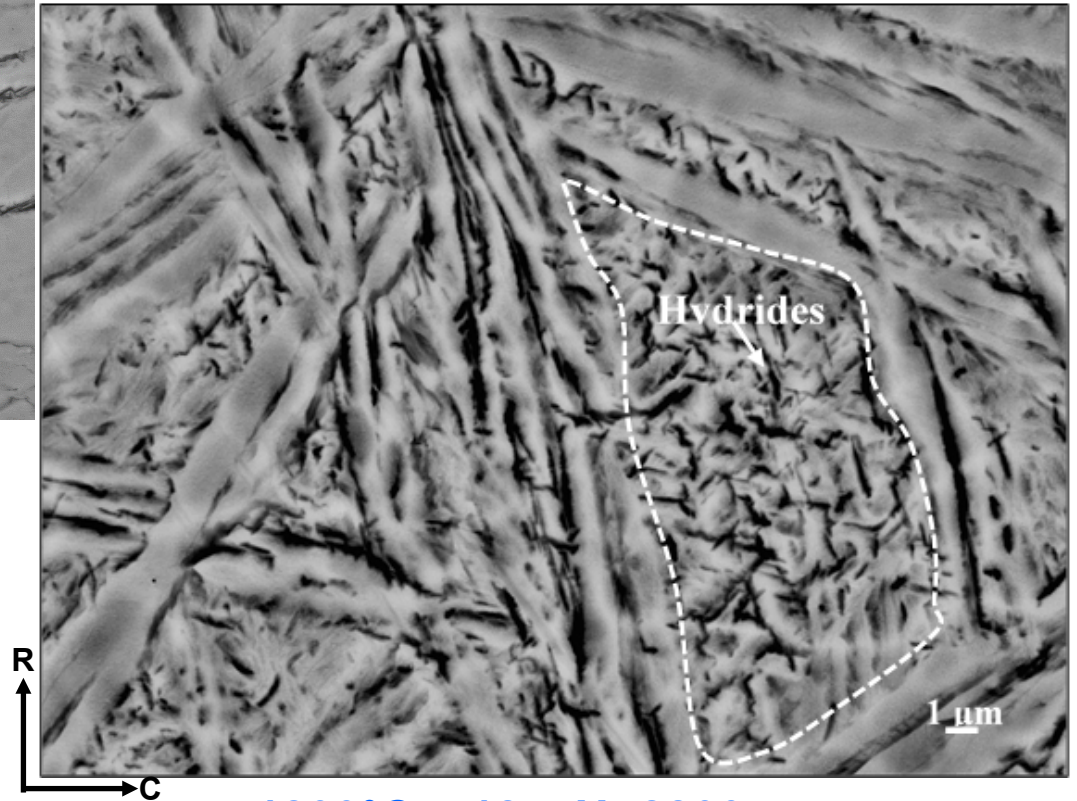
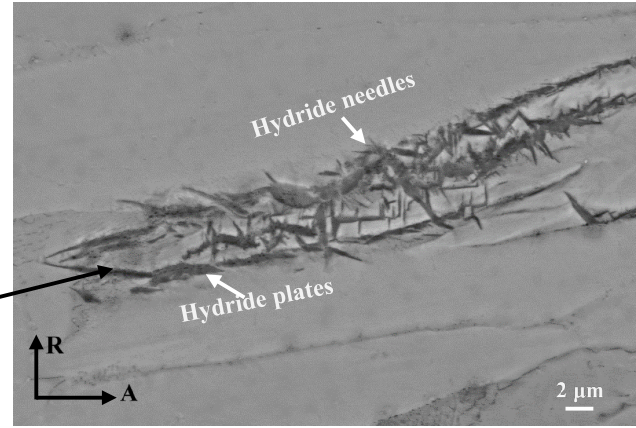
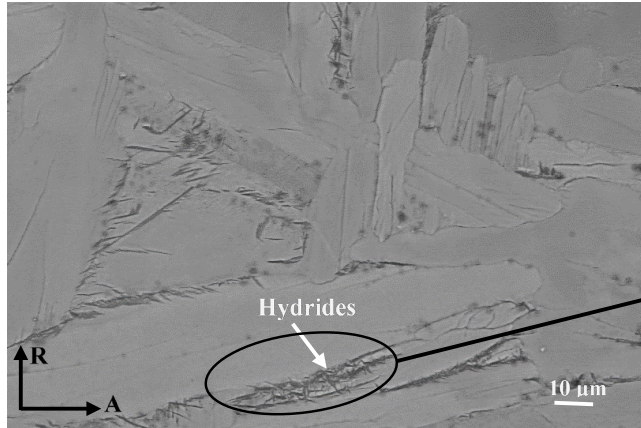
9°C/s-1200°C-12s, O & H in the burst tip region: 1.4 wt.% & 900 wppm respectively



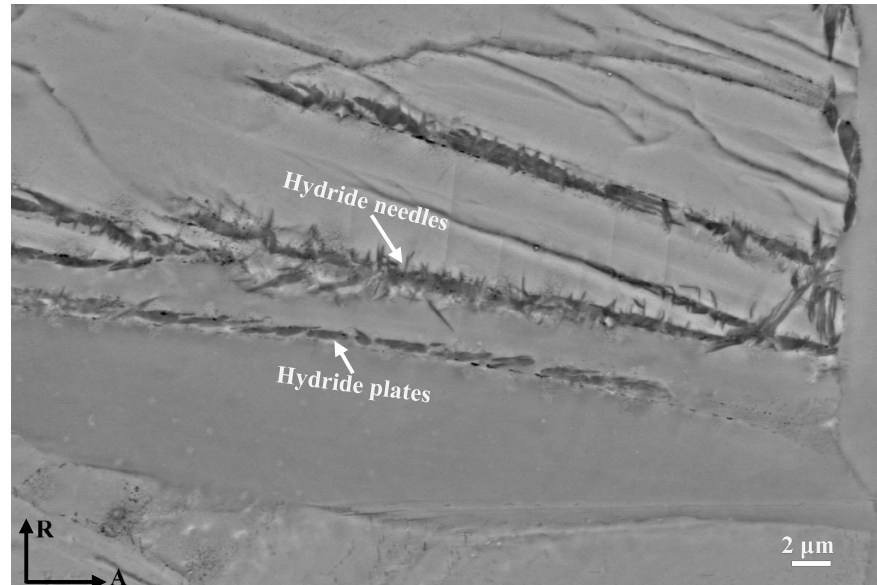
Under the influence of high localised stresses and T gradient, significant amount of hydrogen migrated towards the cladding outer surface and precipitated as hydride blisters.

As O and H concentration increased, hydriding events shift from hydride platelets to hydride blisters.

# Hydrides in the secondary hydriding region



1200°C – 12s, H: 2800 wppm



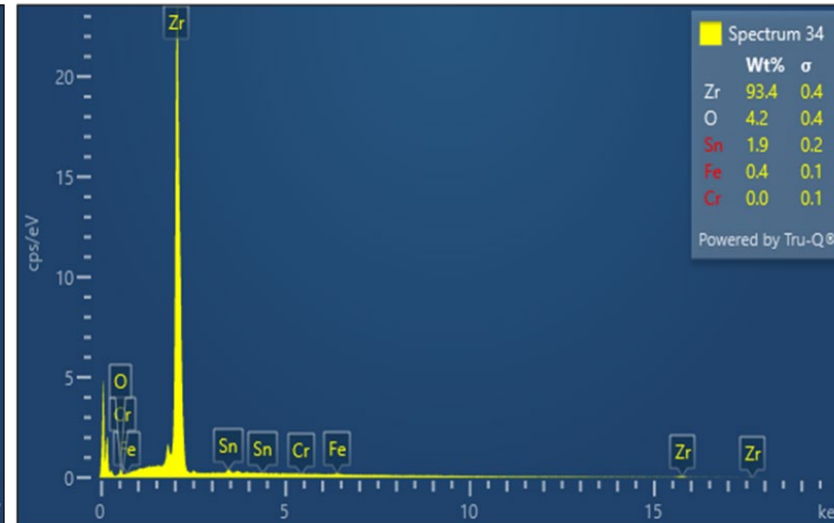
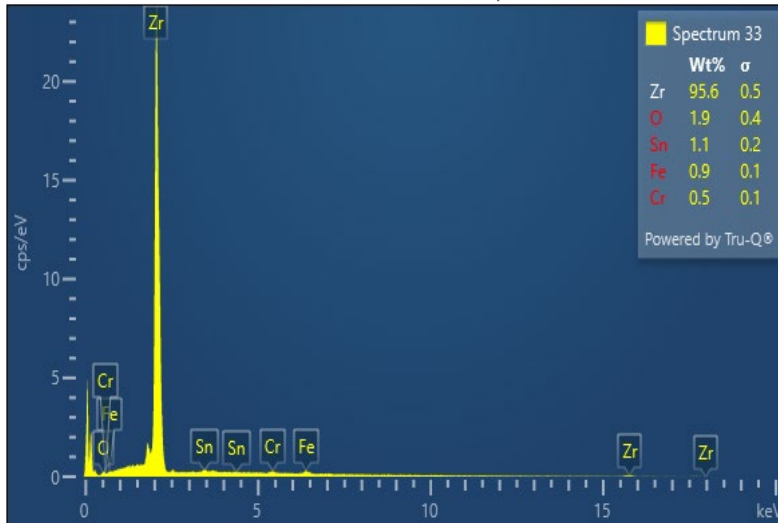
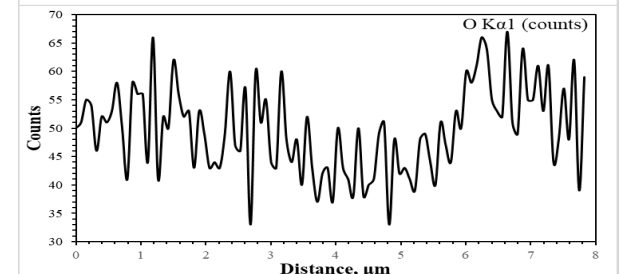
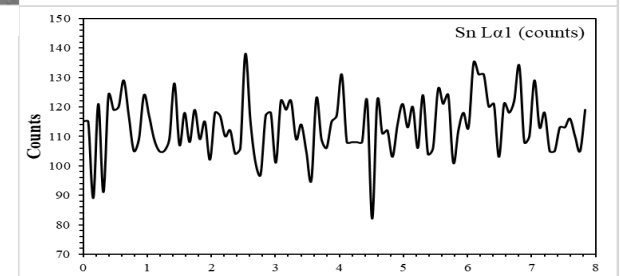
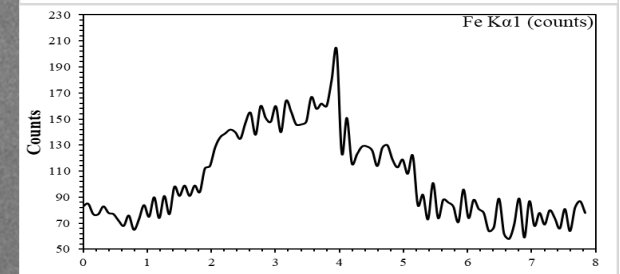
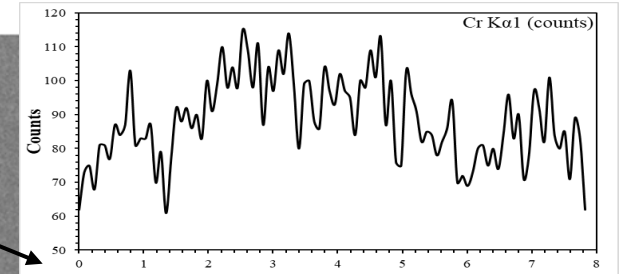
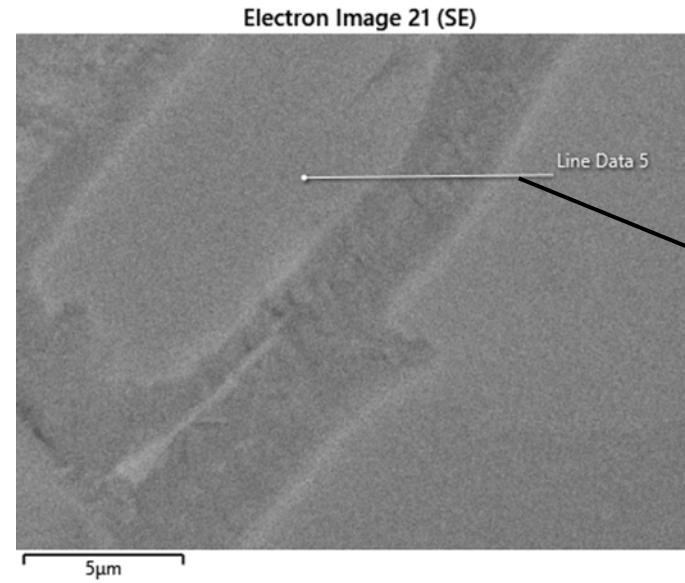
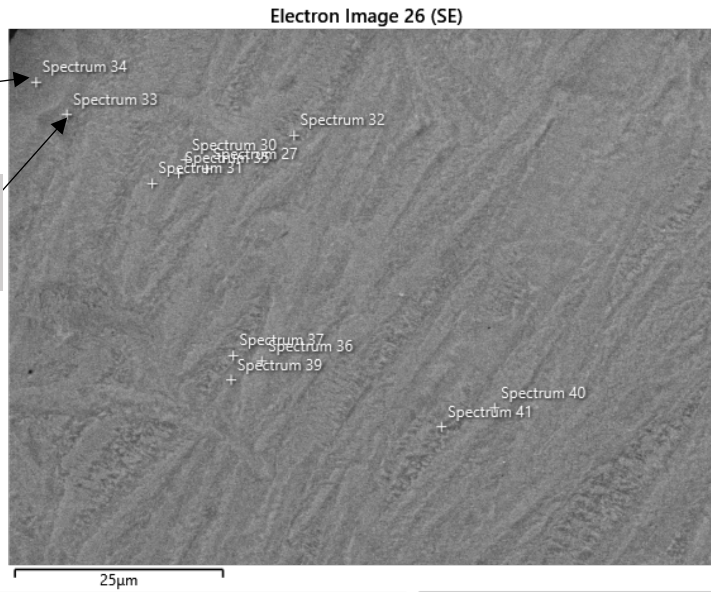
1300°C – 20s, H: 2100 wppm

- Very fine (sub-micron size) hydrides were precipitated.
- Clustering of hydrides also observed.

# Elemental Partitioning

O & Sn-enriched zone

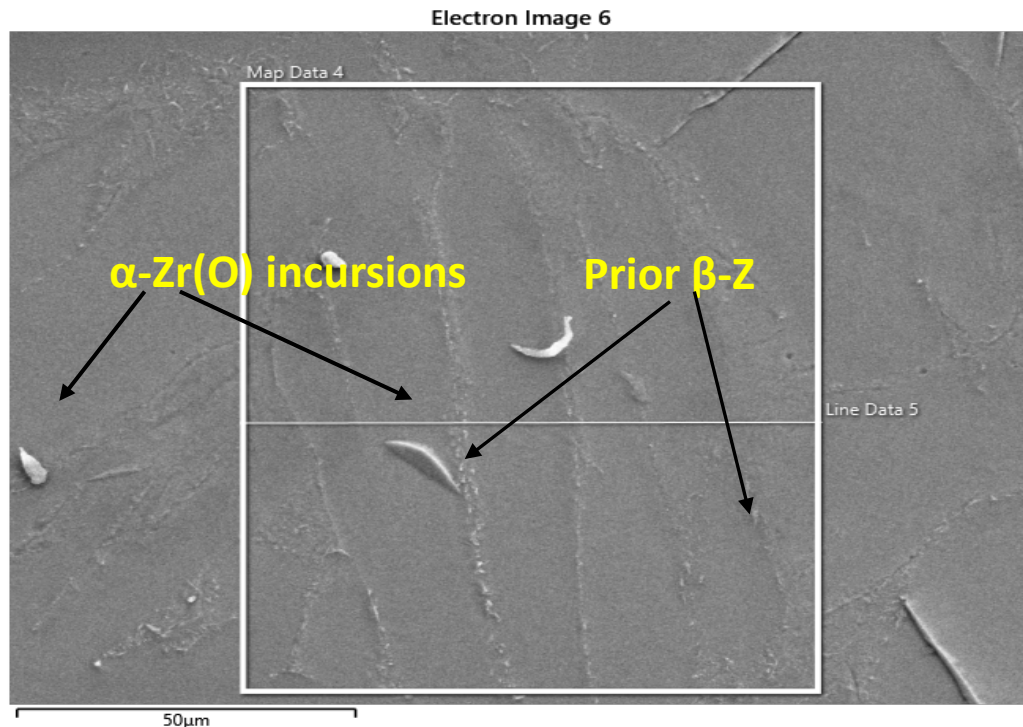
Fe & Cr-enriched zone



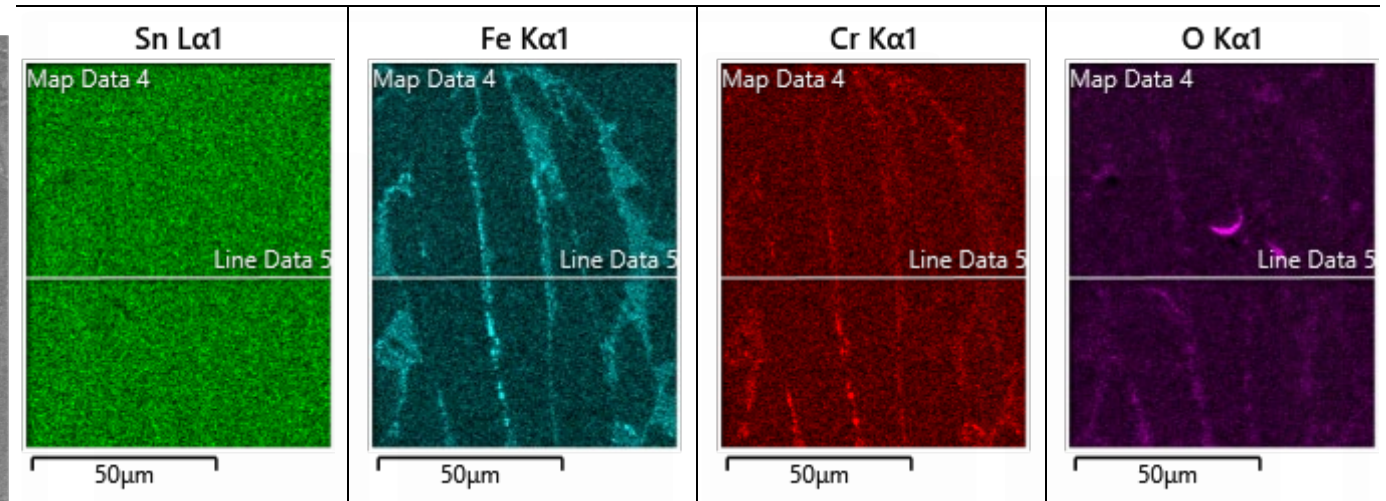
24°C/s-1100°C-12s, O in the burst tip region: 0.25 wt. %

8°C/s-1200°C-12s, O in the burst tip region: 0.7 wt. %

# Elemental Partitioning



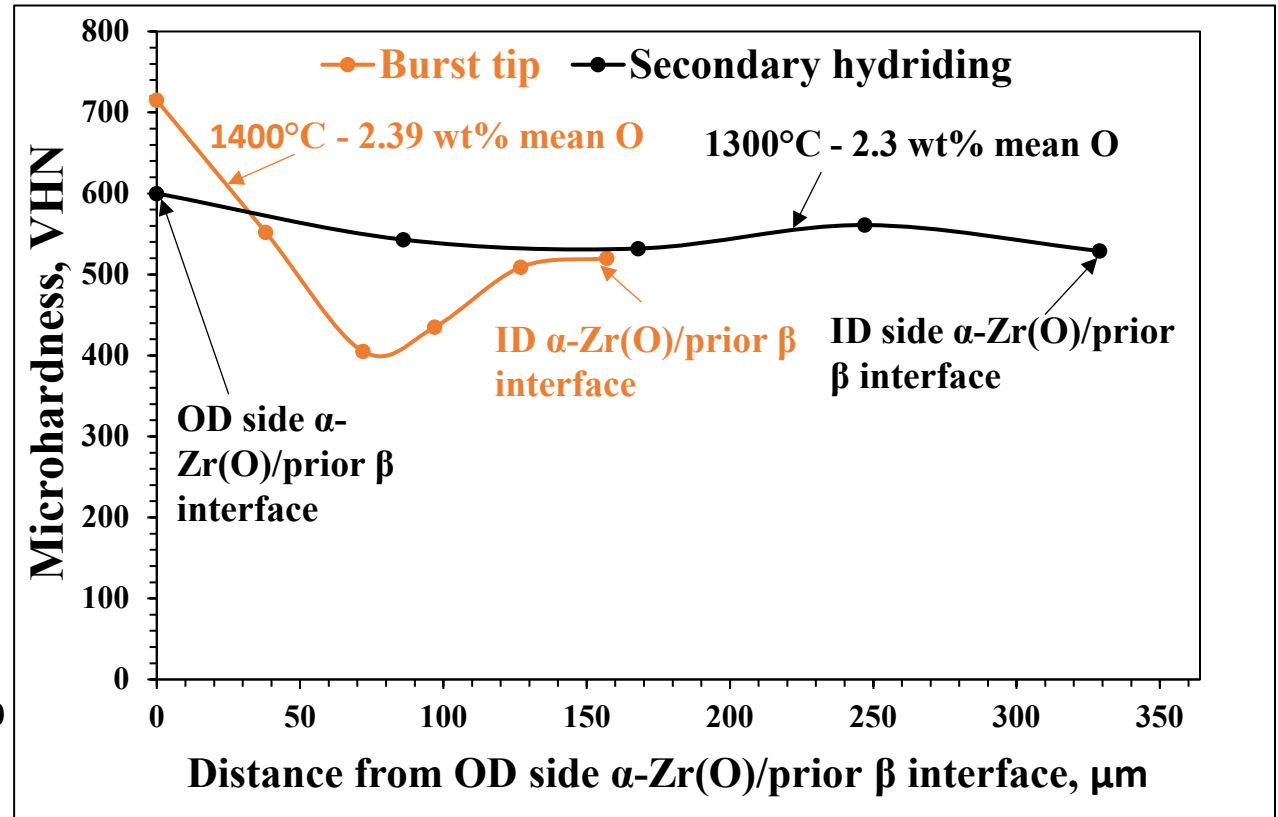
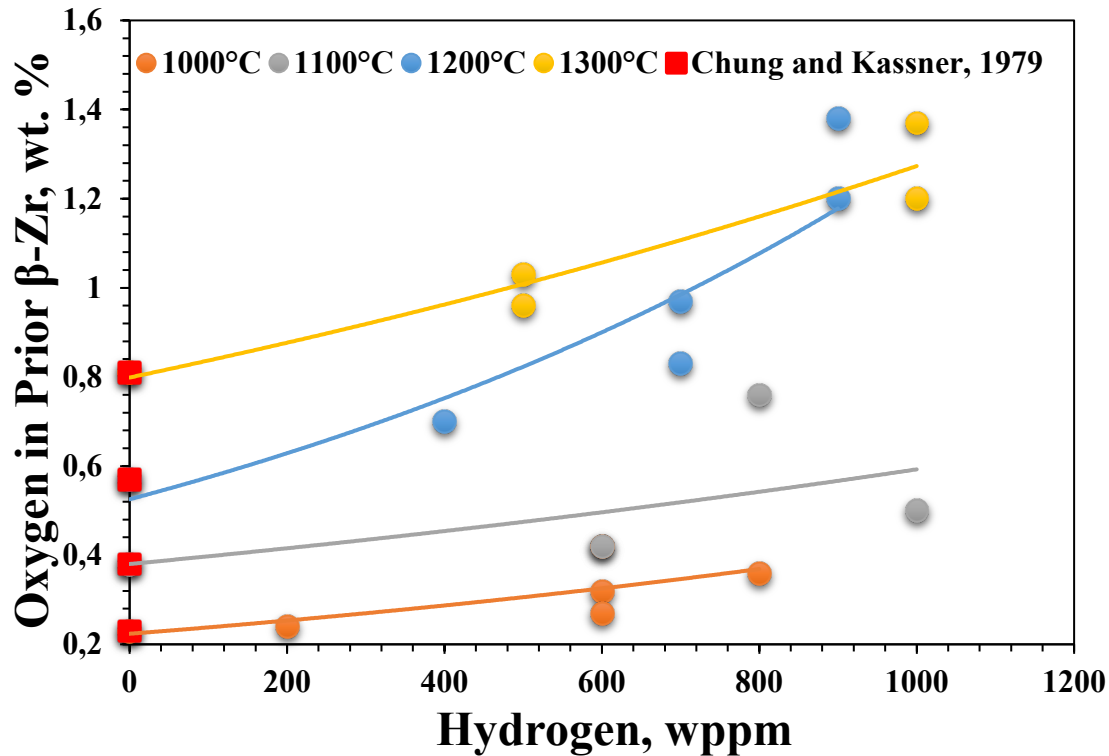
9°C/s-1300°C-12s, O in  
burst tip region- 1.3 wt.%



- O, a potent  $\alpha$ -stabilizing element, concentrates into the first  $\alpha$  platelets to form and encourages the development of " $\alpha$ -Zr(O)-incursions".
- Un-transformed  $\beta$  phase, enriched with  $\beta$ -stabilizing elements like H, Cr, and Fe.
- Sn does not exhibit any discernible partitioning for mean O, 0.7wt.% and beyond.



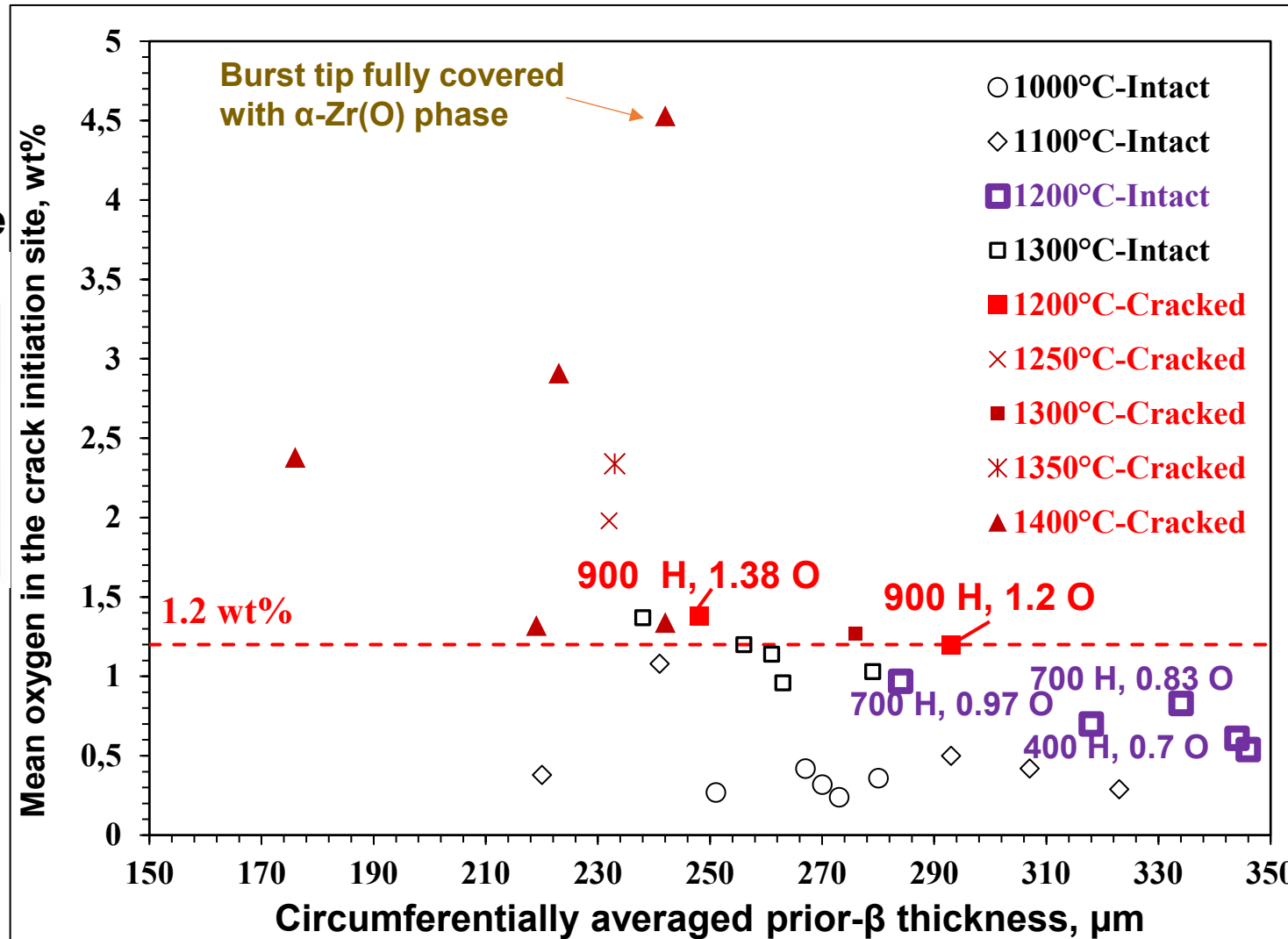
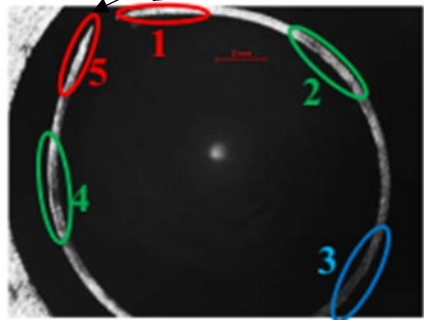
# Influence of hydrogen on oxygen concentration & distribution



- Oxygen content in prior  $\beta$  increased with increased H for a constant oxidation temperature.
- High dissolved hydrogen in the  $\beta$ -Zr increased oxygen diffusivity and solubility in the secondary hydriding zone and delayed oxygen accumulation at the  $\alpha$ -Zr(O)/ $\beta$ -Zr interface, making the entire prior  $\beta$  thickness brittle.

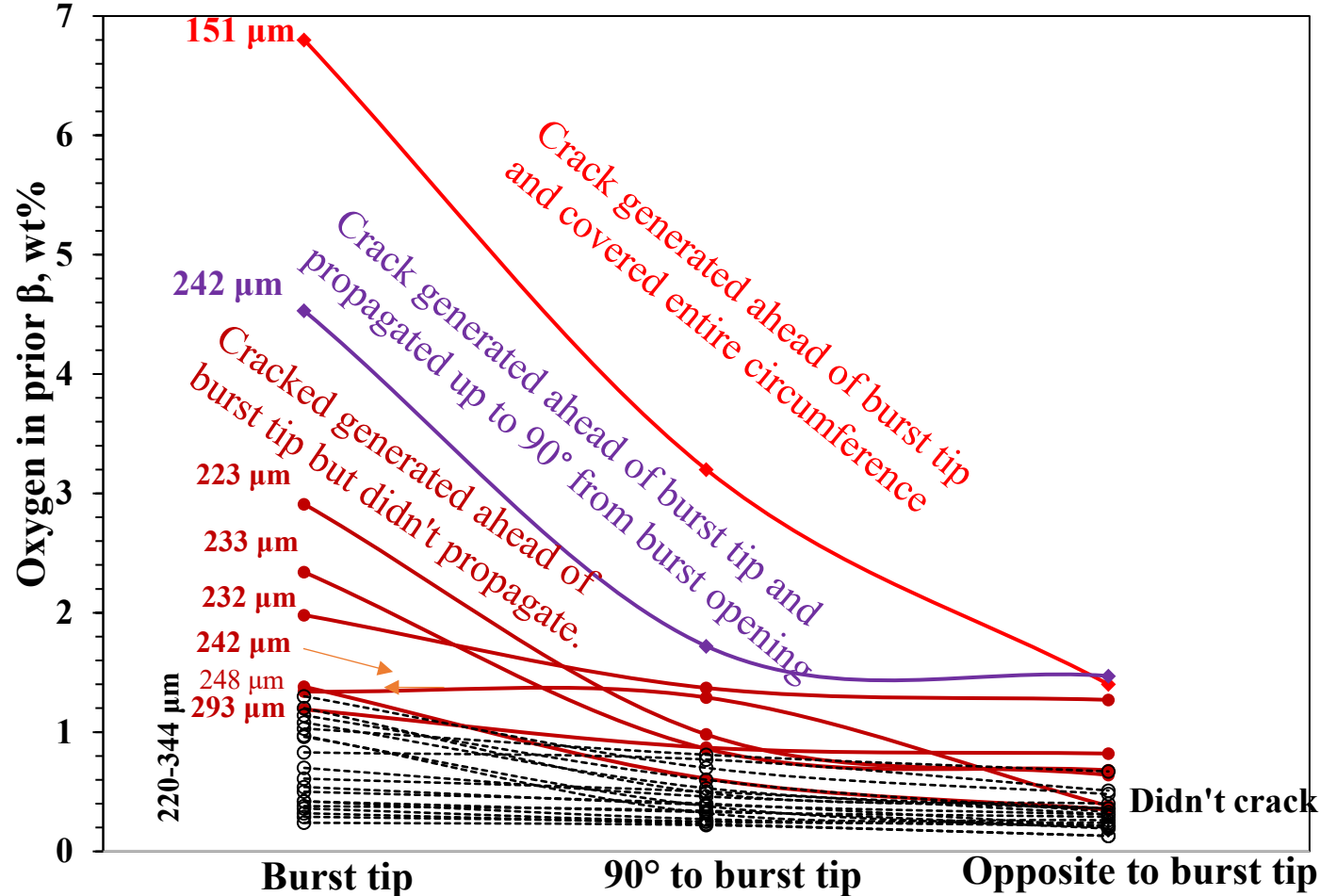
# Crack initiation threshold at the burst tip due to thermal shock

Crack initiation site



- Crack initiation threshold: Oxygen in prior  $\beta$  near the burst tip region 1.2 wt.% .
- There is no effect of hydrogen on thermal shock below 900 wppm.

# Crack propagation during thermal shock

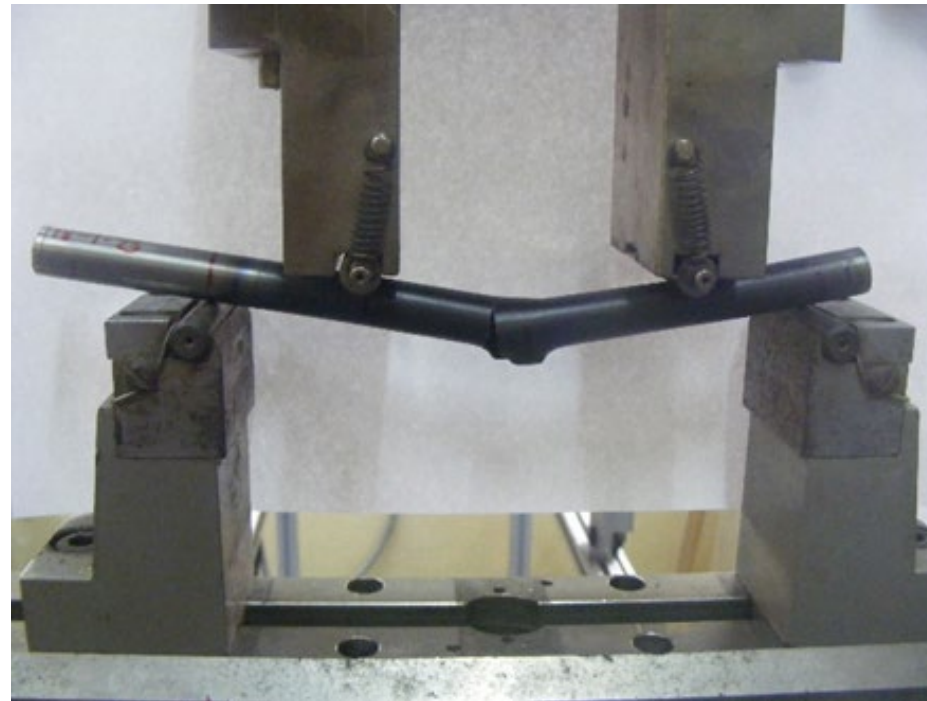


- Circumferential gradient of oxygen concentration existed; highest at the burst tip and lowest at 180°.
- Thermal shock failure initiates at 1.2 wt% oxygen locally in the burst tip region.
- Crack initiated at burst tip could not propagate along the circumference if av. prior  $\beta$  thickness  $>200 \mu\text{m}$

- **Burst tip location was a highly embrittled region on account of synergistic effect of**
  - a. **Thinning of prior  $\beta$  layer due to deformation and formation of thick oxide &  $\alpha$ -Zr(O) layer;**
  - b. **Critical oxygen concentration and**
  - c. **Sharp burst tip acting as a stress raiser.**
  
- **For ballooned and ruptured clad, the threshold for thermal shock failure (crack initiation) 1.2 wt.% O and 900 wppm H.**
  
- **Crack propagation along the circumference stops if av. prior  $\beta$  thickness  $>200 \mu\text{m}$ .**
  
- **Two types of hydride morphologies were observed, viz. hydride blisters near the burst tip and fine hydride platelets near and away from it.**

- **Higher concentration of hydrogen increased the oxygen solubility and diffusivity in the  $\beta$ -Zr at higher temperature, causing**
  - a. **Extensive oxygen partitioning during the cooling from  $\beta$ -Zr to  $\alpha$ -Zr leading to formation of highly embrittled  $\alpha$ -Zr(O) incursions in the burst region.**
  - b. **Oxygen partitioning resulted in segregation of intermetallics along the  $\alpha$ -Zr incursions interfaces.**
  - c. **In the secondary hydriding region high concentration of hydrogen prevented the oxygen built-up near the  $\alpha$ -Zr(O)/prior  $\beta$  interface and flattened the oxygen distribution profile across the prior  $\beta$ -layer, causing brittleness to entire layer.**

**Study of embrittlement mechanism and assessment of fracture strength of integral LOCA tested PHWR cladding using the four-point bend test (4-PBT)**



**Thank you for your attention**



**Anzhelika Khaperskaia**

IAEA

## **Results of the IAEA Coordinated Research Project (CRP) on ‘Testing and Simulation of Advanced Technology and Accident Tolerant Fuels (ATF-TS)’ (2020–2024) and Plans for the Next CRP**

The IAEA Coordinated Research Project on Testing and Simulations for Accident Tolerant and Advanced Technology Fuels (CRP ATF-TS), concluded in 2024, supported Member States in developing and accessing advanced nuclear fuels. Motivated by the Fukushima Daiichi accident, the project focused on near-term ATF solutions, including Cr-coated Zircaloy and FeCrAl claddings and doped fuel pellets, offering safety and operational benefits under normal, design-basis accident (DBA), and design extension conditions (DEC).

CRP ATF-TS encompassed four work tasks: experimental testing of ATF claddings and fuels, benchmarking of fuel performance codes, development of a LOCA fuel safety evaluation methodology, and establishment of an open-source ATF material properties database.

Nine organizations conducted tests on 15 types of ATF cladding materials, including chromium-coated Zr-based alloys, Zr alloys with alternative coatings, FeCrAl alloys, and uncoated Zr alloys (as a reference). Experiments across multiple laboratories generated extensive datasets on ballooning and burst tests, high-temperature oxidation, long-term corrosion, mechanical performance, and bundle tests under extended LOCA and BDBA scenarios. Results showed small benefits in time-to-burst, ballooning size, and burst opening, but improvements in oxidation resistance and post-quench ductility, reducing chemical heat and hydrogen release during hypothetical accidents.

Fuel rod modelling and simulation benchmarks involved 19 organizations from 16 member states, while 9 organizations from 8 member states conducted bundle test simulations for selected ATF concepts, including chromia-doped fuel, FeCrAl claddings, and Cr-coated Zr-alloy claddings. These exercises highlighted the need for modifications to oxidation models for FeCrAl and Cr-coated Zr.

The LOCA evaluation methodology confirmed ATF benefits but also emphasized the need for further improvements in mechanical deformation models and input uncertainties to enhance safety evaluations.

The project also established an open-access material database to support future ATF research and licensing.

The presentation will also summarize outcomes from the proposed new CRP on ATF fuels.

30th International QUENCH Workshop  
Karlsruhe Institute of Technology,  
Germany  
16-18 December 2025

Results of the IAEA CRP on  
'Testing and Simulation of  
Advanced Technology and  
Accident Tolerant Fuels  
(ATF-TS)' (2020–2024)  
and Plans for the Next CRP

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Anzhelika Khaperskaia, Technical Lead  
NFCMS /NEFW, IAEA



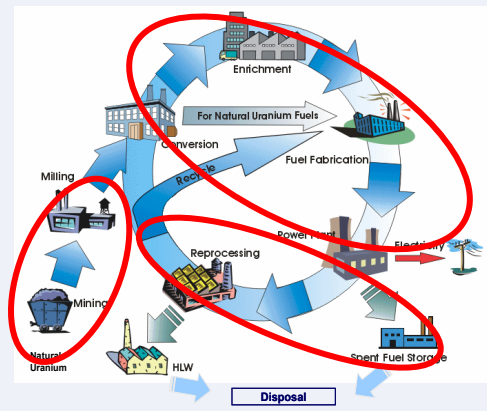
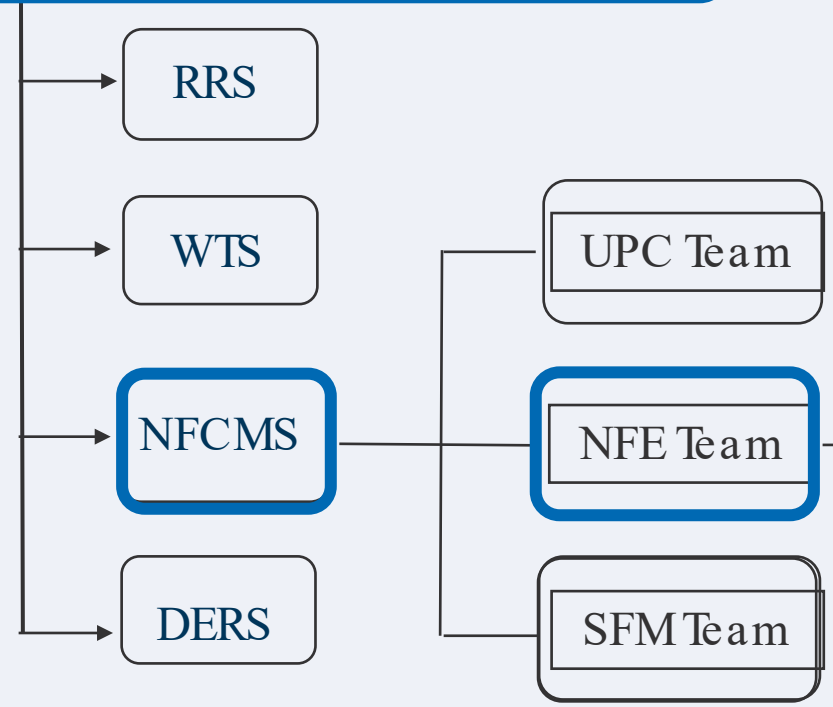
# OUTLINE

- Introduction (IAEA NE structure and activities)
- Completed CRP on ‘Testing and Simulation of Advanced Technology and Accident Tolerant Fuels (ATF-TS)’ (2020–2024)
- Plans for the Next CRP on ATF Testing and Simulation

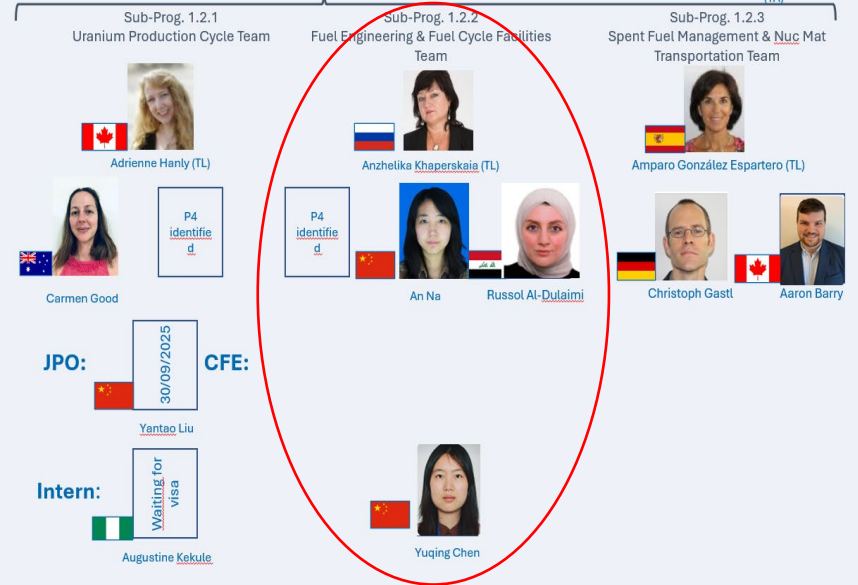
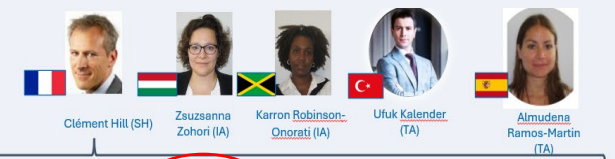
# Nuclear Fuel Cycle and Materials Section (NFCMS)



## Division of Nuclear Fuel Cycle and Waste Technology (NEFW)



### NFCMS today



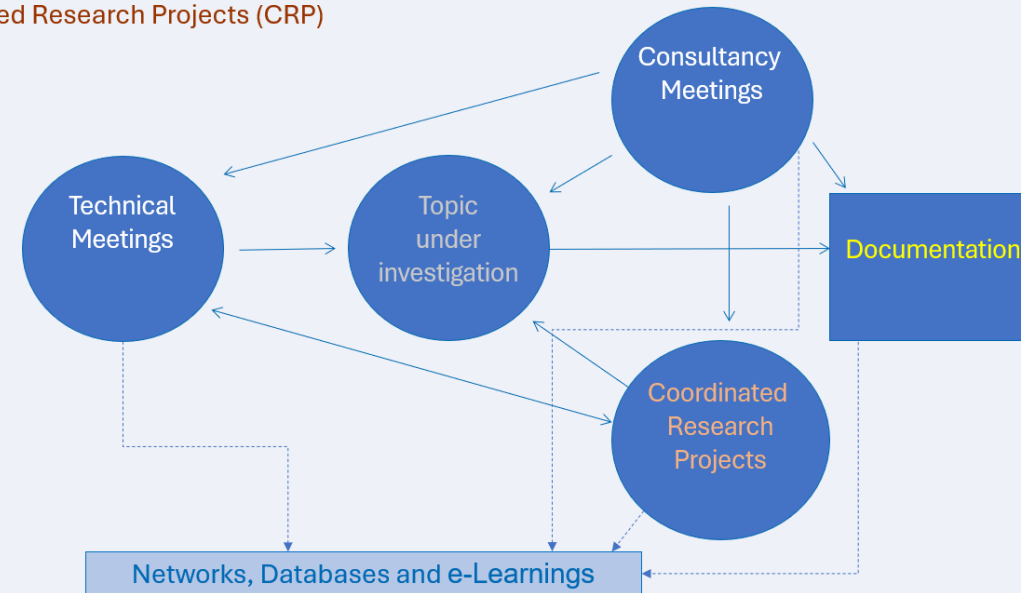
- Project 1.2.2.001 Nuclear Power Reactor Fuel Engineering and Operation: Support Member States (MSs) to understand and address factors affecting the design, fabrication and in-pile behaviour of currently operating and innovative nuclear fuels and materials for power reactors.
- Project 1.2.2.002 Fuel Cycle Facilities Operation and Life Management : Support MSs to technically implement IAEA Safety Standards when operating or upgrading nuclear fuel cycle facilities, and to understand and address factors affecting the ageing of these facilities

# IAEA Sub-Programme 1.2.2: Nuclear Power Reactor Fuel and Fuel Cycle Facilities

- Organizing IAEA meetings and developing IAEA publications
- Coordinating research activities (CRPs)
- Maintaining databases (NFCFs, PIE: [Integrated Nuclear Fuel Cycle Information System - IAEA INFCIS](#)), IAEA Fuel and material database ([The IAEA Fuel and Material Database - IAEA Data Platform](#)) and NFC simulation tools (NFCSS: [Nuclear Fuel Cycle Simulation System \(NFCSS\)](#))
- Developing e-Learning Materials on nuclear fuel and PIE: [OPEN-LMS: All courses](#)
- Building up Networks among experts (NFE-Net): [Pages - NFE Net](#)
- Supporting the IAEA Technical Cooperation Programme

To foster collaboration and information exchange, provide reference data, preserve knowledge, and capacity building

- Consultancy Meetings (Expert Reviews)
- Technical Meetings
- Coordinated Research Projects (CRP)



# Technical Working Group on Fuel Performance and Technology (TWG-FPT)

TWG FPT is a group of recognized experts from MSs providing advice to DDG-NE and supporting programme implementation, reflecting a global network of excellence and expertise in nuclear power reactor fuel engineering

20 Member States (Argentina , Belgium, Brazil, Canada, China, Finland, France, Hungary, India, Japan, Pakistan , RoK, Romania, Russia, South Africa , Spain, Sweden, UK, Ukraine, USA).

TWG-FPT focuses on nuclear fuel and materials technologies with an emphasis on:

- Status and trends in nuclear power reactor fuel technology and performance
- Nuclear core materials research and development, including fuel design, manufacturing, and quality assurance issues, fuel utilization, coolant chemistry, and fuel performance analysis

with consideration for: Safety, Economy, Management systems, Nuclear science, Nuclear power plant operations

TWG-FPT Meeting, 15–17 April 2025



# Technical Working Group on Fuel Cycle Facilities (TWG-FCF)

TWG FCF is a group of recognized experts from MSs providing advice to DDG-NE and DDG-NS and supporting programme implementation, reflecting a global network of excellence and expertise in NFCFs operation areas

20 Member States (Argentina , Belgium, Brazil, Canada, Egypt , France, Germany , India, Japan, Kazakhstan, Netherlands, RoK, Russia, South Africa , Spain, Sweden, UK, Ukraine, USA).

TWG-FCFs focuses on:

- status and trends in nuclear fuel cycle facilities (NFCFs) operation areas, including operating experience, optimization, ageing management, long term operation, refurbishment, modernization, and use for capacity building.

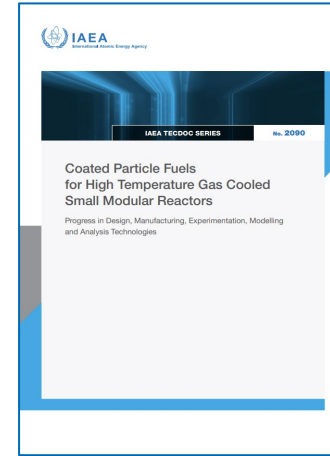
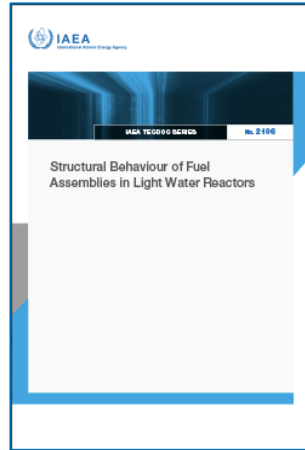
- covers fuel cycle facilities from milling to fuel fabrication, through conversion, enrichment, and re-conversion, as well as nuclear research and development (R&D) related fuel cycle facilities (such as research laboratories, Post Irradiation Examination facilities, etc.).

- with consideration for: Safety, Economy, Management systems

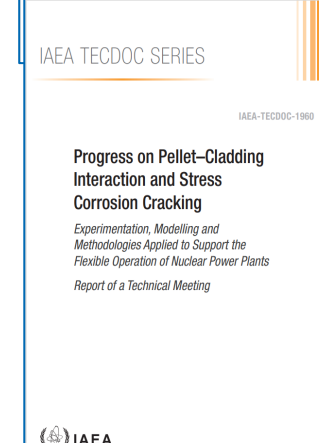
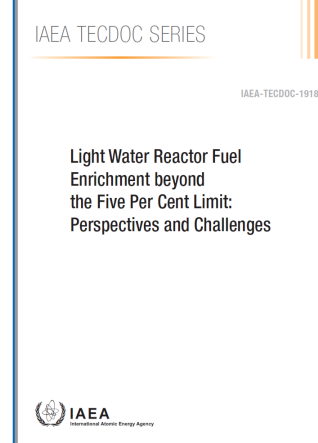
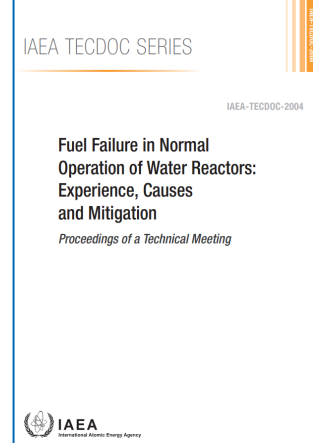
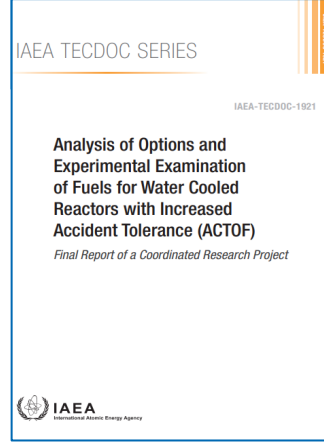
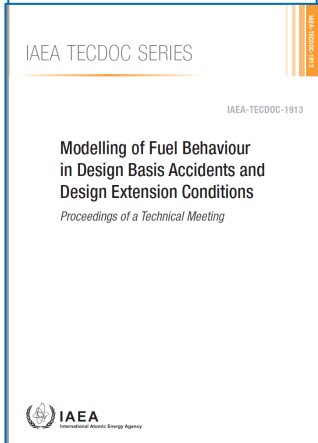
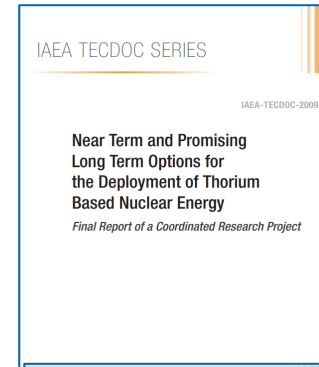
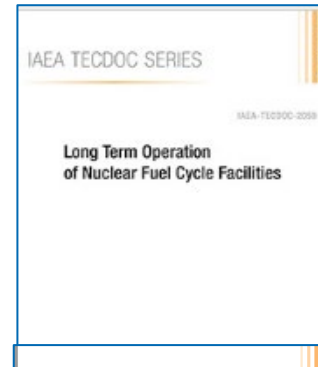
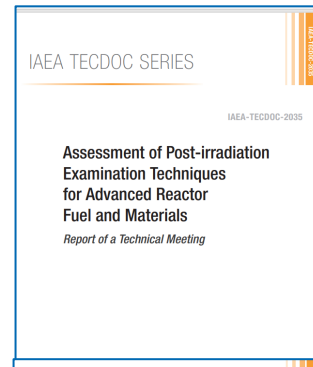
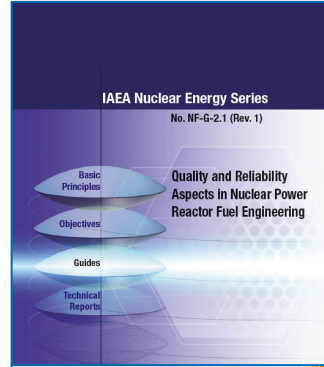
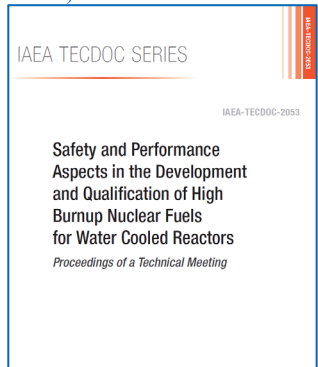
TWG-FCF Meeting, 17-20 June 2025



# Publications on Fuel Engineering & FCF (2020-2025)



IAEA Book on the Metallurgy of Zirconium (3 Volumes)



- IAEA-TECDOC-2106 Structural Behaviour of Fuel Assemblies in Light Water Reactors (2025)
- IAEA-TECDOC-2097 Advances in Fabrication Technologies for Power Reactor Fuels: Proceedings of Technical Meetings held in 2021 and 2023 (2025)
- IAEA-TECDOC-2090 Coated Particle Fuels for High Temperature Gas Cooled Small Modular Reactors (2025)
- IAEA-TECDOC-2059 Long Term Operation of nuclear fuel cycle facilities (2024)
- IAEA-TECDOC-2053 : Safety and Performance Aspects in the Development and Qualification of High Burnup Nuclear Fuels for Water Cooled Reactors (2024)
- IAEA NES No NF-G-2.1: Quality and Reliability Aspects in Nuclear Power Reactor Fuel Engineering (2024)
- IAEA-TECDOC-2035: Assessment of Post-irradiation Examination Techniques for Advanced Reactor Fuel and Materials
- IAEA-TECDOC-2009: Near Term and Promising Long-Term Options for the Deployment of Thorium Based Nuclear Energy - Final Report of a Coordinated Research Project
- IAEA Book on the Metallurgy of Zirconium
- NES NF-T-2.5: Review of Fuel Failures in Water Cooled Reactors in 2006-2015
- IAEA-TECDOC-1889: Fuel Modelling in Accident Conditions - Final Report of a Coordinated Research Project on Fuel Modelling in Accident Conditions – FUMAC, 2014–2018
- IAEA-TECDOC-1918: Light Water Reactor Fuel Enrichment beyond the 5% Limit: Perspectives and Challenges
- IAEA-TECDOC-1942: Coolant Chemistry Control and Effects on Fuel Reliability in Pressurized Heavy Water Reactors
- IAEA-TECDOC-1960: Progress on Pellet-Cladding Interaction and Stress Corrosion Cracking: Experimentation, Modelling and Methodologies Applied to Support the Flexible Operation of Nuclear Power Plants
- IAEA-TECDOC-2004: Fuel Failure in Normal Operation of Water Reactors: Experience, Causes and Mitigation. Proceedings of a Technical meeting

# IAEA ongoing activity to support current generation of nuclear power reactors fuels

## Fuel engineering and operation for current generation of nuclear power reactors

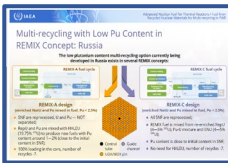
- Accident Tolerant Fuels
  1. **CRP T12032** on “Testing and Simulation of Advanced Technology and Accident Tolerant Fuels (ATF-TS)” (2020-2024)
    2. TM on “Advanced Technology Fuels: Progress on their Design, Manufacturing, Experimentation, Irradiation, and Case Studies for their Industrialization, Safety Evaluation, and Future Prospects” (28-31 October 2025)
    3. **Proposed new CRP** on “Testing and performance simulation of Advanced Technology Fuels (ATF- HBU) (2026 -?)

### Fuels for recycling/multi-recycling

1. TECDOC on “Mixed Oxide Fuels Design, Operation and Management” (in preparation to publishing)
2. IAEA publications on “Challenges and Opportunities in Reprocessed Uranium Fuels” (TECDOC in progress)

### Conventional Water-Cooled Reactor fuels

- 1. NES on “Review of Fuel Failures in Water Cooled Reactors (2016–2020) Rev.1” (preparation for publication)
  2. TM on “Advances in Fuel Design, Manufacturing and Examinations for Pressurized Heavy Water Reactors” (November 2024, Argentina)
  3. TM on “Digitalization and the Use of Artificial Intelligence in Advanced Nuclear Fuel Manufacturing and Quality Control”, June 2026



# IAEA ongoing activities to support advanced reactors fuels development

## Fuel engineering and operation for SMRs and future generations of nuclear power reactors

- Water-cooled SMR fuels

1. TECDOC on “Core and Plant Simulation with an Emphasis on Fuel Behaviour in Light Water Reactor Based Small Modular Reactors” ( based on Workshop 27-29 February 2024, TECDOC in progress )

- Fast reactor fuels

1. **CRP T12031** on “Fuel Materials for Fast Reactors (FMFR)” (2019-2023: Final Report in preparation to publishing)
2. NES Technical Report on “Nuclear Fuel Technologies for Liquid Metal Cooled Fast Reactors (LMFRs)” (in preparation to publishing)
3. Workshop on the “Behaviour of Liquid Metal Cooled Fast Reactors Fuels” (30 June – 04 July 2025)
4. **Proposed new CRP** on “Benchmark Exercises on Testing and Performance Simulation of Advanced Fuels for Liquid Metal-Cooled Fast Reactors” (2026-..)

- HTRs SMR fuels

1. **CRP T12034** on “Fuel Modelling Exercises for Coated Particle Fuel for advanced reactors including SMR”(2024-2029)

### Molten salt SMR fuels

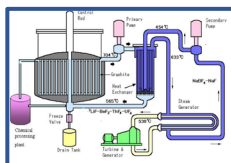
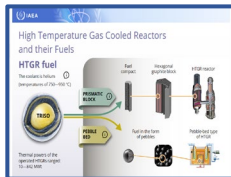
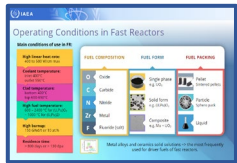
1. New Simulation tool module development for MSR with relevant fuel cycle
2. Workshop on “Molten Salt Reactor Fuel: Recent Development and Future Challenges” (21-25 July 2025)
3. Workshop on “Current Status of Structural Material Development for Molten Salt Reactors and Related Challenges” (July 2026)

### HALEU fuel

1. Workshop on “Operational Aspects of Manufacturing High Assay Low Enriched Uranium Advanced Fuels” (August 2026)

### PIE for SMR fuels

1. **CRP T12033** on “Standardization of Subsized Specimens for Post-Irradiation Examination and Advanced Characterization of Fuel and Structural Materials for Small Modular Reactor and Advanced Reactor Applications (PIE for SMR)”(2024-2028)





# 2026 IAEA Meetings on Nuclear Fuel Engineering

Workshop on the Current Status of Structural Material Development for Molten Salt Reactors and Related Challenges 20–24 July 2026 (Vienna, and virtual participation via Cisco Webex)

Status of MSR technology development with a focus on structural material requirements, Corrosion mechanisms in molten fluoride and chloride salts for MSRs and related fuel cycle applications, Experimental methods and loop testing for structural materials in contact with molten salts, Multi-physics modelling to capture the complex interactions among neutronics, thermal-hydraulics, fuel salt chemistry and materials corrosion phenomena, Advanced manufacturing techniques and robotics. Methods and plans to monitor the integrity of structural materials chosen for MSRs, Lessons learned from pilot-scale MSR projects and industry experience

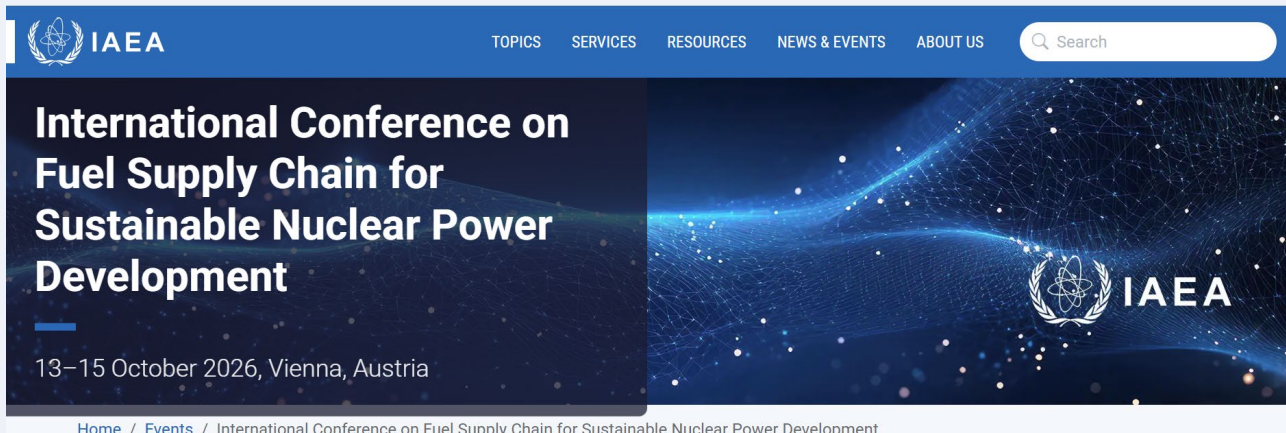
Technical Meeting on Digitalization and the Use of Artificial Intelligence in Advanced Nuclear Fuel Manufacturing and Quality Control, 27-31 July 2026 (Vienna, and virtual participation via Cisco Webex)

AI-based optimisation of fuel and core design; Application of AI/ML in nuclear fuel fabrication and quality control; Application of AI/ML in fuel performance simulation including use of surrogates, and in the material discovering; data management and knowledge retention; Computer and information security, Cross-sectoral insights and best practices from other than nuclear industries experienced in digital and AI technologies

Workshop on Operational Aspects of Manufacturing High Assay Low Enriched Uranium Advanced Fuels, 17–21 August 2026 (Vienna, and virtual participation via Cisco Webex)

National and International Trends Impacting HALEU Deployment, Challenges and Best Practices from Member States, Fabrication Technologies and Process Optimization: Integration of Advanced and Digital Technologies, Criticality Safety and Radiation Protection, Regulatory, Safety, and Security Considerations

# International Conference on Fuel Supply Chain for Sustainable Nuclear Power Development, Vienna, from 13 to 15 October 2026



## Key Deadlines and Dates

### 1 February 2026

- Submission of abstracts through IAEA-INDICO
- Submission of Form B (together with Form A) through the InTouch+ platform

### 31 March 2026

- Notification of acceptance of abstracts for oral or poster presentation

### 10 April 2026

- Submission of Form C (together with Form A) through the InTouch+ platform

[International Conference on Fuel Supply Chain for Sustainable Nuclear Power Development | IAEA](#)

Topic 1. Industry Prospects and Challenges Facing Raising Fuel Supply Demand:

Challenges in supply and front-end services to meet the increasing infrastructure requirements for conversion, enrichment and fuel fabrication

Topic 2. Supply and demand for raw materials for nuclear fuel supply:

Innovations in the front end of the nuclear fuel cycle, from exploration to mining: (new uranium exploration and mining projects, Innovative advancements in uranium exploration and mining, Uranium and thorium resources, processing and mining and the circular economy)

Topic 3. Advanced nuclear fuels for innovative reactor technologies:

Advanced technology fuels and fuels for advanced reactors: design, qualification and operation of ATFs, LEU+ and HALEU fuels, TRISO fuels, fuels for Fast Reactors, MSR and multiple recycling in all types of reactors, advances in nuclear fuel fabrication processes and quality control (automation, additive manufacturing and use of artificial intelligence)

Topic 4. Industrial and Innovative technologies for recycling nuclear materials

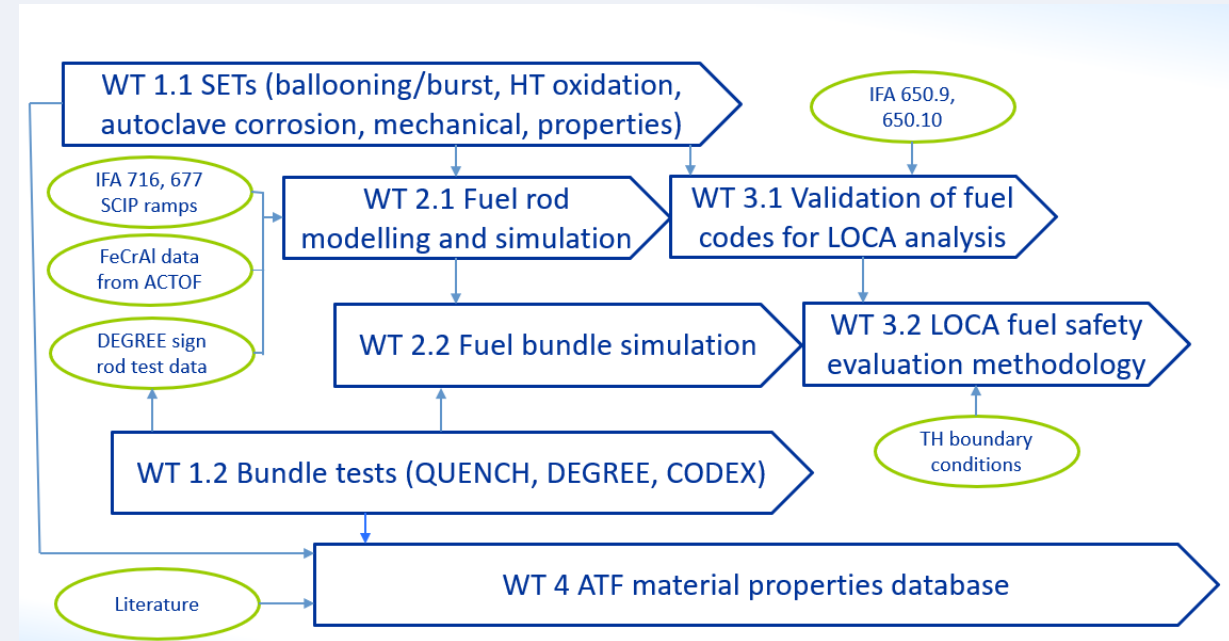
Industrial operating experience and lessons learned in reprocessing for recycling

# CRP T12032 “Testing and Simulation of Accident Tolerant and Advanced Technology Fuels (ATF-TS)” (2020-2024)

## Objectives of the CRP

To support Member States to understand and address factors affecting the design, fabrication and in-pile behaviour of currently operating and innovative nuclear fuels and materials for power reactors, to increase technology readiness for candidate ATF materials

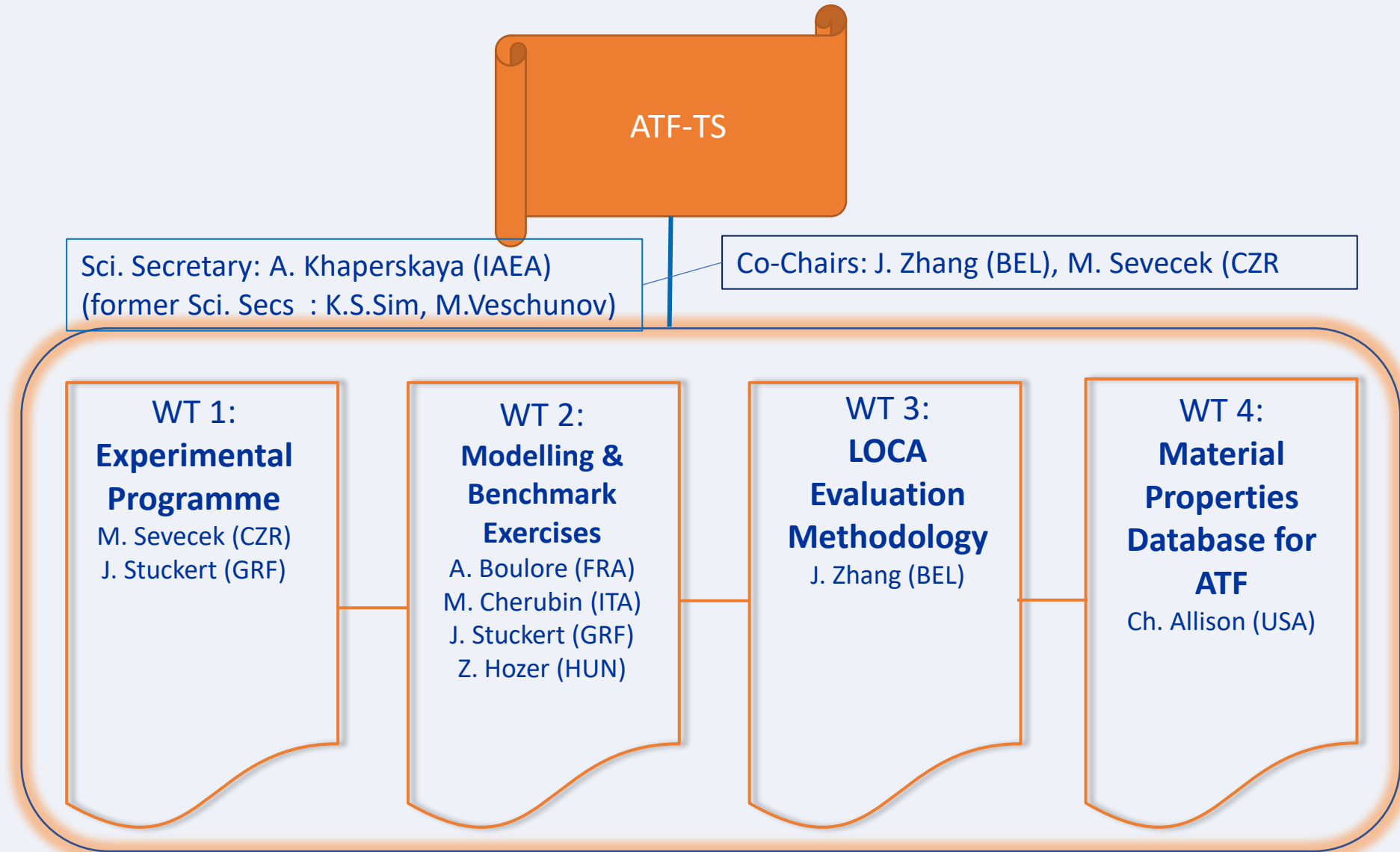
- To perform experimental tests including single rod and bundle tests on ATFs' performance under normal, DB and DE conditions
- To benchmark fuel codes against new test data either obtained during the CRP or from existing data relevant to advanced fuel and cladding concepts from Member States' experimental Programmes
- To develop LOCA evaluation methodology for ATF performance with a view for NPP applications



## Participants: 29 organizations from 22 Member States

Argentina (CNEA), Belgium (Tractebel), Belarus (BSU), Brazil (IPEN/CNEN), Bulgaria (INRNE), Canada (CNL), China (CNPRI, CNPE, NPIC), Czech Republic (CTU), France (CEA), Germany (KIT, GRS), EC (JRC), Hungary (EK), Iran (AEOI), Italy (NINE), Japan (CRIEPI), Korea (KAERI), Poland (IChTj), Russia (IBRAE RAS), Spain (UPM, CIEMAT), Slovakia (B&J NUCLEAR ltd.), UK (NNL), USA (ISSS, UTK)

# CRP T12032 “ATF-TS” structure



# CRP T12032 “Testing and Simulation of Accident Tolerant and Advanced Technology Fuels (ATF-TS) (2020-2024)

## Results achieved

Various ATF options were analyzed resulting in improved understanding of ATFs’ behaviors and developments of ATF technologies in MSs.

Several coated cladding materials (coated Zircaloy claddings, FeCrAl) were manufactured, tested, characterized and analyzed.

Fuel performance codes and severe accident codes from participating organizations were extended to the analysis of several ATF concepts.

The qualified fuel rod codes to develop a hot rod LOCA fuel safety evaluation methodology were applied to assess the performance of ATFs.

The open-source ATF material properties and experimental datasets have been prepared and uploaded the IAEA fuel database

The TECDOC “Testing and Simulation for Advanced Technology and Accident Tolerant Fuels (ATF-TS). Final Report of a Coordinated Research Project” with 3 volumes:

- Vol. 1; Experimental Programme of Accident Tolerant and Advanced Technology Fuels (ATFs);
- Vol. 2: Fuel Modelling and Computer Codes’ Benchmark Exercise for Accident Tolerant and Advanced Technology Fuels (ATFs);
- Vol. 3: LOCA Fuel Safety Evaluation for Accident Tolerant and Advanced Technology Fuels (ATFs).

Under preparation to publication



# CRP ATF-TS: Work Task 1 - experimental programme

9 organizations tested 15 types of ATF cladding materials, including chromium-coated Zr-based alloys, Zr-based alloys with alternative coatings, and FeCrAl alloys. Reference uncoated Zr-based alloys were also tested to establish a baseline for comparison.

**ATF CLADDING MATERIALS TESTED WITHIN THE CRP ATF-TS**

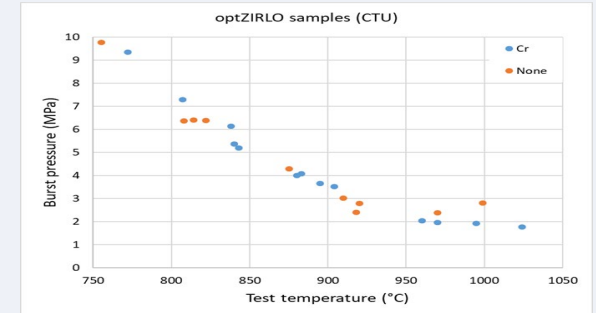
Institute	Country	Coated Zr-based Cladding	Alternative materials
Czech Technical University in Prague	Czech Republic	Cr and CrN-Cr coated Opt. ZIRLO™	
Karlsruhe Institute of Technology (KIT)	Germany	Cr-coated ZIRLO, M5 and Zircaloy-4	FeCrAl B136Y3 – 13Cr-6.2Al-0.03Y (wt.%)
Institute of Nuclear Chemistry and Technology (INCT)	Poland	SiC/ YAG coated Zr1Nb	
Canadian Nuclear Laboratories	Canada	TiAl-coated Zircaloy-4	
Nuclear Power Institute of China	China	Cr-coated Zircaloy-4	FeCrAl 13Cr-4.5Al-2Mo-1Nb-0.4Ta-0.05Y (wt%)
China Nuclear Power Engineering	China	Cr-coated Zircaloy-4	
Belarusian State University	Belarus	Cr-coated and plasma-treated E110	
Atomic Energy Organization of Iran	Iran, Islamic Republic of	Cr and CrN/Cr coated Zr1Nb	

**ATF CLADDING TESTS WITHIN THE CRP ATF-TS**

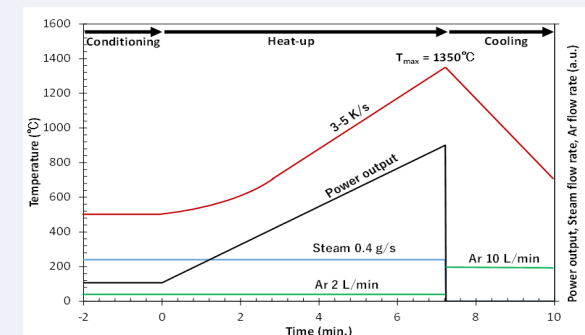
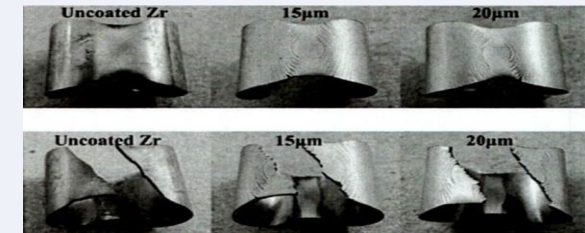
Organization	Country	Experiments Performed
CTU/UJP Praha	Czech Republic	Ballooning/burst tests; high-temperature (HT) steam oxidation; long-term VVER corrosion
JRC Karlsruhe	European Commission	Thermophysical properties
JRC Petten	European Commission	Mechanical tests in the LWR environment
CRIEPI	Japan	Single rod and bundle tests at DEGREE
KIT	Germany	Single rod and bundle tests at QUENCH
INCT	Poland	Neutron activation analysis; long-term corrosion; HT annealing
CNPE	China	Long-term corrosion (PWR); HT oxidation; ballooning/burst
AEOI	Iran	HT oxidation
China Nuclear Power Technology Research Institute (CNPRI)	China	Axial tensile tests; internal burst tests; internal climb tests; autoclave corrosion tests; HT steam oxidation
EK, Centre for Energy Research	Hungary	Ballooning/burst tests; mandrel tests; HT steam oxidation; bundle tests at CODEX-ATF
Universidad Politécnica de Madrid (UPM)	Spain	Cathodic charge; hydriding; ring compression tests; HT creep
Korea Atomic Energy Research Institute (KAERI)	Korea	Microstructural investigations
Seoul National University (SNU)	Korea	LOCA tests; DSC; post-quench ductility evaluation

# CRP ATF-TS: experimental programme: key findings

- Cr-based Coatings: Provided small benefits in time-to-burst, ballooning size, and burst opening, highly dependent on coating quality and methodology used for evaluation
- HT Oxidation Resistance: Both Cr-coated Zr and FeCrAl cladding materials significantly improved oxidation resistance and post-quench ductility, reducing chemical heat and hydrogen release in hypothetical accidents (DBA-A and DEC-A)
- Long-Term Corrosion: Negligible corrosion rates for Cr-based coatings and FeCrAl in all environments
- Mechanical Tests: Showed general agreement across laboratories, with coated Zr claddings performing well in various states. Coated Zr claddings generally exhibited higher strength and lower elongation. Highlighted different coating fracture limits due to microstructure variations. Effects of coating defects and cracks on coated Zr need further investigation
- Supplementary Tests: Demonstrated good resistance of coatings in thermal shock tests. Provided new data on Cr coating mechanical properties and degradation. Indicated that hydrogen uptake mechanisms for coated Zr cladding are not well understood
- Bundle Tests: Proved benefits of Cr-coated claddings in extended LOCA conditions. Revealed significant challenges in DEC after protective coatings fail. Suggested potential benefits of diffusion barriers to limit degradation mechanisms



Item	S1*	S2	S3	S4	S5	S6
Coating thickness and materials	-	10 µm Cr	20 µm Cr	16/10 µm Cr/CrN	10 µm Cr	20 µm Cr
Max. Temp. (°C)	1350			1600		
Steam flow rate (g/s)	0.41	0.41	0.46	0.46	0.50	0.46
Heating rate (K/s)*	3.5-1.5	1.5	2.4-1.8	2.5-2.2	3.0-1.6	3.0-1.8
RIP at RT (MPa, He)	6.0					
Gas plenum volume (ml)	10	15		10		



# CRP ATF-TS : Work Task 2 - Fuel modelling and Benchmark Exercise

19 organizations from 16 MSs participated in fuel rod modelling and simulation benchmarks, and 9 organizations from 8 MSs participated in bundle tests simulation, focusing on selected ATF concepts (Chromia doped fuel, FeCrAl, and Cr-coated claddings)

Benchmark of codes for simulation of selected separate effect tests (WT2.1)

Organization	Country	Code	UO2 Cr- doped			FeCrAl	Coated Zr claddings	Coated Zr claddings
			IFA716	IFA677	SCIP II power ramps	ACTOF cases + ATF-TS SET	ATF-TS SET	DEGREE Single rod test
CNEA	Argentina	DIONISIO	x	x	x	x	x	x
Tractebel	Belgium	FRAPCON/ FRAPTRAN					x	
IPEN	Brazil	TRANSURANUS				x		
INRNE-BAS	Bulgaria	TRANSURANUS				x		
CNPRI	China	JASMINE	x	x		x	x	
CNPE	China	FRAPCON/ FRAPTRAN				x		
NPIC	China	FUPAC	x	x		x	x	
CTU	Czech Republic	FRAPCON/ FRAPTRAN TRANSURANUS	x		x		x	
CEA	France	ALCYONE	x	x	x			
GRS	Germany	TESPA-ROD				x		
ANCC	Iran	PARS/PART	x	x	x		x	
NINE	Italy	TRANSURANUS	x	x	x	x		
CRIEPI	Japan	FRAPCON						x
KAERI	Korea	FRAPCON/ MERCURY	x			x	x	x
IBRAE	Russia	SOCRAT					x	x
B&J	Slovakia	FEMAXI	x	x	x			
UPM	Spain	TRANSURANUS				x		
CIEMAT	Spain	FRAPCON/ FRAPTRAN	x	x	x	x		
UTK	USA	BISON	x	x	x	x		

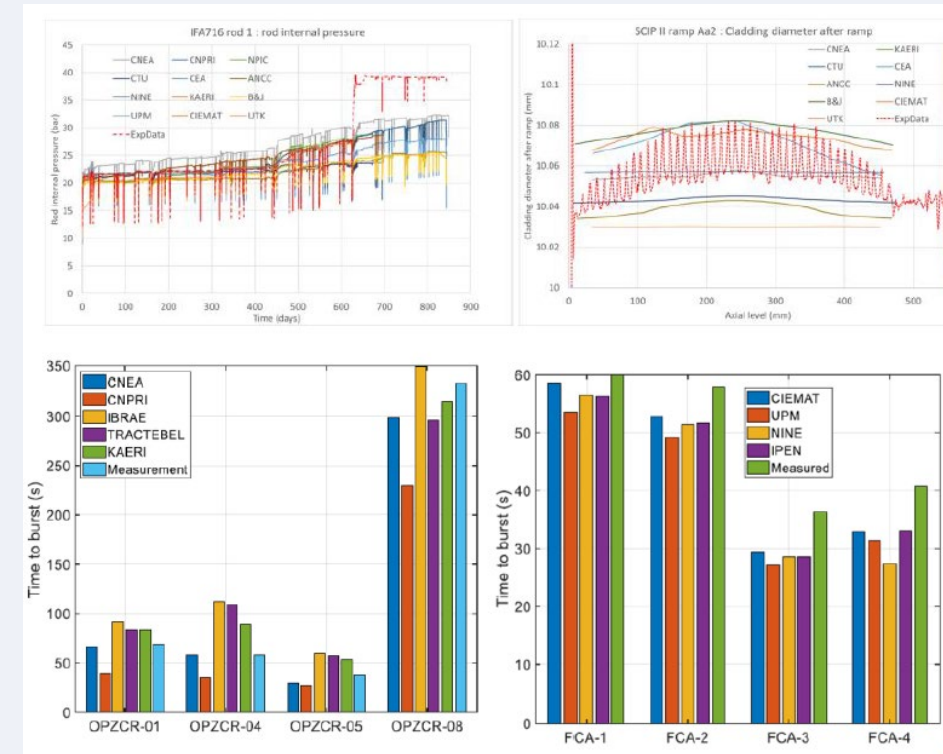
Benchmark of codes for simulation of bundle tests (WT2.2)

Organization	Country	Code	QUENCH-19 with FeCrAl	DEGREE Bundle test B3 with Cr coated Opt. ZIRLO	CODEX-ATF with Cr coated Opt. ZIRLO (pre-test calculations)
CNEA	Argentina	DIONISIO	x		
CTU	Czech Republic	MELCOR	x		
GRS	Germany	ATHLET-CD	x		
KIT	Germany	ASTEC	x	x	x
NUBIKI	Hungary	ASTEC			x
NINE	Italy	MELCOR	x		
CRIEPI	Japan	FRAPTRAN		x	
IBRAE	Russia	SOCRAT	x	x	x
UPM	Spain	MELCOR	x		



# CRP ATF-TS : Work Task 2 - Fuel modelling and Benchmark Exercise: key findings

- Chromia Doped Fuel:
  - Benchmark results aligned well with experimental data, highlighting the importance of uncertainty analysis in fuel performance code validation
- ATF Claddings:
  - Burst pressure predictions were accurate with available data, though hoop strain predictions varied.
  - Improvements suggested in code predictions and the need for further work on material properties
- Bundle Tests:
  - Showed potential for adapting codes for new materials, with modifications to oxidation models for FeCrAl and Cr-coated Zr
  - Thermal-hydraulic parameters were calculated using existing algorithms, while oxidation models were modified for FeCrAl and Cr oxidation
  - FeCrAl oxidation covered the entire temperature range, and Cr coating behavior was modeled up to the Cr/Zr eutectic melt point: further enhancements are needed for processes above this eutectic point and after coating failure



# CRP ATF-TS: Work Task 3 - LOCA fuel safety evaluation methodology

11 organizations from 10 MSs used 9 fuel rod codes and 1 system thermal hydraulic code to simulate and predict the fuel behaviours for reference fuel and ATFs (Cr-coated cladding, FeCrAl cladding, doped pellet, and micro-cell pellet)

## LOCA cases:

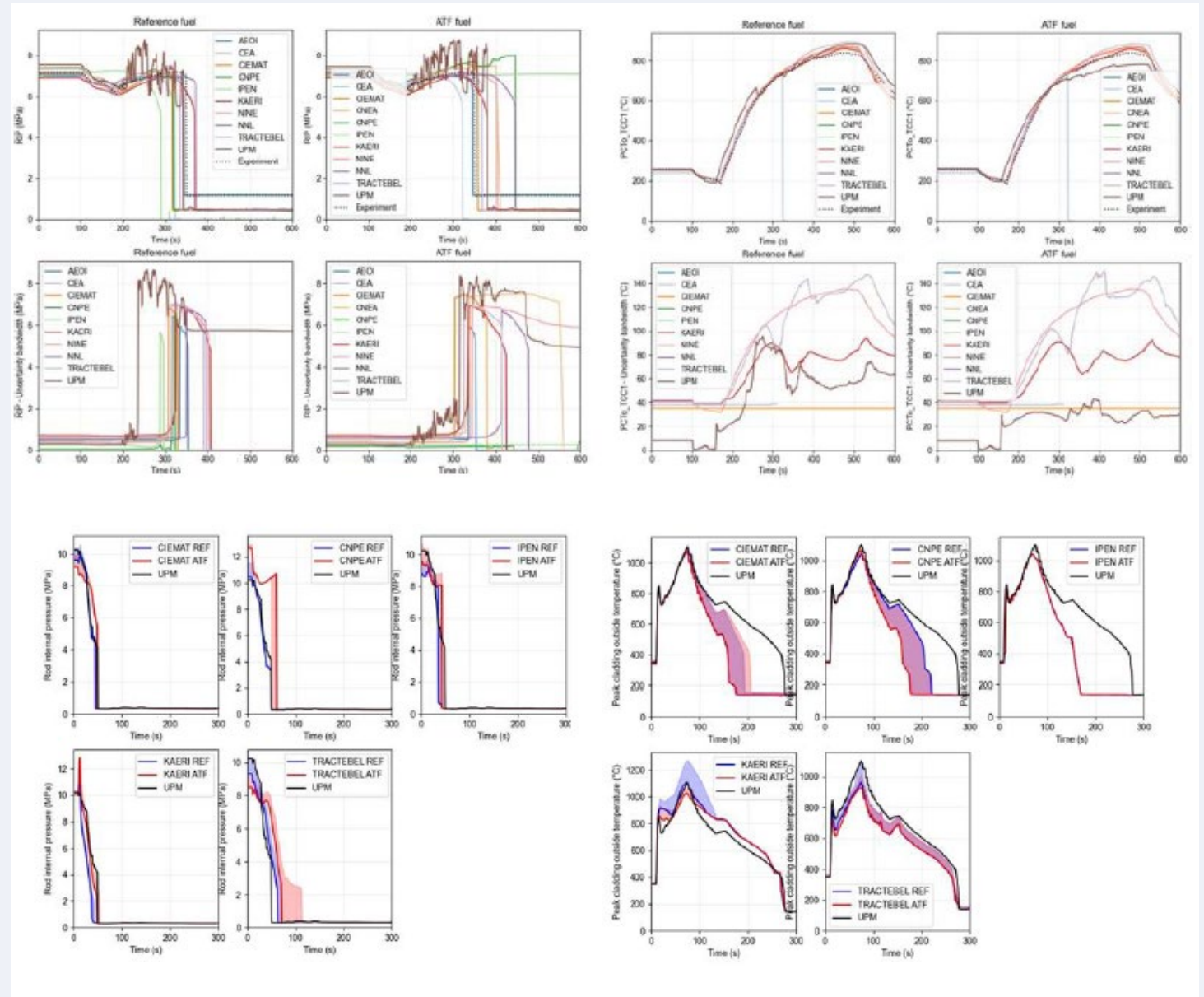
- Halden LOCA tests IFA-650.9 and IFA-650.10
- DBA large-break LOCA (LBLOCA) of a real NPP
- DEC small-break LOCA (SBLOCA) of a real NPP

Organization	Country	Fuel Rod Code	UA/SA Code	ATF concept	WT3.1. Code validation & prediction for ATF		WT3.2. LOCA FSEM for NPP & prediction for ATF	
					IFA-650.9	IFA-650.10	LBLOCA	DEC SBLOCA
CNEA	Argentina	DIONISIO	DAKOTA	FeCrAl, Doped pellet	x	x		
Tractebel	Belgium	FRAPCON/ FRAPTRAN-TE-1.5	DAKOTA	Coated Zr cladding	x	x	x	
IPEN/USP	Brazil	TRANSURANUS	SUNSET	FeCrAl	x	x	x	x
CNPE	China	FRAPCON/ FRAPTRAN-2.0P1	DAKOTA	FeCrAl	x	x	x	x
CEA	France	ALCYONE	URANIE	Doped pellet Coated Zr cladding		x		
AEOI	Iran	PARS/PART	SUAP	Doped pellet	x	x		
NINE	Italy	TRANSURANUS	MC built-in	FeCrAl	x	x		
KAERI	Korea	MERCURY	OpenTURNS	Coated Zr cladding, doped pellet, micro-cell pellet	x	x	x	x
UPM/Nfq	Spain	TRACE	DAKOTA	FeCrAl		x	x	x
		TRANSURANUS	DAKOTA	FeCrAl		x		
CIEMAT	Spain	FRAPCON/ FRAPTRAN-2.0P1	DAKOTA	FeCrAl	x	x	x	x
NNL	UK	ENIGMA	CASINO	Coated Zr cladding		x		

List of participants, used codes and simulated tests in WT3

# CRP ATF-TS: Work Task 3 - LOCA fuel safety evaluation methodology: results

- Reasonable agreement for reference fuel, with some dispersions and large uncertainty bands
- Limited benefits with ATF concepts and large uncertainty bands
- Further improvements are needed in modelling and simulation, particularly in mechanical deformation models and input uncertainties



# IAEA fuel experimental database

**Fuel Experimental Data**

Improved understanding of fuel performance can lead to a reduction in operating margins, increased flexibility in fuel management and improved operating economics.

To better understand fuel performance, the IAEA has addressed different aspects of fuel behaviour modelling in a series of coordinated research projects aimed at:

- assessing fuel performance codes and supporting countries with code development and application needs,
- building a database of well-defined experiments suitable for code validation,
- transferring a mature fuel modelling code to developing countries and supporting its adaptation to the requirements of reactors,
- providing guidance on applying that code to reactor operation and safety assessments, and
- providing guidelines for code quality assurance, code licensing and code application to fuel licensing.

The IAEA Fuel database is a collection of fuel performance experimental data on power reactor fuel performance (water-cooled and fast neutron reactors) derived from IAEA coordinated research projects.

The purpose of this database is to preserve information from fuel performance experiments, such that the data is useful and in a form that can be used for code development and validation. Therefore, each dataset includes sufficient information to assemble an input file to run a code and information against which to compare predictions (data on fuel temperatures, fission gas release (FGR), fuel swelling, clad deformation (e.g., creep-down, ridging) and mechanical interactions. In addition to direct in-pile measurement, PIE information is included on clad diameters, oxide thickness, hydrogen content, fuel grain size, porosity, Electron Probe Micro Analysis (EPMA) and X-ray Fluorescence (XRF) measurements on cesium, xenon, other fission products and actinides.

The IAEA would like to thank the OECD/NEA Halden Reactor Project for providing data for some of the IAEA coordinated research projects.

**Datasets relating to fuels for thermal reactors can be found here:**

- AEKI Burst Tests
- Halden Reactor Test IFA-650.9 (PWR)
- Halden Reactor Test IFA-650.10 (PWR)
- Halden Reactor Test IFA-650.11 (PWR)
- KIT CORA-15
- KIT QUENCH-L0 Bundle Test
- KIT QUENCH-L1 Bundle Test
- Studsvik LOCA test (NRC-192)
- CRIEPI - DEGREE Single Rod and Bundle Tests
- Database of separate effect tests carried out at HUN-REN EK with cladding samples provided by IAEA CRP "ATF-TS" partners

**Datasets relating to fuel for fast reactors can be found here:**

- METAPHIX-1#1
- METAPHIX-2#1
- Sentenay, Phenix (MOX fuel)
- SUPERFACT (MOX fuel)

## Datasets relating to fuels for thermal reactors can be found here:

- AEKI Burst Tests
- Halden Reactor Test IFA-650.9 (PWR)
- Halden Reactor Test IFA-650.10 (PWR)
- Halden Reactor Test IFA-650.11 (PWR)
- KIT CORA-15
- KIT QUENCH-L0 Bundle Test
- KIT QUENCH-L1 Bundle Test
- Studsvik LOCA test (NRC-192)
- CRIEPI - DEGREE Single Rod and Bundle Tests
- Database of separate effect tests

## Datasets relating to fuel for fast reactors can be found here:

- METAPHIX-1#1
- METAPHIX-2#1
- Sentenay, Phenix (MOX fuel)
- SUPERFACT (MOX fuel)
- FBTR MOX
- The JOYO B5D-2 test

# ATF-TS experimental datasets.

## ATF Database of SET, HUN-REN\_EK

At HUN-REN EK, extensive work has been carried out to characterize the behaviour of candidate materials for ATFs and to compare newly measured data with the parameters of traditional cladding alloys

The database includes the main characteristics and results of the separate effect tests: ballooning and burst tests, oxidation tests in high-temperature steam, tensile testing using ring samples, ring compression tests, mandrel tests, scanning Electron Microscopy (SEM) examinations

13 cladding types were tested:

Reference Claddings: Zircaloy-4, ZIRLO™, Optimized ZIRLO™ (optZIRLO™), Zr-1%Nb alloy

Coated Claddings (Zr alloy base): Cr coating, CrN coating, CrN/Cr multilayer coating, TiAl coating

Alternative Alloy: FeCrAl alloy

[Database of separate effect tests carried out at HUN-REN EK with cladding samples provided by IAEA CRP “ATF-TS” partners - Database of separate effect tests carried out at HUN-REN EK with cladding samples provided by IAEA CRP “ATF-TS” partners - Datasets - IAEA Data Platform](#)

Database of separate effect tests carried out at HUN-REN EK with cladding samples provided by IAEA CRP “ATF-TS” partners

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### Data and Resources

-  IAEA ATF-TS Burst Data Hun-Ren EK data valid
-  ATF-TS Burst Test Research Report...
-  ATF-TS Burst Test Balloon Pictures
-  ATF-TS Ring Compression HUN-REN EK data valid
-  ATF Ring Compression Tests Research Report...
-  ATF-TS Ring Compression Graphs
-  ATF-TS Mandrel EK-FRL-2024-120-1-2-M0
-  ATF-TS Mandrel Data HUN-REN EK data valid
-  EK Oxidation Tests Research Report...
-  ATF-TS Oxidation Data data valid
-  Photos of ATF Samples
-  ATF SEM AEOI Samples Research Report...
-  ATF SEM BSU Samples Research Report...

-  ATF SEM CNL Samples Research Report...
-  ATF SEM Cr Coated Zr Cross Research Report...
-  ATF SEM Cr Coated Zr EK-FRL-2021-161-1-1-M0
-  ATF SEM FeCrAl Sample Research Report...
-  ATF SEM Oxidised Samples Research Report...
-  ATF Tensile Tests Research Report...
-  ATF-TS Tensile Data HUN-REN EK data valid
-  ATF-TS Tensile Graphs
-  ATF-TS Database Research Report EK-FRL-2024-120-1-1-M0

# ATF-TS experimental datasets.

## CRIEPI - DEGREE Single Rod and Bundle Tests

Series of single rod tests (S1–S13) and 3x3 bundle tests (B1–B7) were performed at the DEGREE facility, CRIEPI (Japan) for simulation Design Extension Conditions (DEC) LOCA scenarios using an induction heating furnace.

Cladding types tested: Zircaloy-4, Optimized ZIRLO, E110, all coated with either chromium (Cr) or Cr/CrN.

Heating conditions: Peak temperatures: 1350°C, 1500°C, 1600°C; heating rate: 3–5 K/s, atmosphere: Steam/Ar mixture

Test phases: Pre-heating to 500°C, conditioning at 500°C; heat-up to target temperature, cool-down in Ar atmosphere

The screenshot shows the dataset page for 'CRIEPI - DEGREE Single Rod and Bundle Tests'. It includes a 'Data and Resources' section with two entries for 'CRIEPI - DEGREE Single Rod Test S3' and 'CRIEPI - DEGREE Single Rod Test B3', both marked as 'data valid' and having 'Explore' buttons. Below this is a table with the following fields and values:

Field	Value
Source	CRIEPI
Version	1.0
Author(s)	K. Nakamura, K. Inagaki
Maintainer	NFCMS
Maintainer Email	NFCMS
Update Frequency	Never
Preferred Form of Citation	Dataset provided by CRIEPI in the framework of IAEA Coordinated Research Project (CRP T12032) on Testing and Simulation for Advanced Technology and Accident Tolerant Fuels (ATF-TS).

# Thermohydraulic Boundary Conditions for Simulation

Thermohydraulic Boundary Conditions for Simulation were developed in the framework of IAEA CRP “Fuel Modelling in Accident Conditions” (FUMAC, IAEA-TECDOC-1889)

project partner for three Halden LOCA tests:

- IFA-650.9 (PWR fuel)
- IFA-650.10 (PWR fuel)
- IFA-650.11 (VVER fuel)

and calculated by the integral code SOCRAT/V3

IFA-650.10 (PWR fuel) - Cladding Surface Temperatures  
Cladding Surface Temperatures (C) : TcI\_09125 at 912.5 mm, TcI\_09375 at 937.5...

IFA-650.10 (PWR fuel) - Coolant Temperatures

IFA-650.9 (PWR fuel) - README socrat

IFA-650.9 (PWR fuel) - Summary socrat

IFA-650.9 (PWR fuel) - html socrat data valid

IFA-650.9 (PWR fuel) - QA socrat data valid

IFA-650.9 (PWR fuel) - Total Heat Flux from...  
Total (radiative+convective) Heat Flux from Cladding Surface (W/m) ...

IFA-650.9 (PWR fuel) - Cladding Surface Temperatures  
Cladding Surface Temperatures (C) : TcI\_09125 at 912.5 mm, TcI\_09375 at 937.5...

IFA-650.9 (PWR fuel) - Coolant Temperatures

Thermohydraulic Boundary Conditions for Simulation

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Openness  
☆☆☆☆☆ 0 out of 5

Data and Resources

IFA-650.11 (VVER fuel) - README socrat Explore

IFA-650.11 (VVER fuel) - Summary socrat Explore

IFA-650.11 (VVER fuel) - html socrat data valid Explore

IFA-650.11 (VVER fuel) - QA socrat data valid Explore

IFA-650.11 (VVER fuel) - Total Heat Flux from...  
Total (radiative+convective) Heat Flux form Cladding Surface (W/m) ... Explore

IFA-650.11 (VVER fuel) - Cladding Surface Temperatures  
Cladding Surface Temperatures (C) : TcI\_09125 at 912.5 mm, TcI\_09375 at 937.5... Explore

IFA-650.11 (VVER fuel) - Coolant Temperatures Explore

IFA-650.10 (PWR fuel) - README socrat Explore

IFA-650.10 (PWR fuel) - html socrat data valid Explore

IFA-650.10 (PWR fuel) - QA socrat data valid Explore

IFA-650.10 (PWR fuel) - Summary socrat Explore

IFA-650.10 (PWR fuel) - Total Heat Flux from...  
Total (radiative+convective) Heat Flux form Cladding Surface (W/m) ... Explore

IFA-650.10 (PWR fuel) - Cladding Surface Temperatures  
Cladding Surface Temperatures (C) : TcI\_09125 at 912.5 mm, TcI\_09375 at 937.5... Explore

[Thermohydraulic Boundary Conditions for Simulation - Thermohydraulic Boundary Conditions for Simulation - Datasets - IAEA Data Platform](#)

# Open-source ATF material properties database

## Advanced Material Database

IAEA Material database covers thermodynamic, electro-chemical, phase-diagram, and physical properties of advance materials for nuclear fuels for the current and future nuclear fleet.

Datasets relating to fuels for the advanced materials database can be found here:

- [Minor Actinide Property Database \(MADB\) - Datasets - IAEA Data Platform](#)
- [ATF open sources material properties database](#)


### ATF Open Sources Material Properties Database

Developed by IAEA CRP “ATF-TS” Partners

In the framework of the IAEA CRP “Testing and Simulation for Advanced Technology and Accident Tolerant Fuels (ATF-TS)” project the open sources material properties for FeCrAl and Cr-coated Zr cladding were collected.

Last Update: July 14, 2025, 7:50 AM (UTC+02:00)

[Contact dataset maintainer](#)



**Dataset Info**

ATF Open Sources Material Properties Database Developed by IAEA CRP “ATF-TS” Partners

Followers: **0**

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Openness: Openness








































☆☆☆☆☆ 0 out of 5

**Data and Resources**

ATF Open Sources Material Properties Database data valid [Explore](#)

Energy Nuclear Fuel Cycle ...

Field	Value
Source	Innovative Systems Software (ISSS, USA)
Version	1.0
Author(s)	Chris Allison
Maintainer	NFCMS
Maintainer Email	NFCMS
Update Frequency	Never
Preferred Form of Citation	Dataset provided by Dr. Chris Allison, Innovative Systems Software (ISSS, USA) in the framework of IAEA Coordinated Research Project (CRP T12032) on Testing and Simulation for Advanced Technology and Accident Tolerant Fuels (ATF-TS).

	Measurements of the thermal conductivity of uranium dioxide by the Flashing Method.pdf
	Mechanical Behavior of FeCrAl and Other Alloys Following Exposure to LOCA Conditions Plus Quer
	Mechanical performance of SiC three-layer cladding in PWRs.pdf
	Mechanical property and damping capacity of ultrafine-grained Fe-13Cr-2Al-1Si alloy produced by
	Microstructural characterization of accident tolerant fuel cladding with Cr-Al alloy coating layer aft
	Microstructure dependent thermal conductivity measurement of Zircaloy-4 using an extended Ram
	Mid-Term Review of Predictive Modelling Activities.pdf
	Modeling QUENCH-14 with RELAP5SCDAP MOD3.5.pdf
	Modelling of Fuel Behaviour in Design Basis Accidents and Design Extension Conditions _IAEA-TE-
	Modification of MELCOR for severe accident analysis of candidate.pdf
	Morphology_and_Phase_Distributions_of_Molten_Core_in_a reactor vessel.pdf
	Neutronic performance of fully ceramic microencapsulated of uranium oxycarbide and uranium nit
	Nitriding and Re-oxidation Behavior of Zircaloy-4 at High Temperatures- PhD_Thesis_Park_OfficialL:
	Nitriding and Re-oxidation Behavior of Zircaloy-4 at High Temperatures-PhD_Defense_Park_13Oct2
	On the oxidation mechanism of U3Si2 accident tolerant nuclear fuel.pdf
	Oxidation and phase separation of U3Si2 nuclear fuel in high-temperature steam environments.pdf
	Oxidation and Quench Behavior of Cold Spraying Cr-Coated Zircaloy Fuel Cladding Under Severe A
	Oxidation of AISI 304L and 348 Stainless Steels in Water at High Temperatures.pdf
	Effects of ZrC addition on the microstructure and mechanical properties of Fe-Cr-Al alloys fabricated by spark pl
	Environmental behavior of light water reactor accident tolerant candidate cladding materials under design condi
	Evaluation of Accident Tolerant FeCrAl Coating for PWR Cladding under Normal Operating Conditions with Coup
	Evaluation of Equivalent Cladding Reacted parameters of Cr-coated claddings oxidized in steam at 1200C in relat
	EVALUATION_METRICS_APPLIED_TO_ACCIDENT_TOLERANT_FU.pdf
	Experimental Results of Reflood Bundle Test QUENCH-15 with ZIRLO™ Cladding Tubes.pdf
	Fabrication and Mechanical Aspects of Using FeCrAl for Light Water Reactor Fuel Cladding.pdf
	Fabrication and mechanical properties of an oxide-dispersion-strengthened FeCrAl alloy.pdf
	FEM MODELLING OF THE EXPANDING MANDREL TEST SIMULATING OUT-OF-PILE PCI SCC OF FUEL CLADDING, p
	Fission gas diffusion and release for Cr2O3-doped UO2_ From the atomic to the engineering scale.pdf
	Fission gas release in the micro-cell fuel pellet under normal operating conditions A simplified approach based c
	Handbook on the Material Properties of FeCrAl Alloys for Nuclear Power Production Applications(FY18 Version R
	High temperature steam oxidation of chromium-coated zirconium-based Alloys- Kinetics and process.pdf
	High-temperature oxidation resistance of chromium-based coatings deposited by DLI-MOCVD for enhanced pro
	High-temperature tests of silicon carbide composite cladding under GFR conditions.pdf
	HRTEM and chemical study of an ion-irradiated chromium-zircaloy-4.pdf
	Influence of composition and heating schedules on compatibility of FeCrAl alloys with high-temperature steam, p
	Influence of Ta-Zr minor-alloying on the high-temperature microstructural stability of cladding Fe-Cr-Al ferritic s
	Investigation of Corrosion and High Temperature Oxidation of Promising ATF Cladding Materials in the Framewo
	Large eddy simulation on turbulent heat transfer in reactor vessel lower head corium pools.pdf
	Long-Term Management and Actions for a Severe Accident in a Nuclear Power Plant.pdf



# Technical Meeting on Advanced Technology Fuels: Progress on their Design, Manufacturing, Experimentation, Irradiation, and Case Studies for their Industrialization, Safety Evaluation, and Future Prospects, 28 - 31 October 2025

89 experts from 33 MSs and 2 IOs (NEA OECD +EC) participated in the Workshop.

A total of 39 presentations were provided during its sessions.



Participants represented research organizations, nuclear fuel design institutions, nuclear power plant operators and engineering companies, regulatory bodies and technical support organizations, universities, and other entities engaged in near- and mid-term ATF fuel development, design, manufacturing, licensing, and operation for both large and small water-cooled reactors.

The meeting was highly successful, featuring high-quality presentations and extensive technical discussions. Valuable recommendations were provided to guide future IAEA activities related to ATF testing, modelling and simulation, and safety analysis.

# Technical Meeting on Advanced Technology Fuels Sessions

1. Advances in ATF Materials and Manufacturing (ATF cladding and fuel fabrication; Coating designs and optimization; Industrialization of ATFs and associated challenges) ( N.Doncel (Spain) and Mr K. Sakamoto (Japan),
2. Experimental Testing of ATF Materials and Validation Database ( Bundle Tests – Bundle tests with ATFs simulating DBA, DEC-A and DEC-B conditions including tests with air ingress; Separate Effect Tests (SETs) – SETs focused on nominal operating conditions and anticipated occupational occurrences (long-term corrosion testing, mechanical tests, coating defects), accidental scenarios (HT steam/air oxidation, LOCA- and RIA-related SETs) ; In-pile Testing– Irradiation testing of candidate ATF materials (LTRs, LTAs) (R. Hansen (USA) and Mr Z. Hózer (Hungary)
3. ATF Modelling (Verification, Validation, and Uncertainty Quantification of fuel performance codes ; Multi-physics and Multi-scale Modelling; Benchmarking of fuel performance codes for ATF materials in operational and accident conditions; Data-driven and artificial intelligence (AI) applications) (P. Van Uffelen (JRC) and A. Bouloré (CEA, France),
4. ATF Safety Analysis and Licensing Practices (New Safety Criteria for ATFs, Innovative Qualification & Licensing Approaches for DBA and DEC scenarios; Risk-Informed Approaches; Margin Quantification and Management (J. Zhang (Belgium),
5. Future prospects of ATF (Effect of ATFs on occurrence and consequences of Fuel Fragmentation, Relocation, and Dispersal (FFRD), Definition of Post- Critical Heat Flux (CHF) Time at Temperature Limits; Improved ATF designs; Use of LEU+ with ATFs for High Burnup (HBU); Deployment of ATFs in Small Modular Reactors (SMRs) (Yongjun Jiao (China) and Mr Zoltan Hozer (Hungary)

Panel - “What is the future for ATFs?” (Martin Ševeček)

# Proposed scope of new CRP on ATF testing and simulation including for SMRs

General objective: to complement the completed CRP ATF-TS by

Addressing high-burnup applications for existing LWRs.

Advancing testing and simulation frameworks for innovative fuels and SMRs

## Specific Objective 1: Experimental Program and Test Data

- Investigate behaviour of advanced claddings: Cr-coated, FeCrAl, SiC —focusing on improved integrity and oxidation resistance beyond LOCA. Activities will include microscale, temperature-dependent testing for coating creep and integrity characterization, assessment of pre-corroded coatings, and development of coating-specific creep laws.
- Published FeCrAl data (e.g. from ORNL) and open literature on coating technologies will be compiled and include into the IAEA ATF materials database.
- Harmonize ATF testing procedures to ensure reproducibility and comparability.
- Expand ATF datasets under representative thermal–hydraulic conditions for design-basis (DB) and beyond-design-basis (BDB) scenarios.
- Support bundle-scale Integral Effect Tests (IETs) (QUENCH, CODEX, DEGREE) engaging at least three institutions.
- Strengthen cooperation with OECD for quench and transient test data exchange

# Proposed scope of new CRP on ATF testing and simulation including for SMRs:

## Specific Objective 2: Simulation and Modelling

- Develop cross-scale models for:
  - Fission gas behaviour, creep, swelling in large-grain pellets.
- Improve modelling of:
  - Cladding ballooning, burst, oxidation, and FFRD at high burnup.
- Apply multi-physics coupled codes (fuel performance + thermal-hydraulics) for steady-state and transients.
- Conduct comparative assessments of simulation vs experimental data to quantify ATF benefits.
- Expand benchmarking:
  - Include semi-integral and integral irradiation tests.
  - Harmonize user-input effects;
  - Use system-code-derived boundary conditions when LOCA data unavailable.

# Proposed scope of new CRP on ATF testing and simulation including for SMRs

## Specific Objective 3: PCMI, LOCA & RIA Safety Evaluation

- Address gap in fuelled ATF LOCA and RIA experiments; aim for experimental validation
- Improve hot rod LOCA safety evaluation for ATF and SMRs,
  - Provide detailed thermal–hydraulic boundary conditions (THBCs) for nominal and upper-bound cases.
  - Verify THBC applicability;
  - Refine uncertainty quantification.
- Incorporate PCMI, multiple LOCA and RIA scenarios in benchmarks
- Consider RIA scenarios for high-burnup fuels (e.g., JAEA data with doped pellets).
- Integrate ATF models into coupled fuel performance–safety analysis codes for operational and accident conditions.
- Emphasize:
  - Uncertainty analysis and material property verification.
  - Improved methodologies for quantifying ATF safety and economic benefits, especially for near-term and SMR applications.

# Planned Timeline for the New CRP on ATF

- March 2026 – Convening of a Consultancy Meeting to shape the new CRP, including:
  - Detailed discussions on available experimental datasets, experimental and code benchmark, and margin quantification activities within CRP
  - Defining the scope of the CRP and specific tasks
  - Drafting the CRP Proposal
- Mid 2026 – Finalization of the CRP Proposal
- Q3 2026 – Submission of the CRP Proposal for review and approval by the Committee for Coordinated Research Activities (CCRA)
- Q4 2026 – Official launch of the CRP on ATF

## Conclusion

- The completed IAEA CRP on ATF-TS (2020–2024) has supported IAEA MSs to understand and analyse ATF behaviours in normal and accident conditions by sharing experimental data and best practices in fuel modelling, increasing technology readiness for candidate ATF materials
- Building on this foundation, the new CRP will further advance testing and simulation of ATF concepts through coordinated experiments, expanded material datasets, and harmonized methodologies. It will enhance high-burnup fuel modelling, incorporate PCMI and multiple LOCA and RIA scenarios in benchmarks with improved boundary-condition and refined uncertainty quantification, and apply multi-physics coupled codes (fuel performance + thermal-hydraulics) to support advanced fuel development.

Thank you

[A.Khaperskaia@iaea.org](mailto:A.Khaperskaia@iaea.org)





## **Martin Ševeček**

CTU

### **Separate effects tests with ATF cladding materials within the IAEA ATF-TS CRP**

The presentation by Martin Ševeček reviewed the outcomes of the IAEA Coordinated Research Project on Advanced-Fuel-Cladding-Technologies (ATF-TS) and highlighted key experimental findings on a broad portfolio of coated-zirconium and alternative cladding concepts. Ten institutes supplied nine zirconium-based reference alloys (Zircaloy-4, Opt. Zirlo, Zr1Nb, HANA6, M5, E110) together with various chromium-based, CrN/Cr, TiAl, SiC and FeCrAl coatings. Over a dozen laboratories performed high-temperature steam oxidation, balloon-/burst, autoclave corrosion and mechanical tests, generating extensive datasets for model validation.

Chromium-coated Zr showed modest benefits for ballooning and burst resistance, but the gain depends strongly on test conditions, coating thickness and substrate alloy. New failure criteria and creep correlations for coated claddings were derived and supplied to the WT2 fuel-performance model. FeCrAl alloys exhibited markedly different behavior compared with Zr, with a strengthening effect that is partially offset by thinner wall limitations; their high-temperature oxidation kinetics were investigated at 1350–1375 °C under various dwell times. TiAl coatings on Zr-4 were targeted to 10 µm thickness for CANDU applications. Overall, the ATF-TS project delivered more than 100 open datasets, numerous publications, and validated correlations for HT oxidation, ballooning, burst and corrosion, establishing a solid experimental basis for the upcoming ATF-HBU program.

# Separate effects tests with ATF cladding materials within the IAEA ATF-TS CRP

Martin Ševeček

30th International QUENCH Workshop  
18th of December, 2025  
KIT, Karlsruhe, Germany



# ATF-TS Experimental Programme - SETs

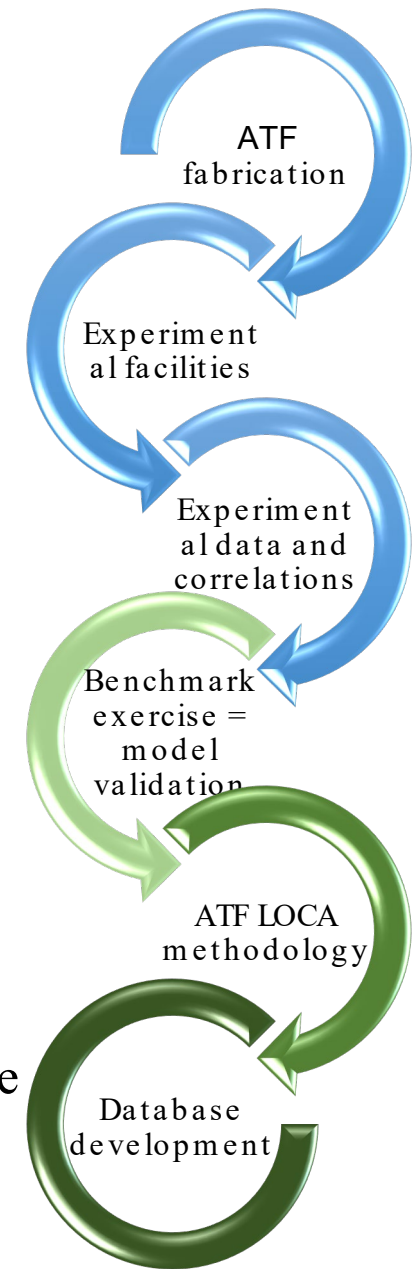
Participants proposed to provide ATF cladding materials for testing

- ✓ Quantity and geometry limitations – e.g. tubes vs. coupons
- ✓ Limited volume of materials – e.g. FeCrAl B136Y
- ✓ Priorities of sample suppliers

Other participants proposed testing campaigns using their facilities

- ✓ Different testing capacities, geometry, test parameters, methodologies, manpower, and resources

Low TRL concepts were investigated in the previous CRP. In ATF-TS, suppliers were asked to provide optimized high TRL products. The optimization was not part of the project, and the fabrication parameters were selected solely by material providers.







# ATF Cladding Materials

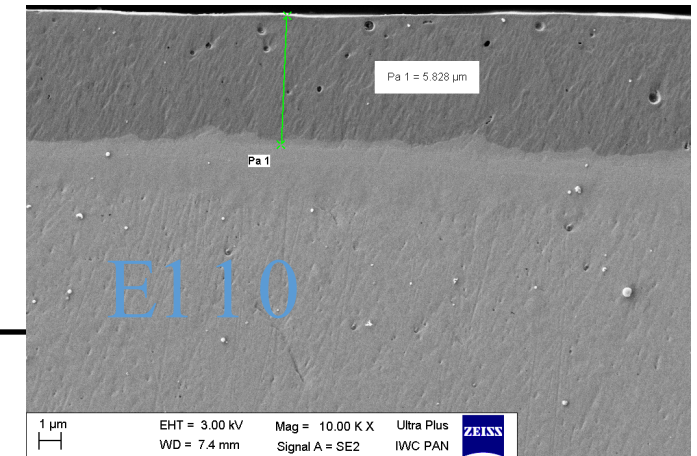
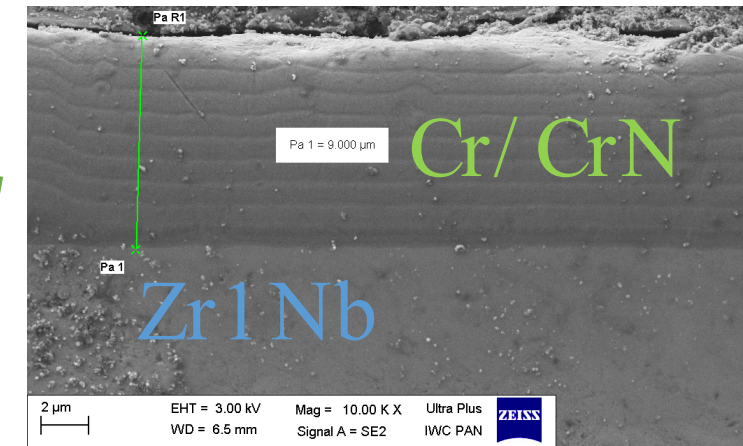
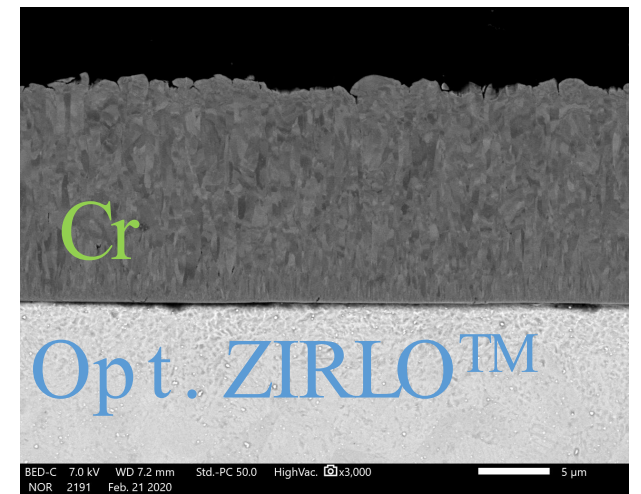


# ATF concepts fabricated within ATF-TS

- institutes fabricated ATF cladding materials for testing
- fabricated Zr-based alloys to be used as a reference (Zr1Nb, Zr1Nb-6Y, Zr1Nb-6Y-2M5, E110)

**In total, more than 160 meters of reference and ATF tubes and several m<sup>2</sup> of reference and ATF plates were shared and tested.**

- CRN
- TiAl – CNL 
- SiC/ YAG– INCT  (Zr1Nb plates)
- FeCrAl, SiC
  - KIT FeCrAl B136Y (ORNL) 
  - NPIC FeCrAl, SiC/ SiC 



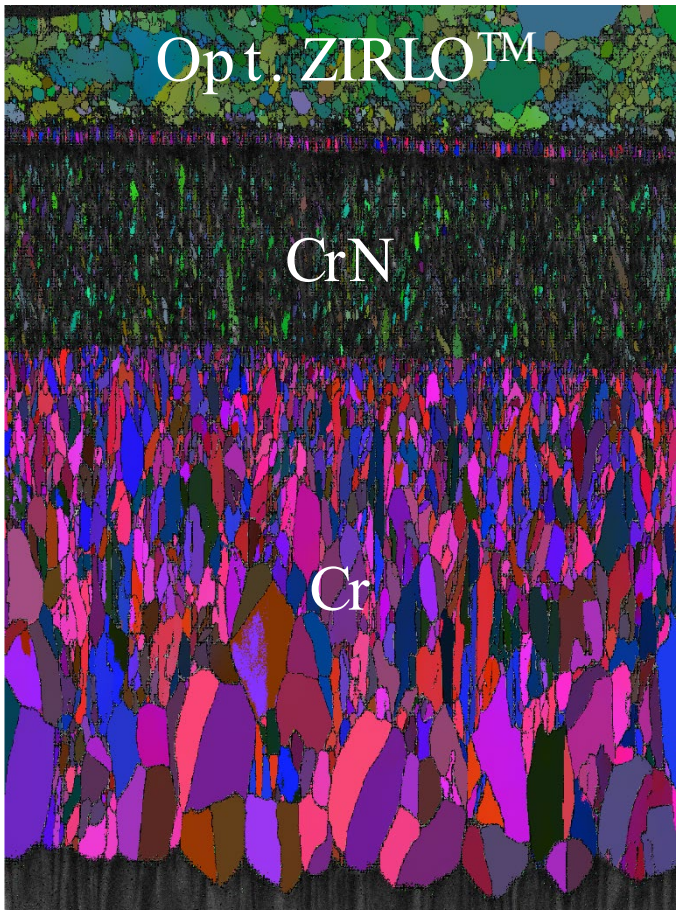
# CTU – Cr and Cr/ CrN coated Opt. ZIRLO™

*Opt. ZIRLO (OD=9.144mm), kindly provided by Westinghouse Electric Company for the ATF -TS CRP project*

Two coating machines/chambers, optimized power sources and deposition parameters:

- Semi-industrial - Hauzer Flexicoat 850
- Industrial – Hauzer Flexicoat 1500



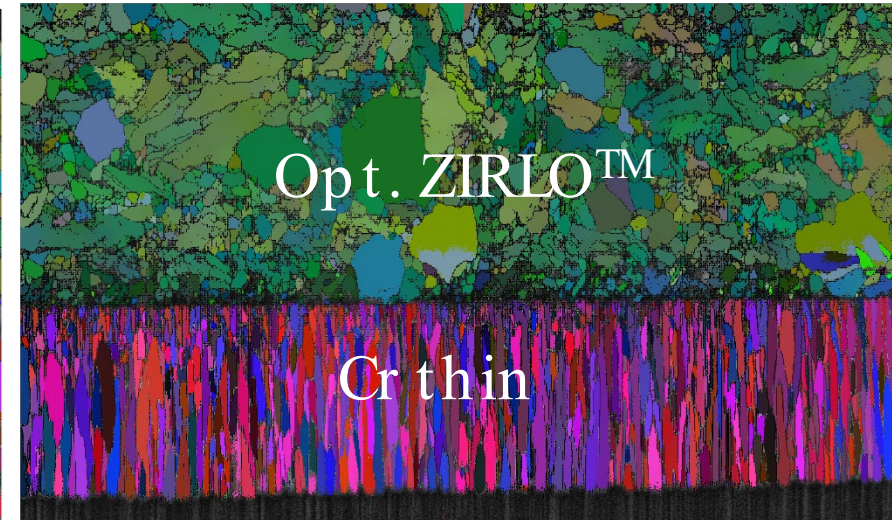


6 μm



8 μm

Step size: 0.035μm Resolution: 887x879 Index. Rate: 74% Magnification: x3800 Tension: 20kV  
Minimum: 0 Maximum: 2 Average: 0.61 S. Dev: 0.3 Entropy: 0  
Median: 0.52 Mode: 0.42



8 μm

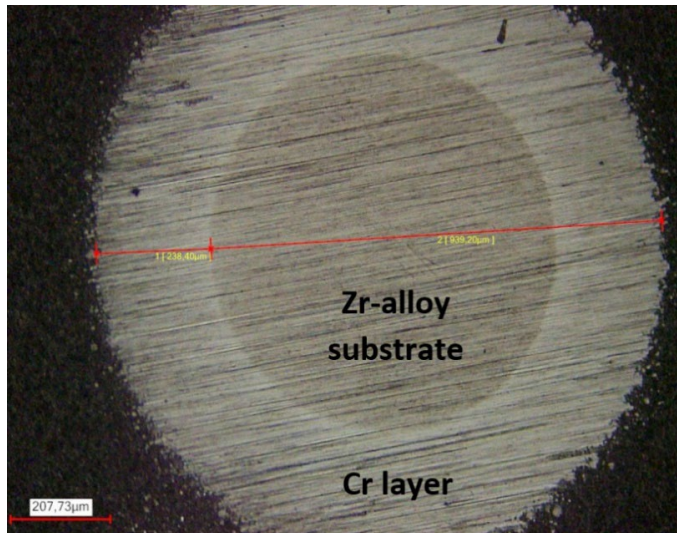
Step size: 0.03μm Resolution: 1001x592 Index. Rate: 81% Magnification: x4000 Tension: 20kV  
Minimum: 0 Maximum: 2 Average: 0.65 S. Dev: 0.33 Entropy: 0  
Median: 0.57 Mode: 0.37

Martin SEVECEK - 21/6/2024  
RunFinal01\_PhMain - EBSD DataRunFinal01\_PhMain  
www.aber-software.eu

## KIT - Cr-coated Zr

Oerlikon Balzers coating company GmbH

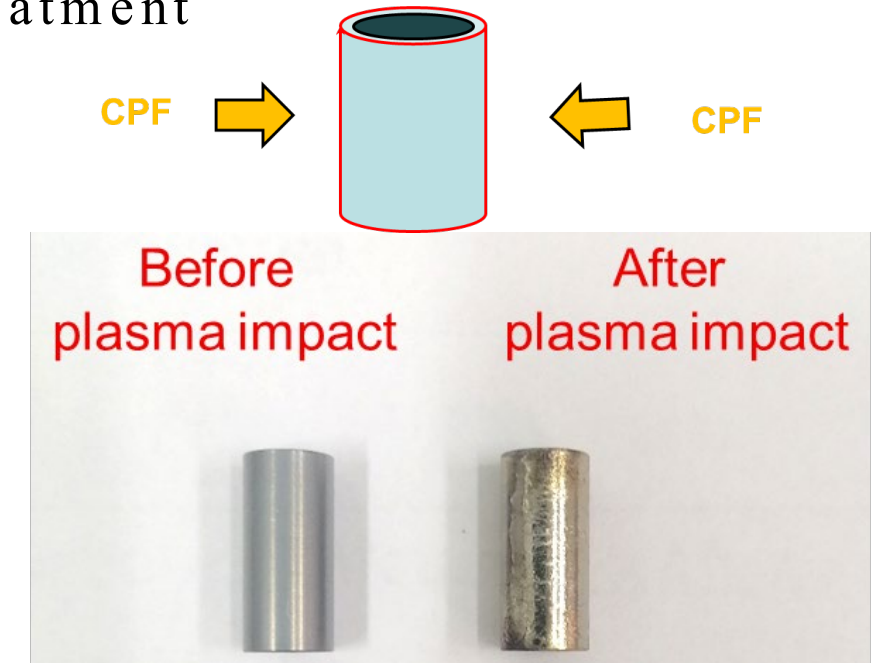
- Variety of Zr -based tubes provided by KIT, proprietary deposition parameters (deposition temperature  $\sim 270^\circ\text{C}$ )
- Coating thicknesses – 7.5 and 10.5 microns



## BSU – Cr coated plasma treated Zr

Zr1Nb (E110) – 20mm used as a substrate

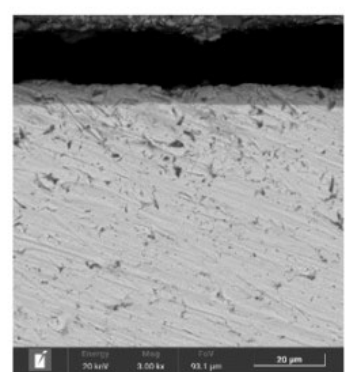
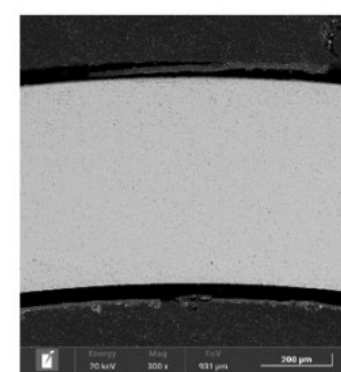
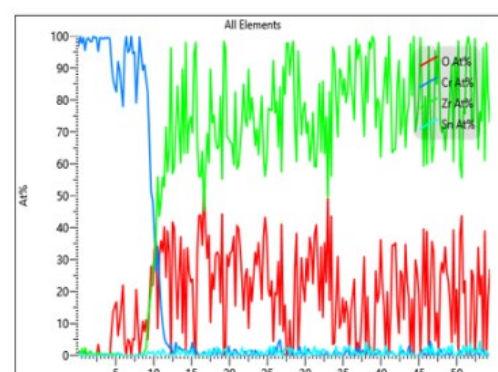
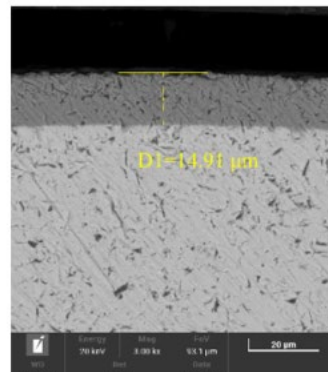
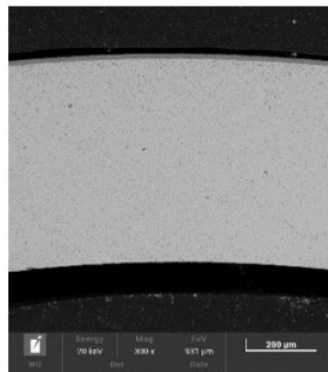
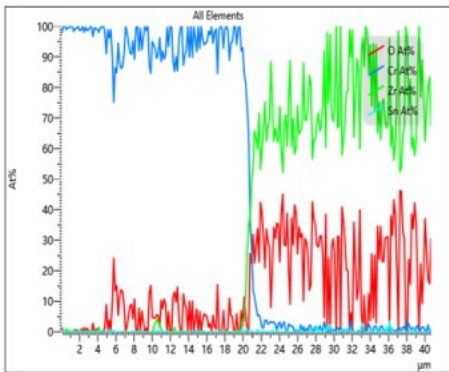
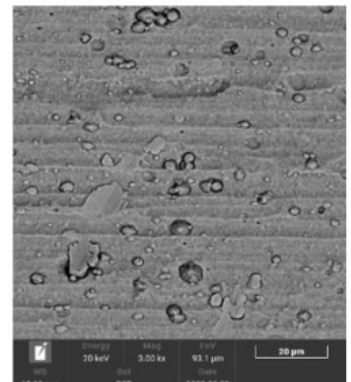
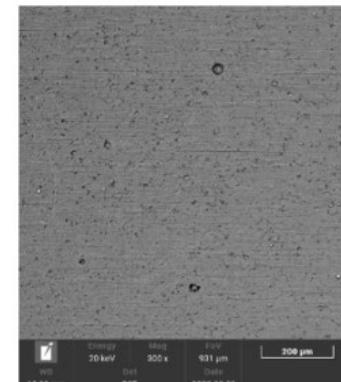
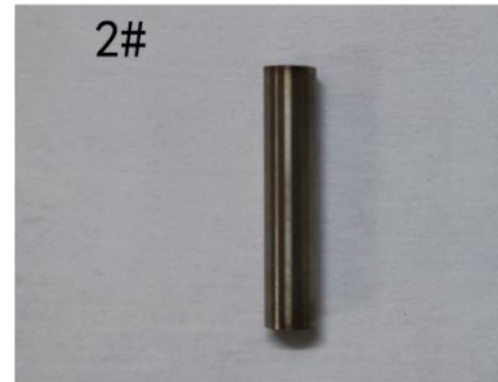
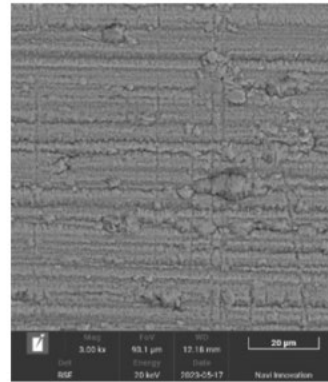
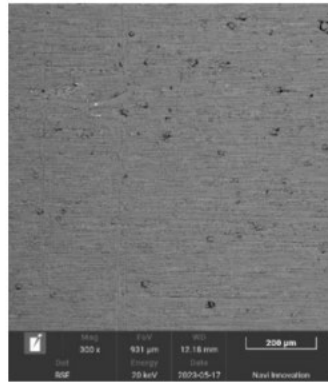
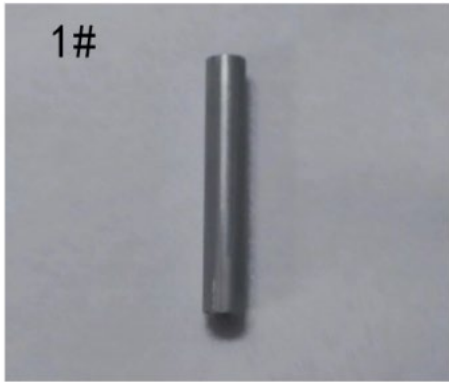
- 1<sup>st</sup> step – Cr deposition
- 2<sup>nd</sup> step - compression plasma flow treatment





# CNPE – Cr coated Zr

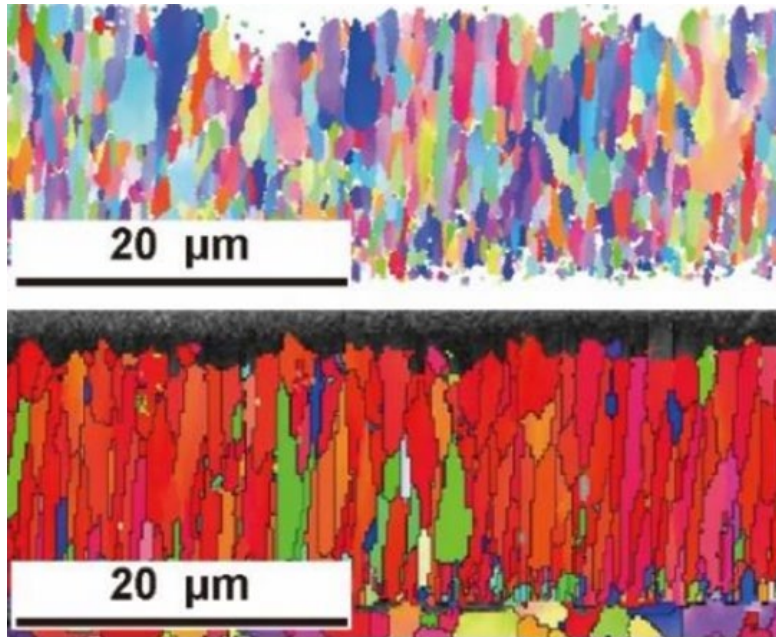
- Type 1 – Zr-Sn-Nb alloy – MS Cr
- Type 2 – Zircaloy -4 – arc ion plated Cr



## NPIC – Cr coated Zircaloy-4

Zircaloy -4 (Zr-1.5Sn-0.2Fe-0.1Cr), outer diameter 9.5 mm, wall thickness 0.57 mm

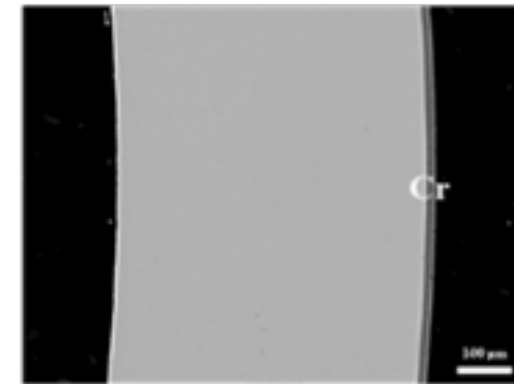
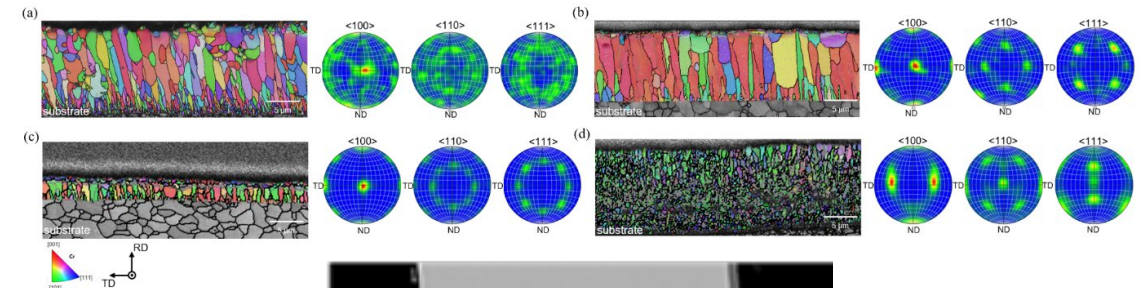
- Multi-arc ion plating technology (15–17  $\mu\text{m}$ )



## KNF – Cr coated HANA6

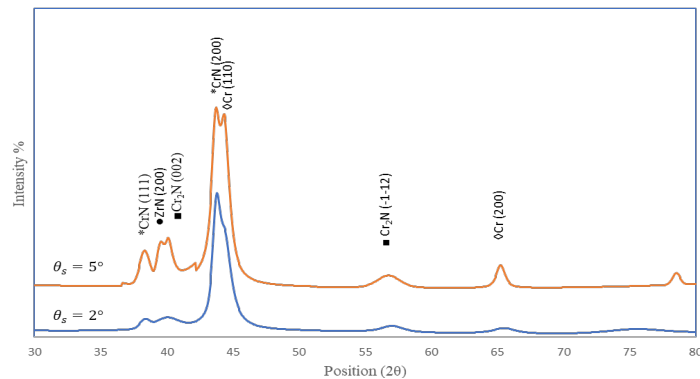
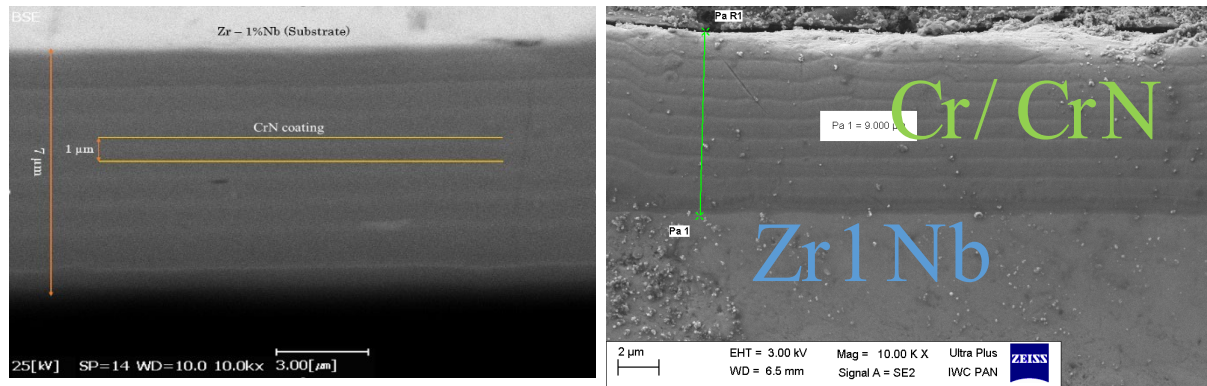
HANA-6 manufactured by KNF used as a substrate

- Arc Ion Plating – 9 and 19 microns
- LTRs inserted in Korea in spring 2025



# AEIOI – CrN and CrN/ Cr

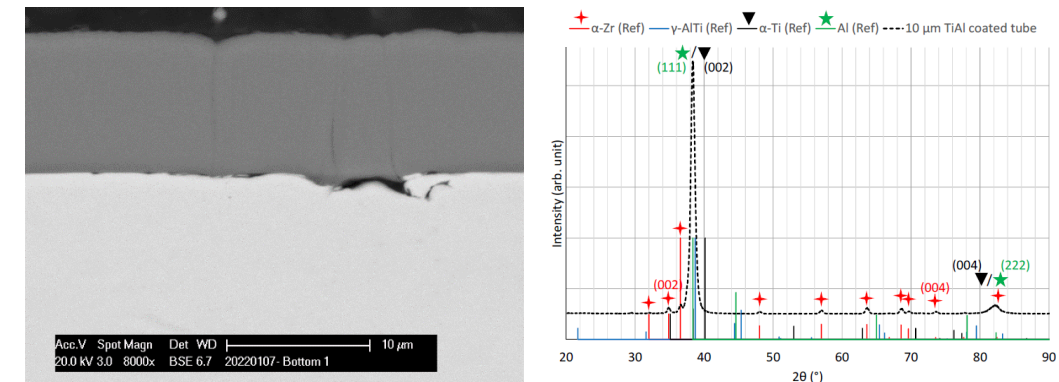
CrN, and Cr/ CrN multilayer coatings deposited on AEIOI's Zr-1%Nb by AIP



# CNL – TiAl coated Zry-4

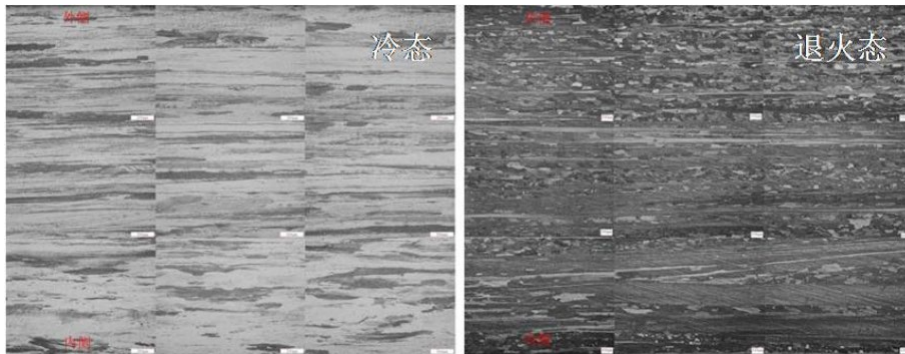
Focus on CANDU – two dimensions – OD= 5.3 and 13.08 mm

- TiAl MS, target thickness of 10 μm and a composition of 45–50 at.% Ti to 55–50 at.% Al on the tubes
- Unbalanced closed field UMS-PVD coater (Teer 650) using two Ti and two Al targets, with argon as the working gas.



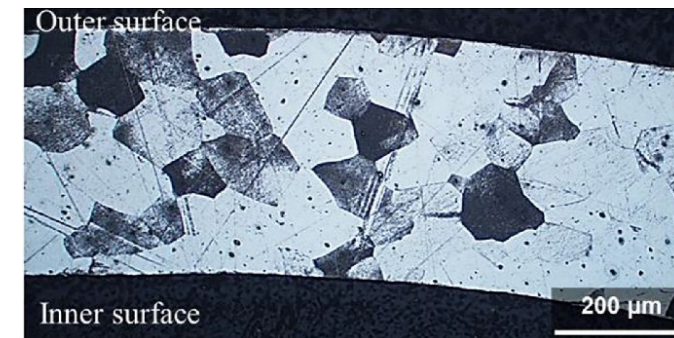
## FeCrAl NPIC

- 13Cr-4.5Al-2Mo-1Nb-0.4Ta-0.05Y (wt.%)
- Vacuum induction melting → homogenization → red feeding forging → extrusion → warm rolling (three passes) → cold rolling (seven passes) → recrystallization annealing
- The final geometry of the cold pilgered thin-wall tube are 9.5\*0.38 mm

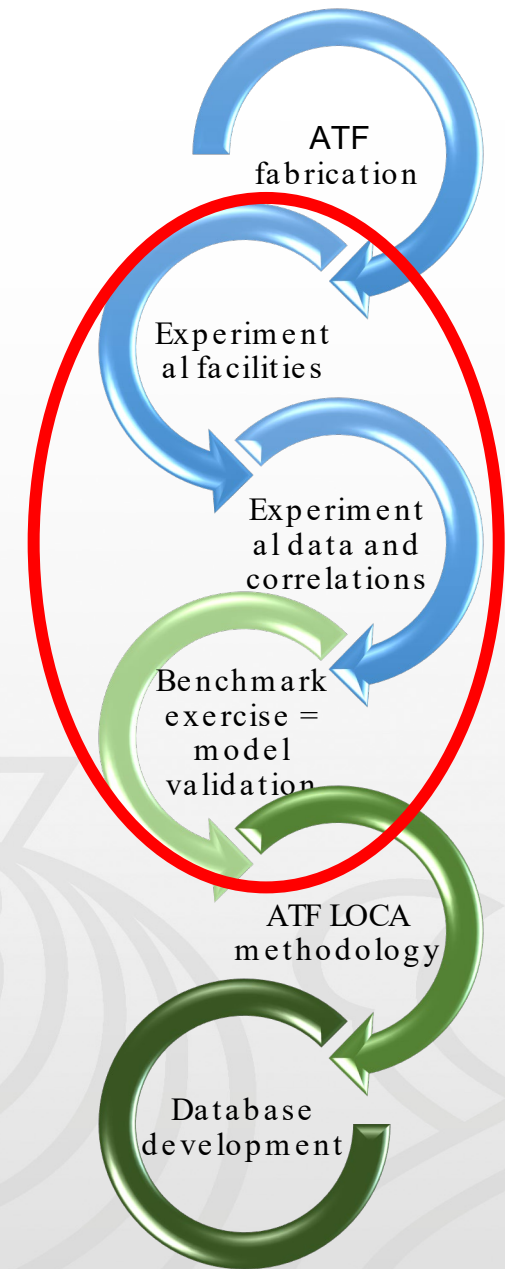


## FeCrAl B136Y3 (KIT/ORNL)












- 13Cr-6.2Al-0.03Y-0.01C (wt.%)
- Produced by ORNL – B-type alloy
- Used in the QUENCH-19 bundle test = link to Q19 benchmark exercise + support with SETs



# Experiments – DBA/ DEC



# Experimental facilities

- 12 laboratories/institutes proposing various testing campaigns
  - CNPE  – HT oxidation; Ballooning/burst
  - CNPRI  – axial tensile tests; internal burst tests; internal creep tests; autoclave corrosion tests; HT steam oxidation
  - CRIEPI  – bundle/single rod tests
  - CTU/UJP  – ballooning/burst tests; HT steam oxidation; Autoclave corrosion
  - EK  – HT oxidation; ballooning/burst tests; Mechanical tests; CODEX bundle test
  - INCT  – autoclave corrosion tests; HT air oxidation; NAA
  - JRC  – thermal characterization; mechanical tests
  - KAERI/SNU  – LOCA testing; PQD evaluation; DSC -eutectic study; Micro -mechanics
  - KIT  – HT oxidation tests; single rod tests
  - NPIC  – FeCrAl-thermomechanical tests; SiC – thermal shock tests; irradiation tests
  - UPM  – Autoclave corrosion; Ring compression tests; Cathodic charge; Burst tests







# Ballooning/ burst tests



## TASK 2: HT creep/ ballooning/ burst

Originally defined for a round robin exercise. But due to different limitations, the tests are not standard RRTs but rather complementary tests of several cladding candidates. However, RRTs was possible in several instances.

HT creep/ ballooning/ burst

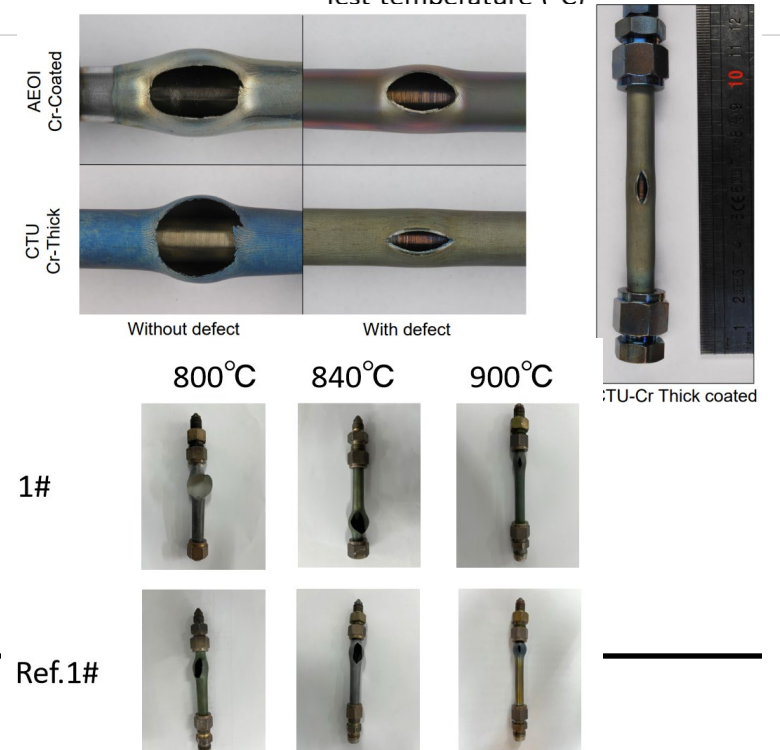
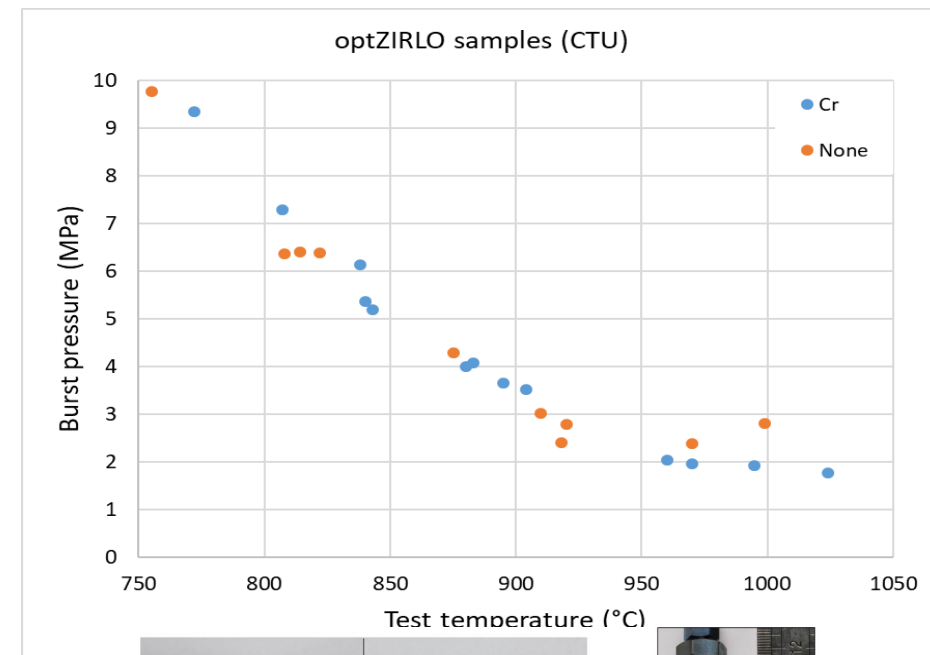
- CTU/ UJP 
  - Constant pressure-temperature ramp (0.7K/sec and 7K/sec)
  - Isothermal isobaric creep tests (constant moles of gas vs. infinite volume) at 750 and 950 °C
- EK 
  - Constant temperature (750, 850 and 950 °C; 800, 900 and 1000 °C) – pressure ramps (5; 100 kPa/s)
  - As-received and pre-oxidized samples
- UPM 
  - Isothermal pressure ramps (1 bar/s) – 100mm; 600 °C
  - Autoclave pre-oxidized and as-received
- CNPE 
  - Isothermal (800, 840, 900 °C) pressure ramps (6 and 100 kPa/s)
- CNPRI 
  - Lower temperature (350 °C) pressure ramps (13.8 MPa/s)
- SNU 
  - Single rod LOCA tests with surrogate pellets/ fragments; (closed volume, 60–80 °C/s using IR heating)



# HT creep/ ballooning/ burst – Main Findings

## Coated Zr cladding

- Limited benefit of coatings in time-to-burst (within the uncertainty range)
- Ballooning and opening size – coated Zr provides some benefits but the magnitude depends on the specific test conditions and methodology.
- New creep correlation and burst criteria derived (both stress- and strain-based for coated cladding) and provided to WT2 for model implementation and validation. Correction coefficients proposed for fuel performance models.



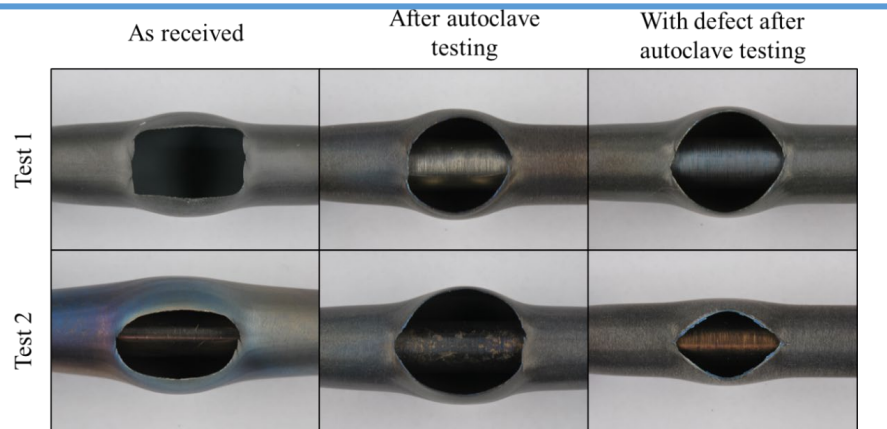


CTU

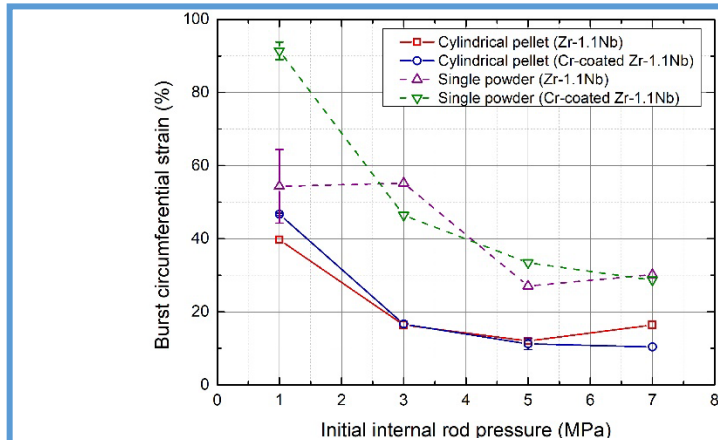
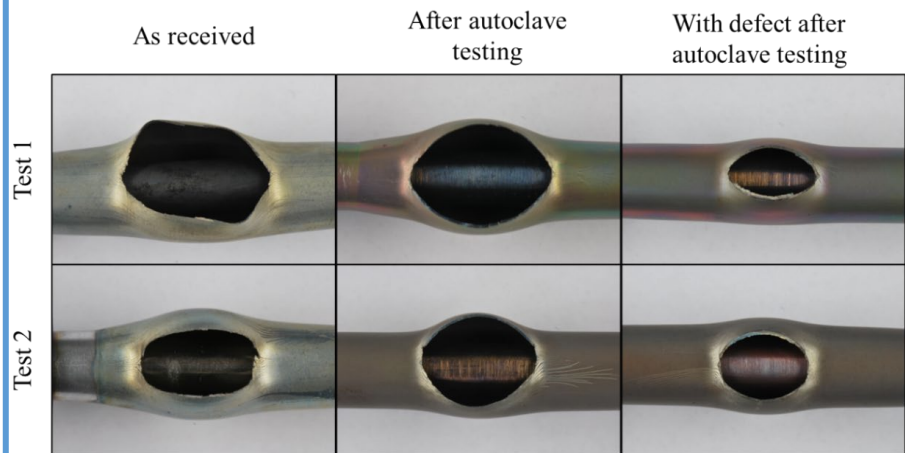
CZECH TECHNICAL UNIVERSITY IN PRAGUE



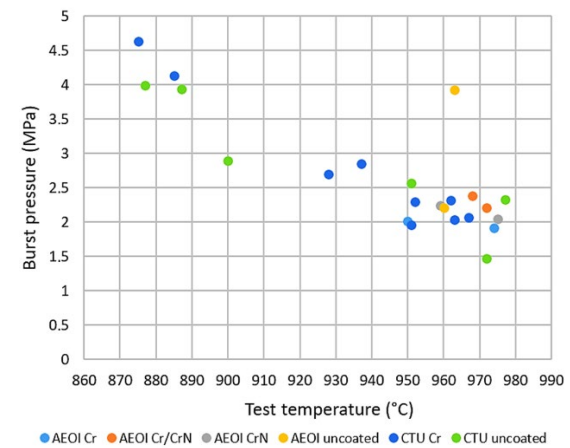
*Coating cracking - different patterns and consequences for each type*



*Ballooning size reduction – closely linked to chosen Zr alloy (more beneficial for softer Zr/Nb alloys)*



*Strong effect of methodologies – pre-oxidation, geometry of fuel matrix, closed/infinite volume...*

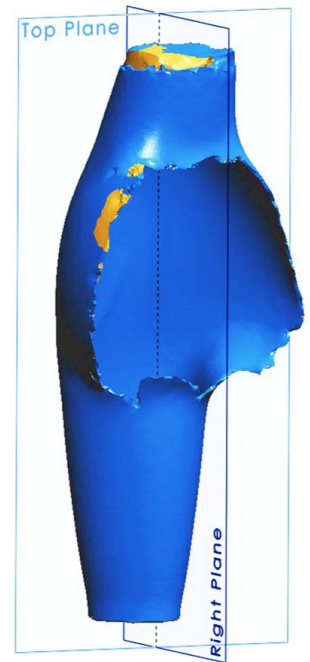
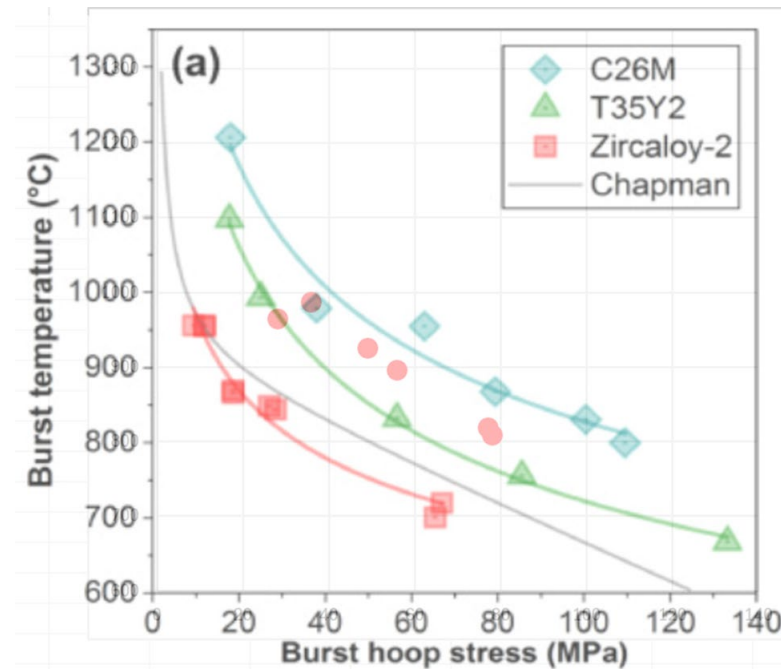
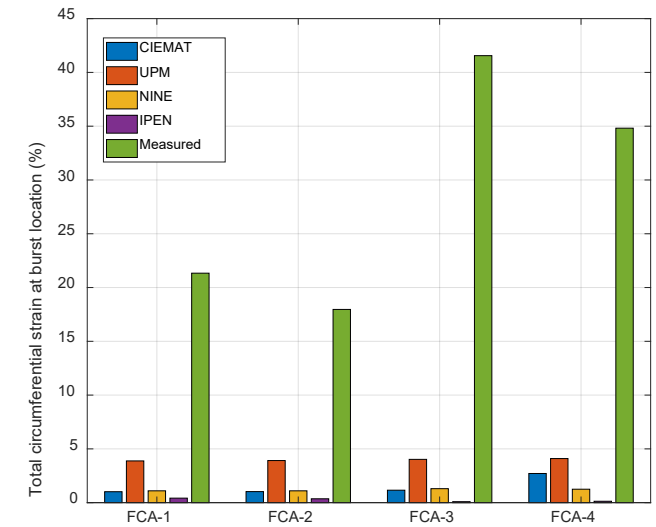


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# HT creep/ ballooning/ burst – Main Findings

## FeCrAl

- Very different performance of FeCrAl compared to Zr.
- Strengthening effect confirmed but partially eliminated by thinner wall.
- Fuel performance codes were not able to predict this behavior because the models were historically developed and tuned for Zr-based materials.












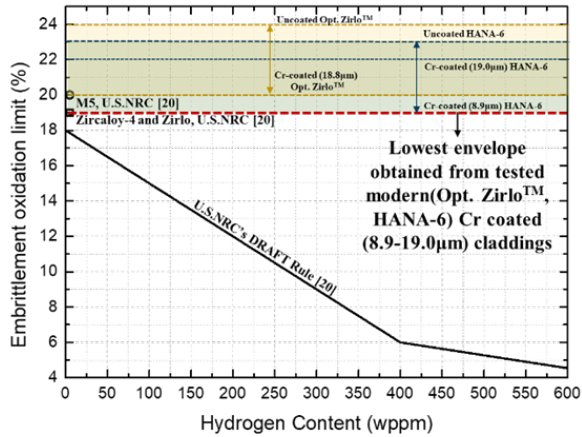
# High-temperature oxidation



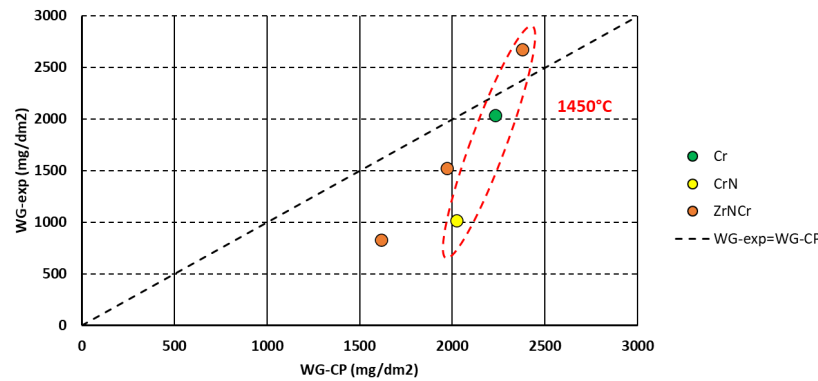
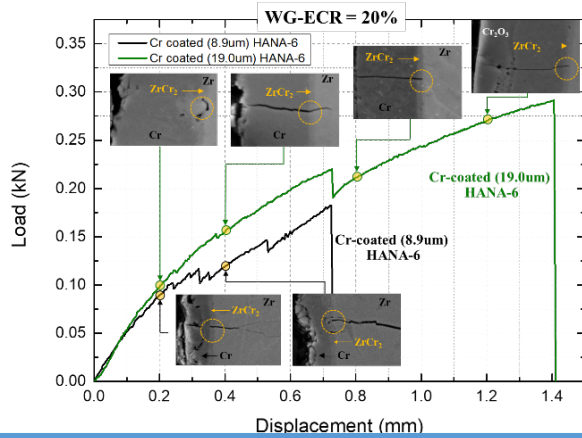
## TASK 3: HT oxidation

### High-temperature oxidation tests

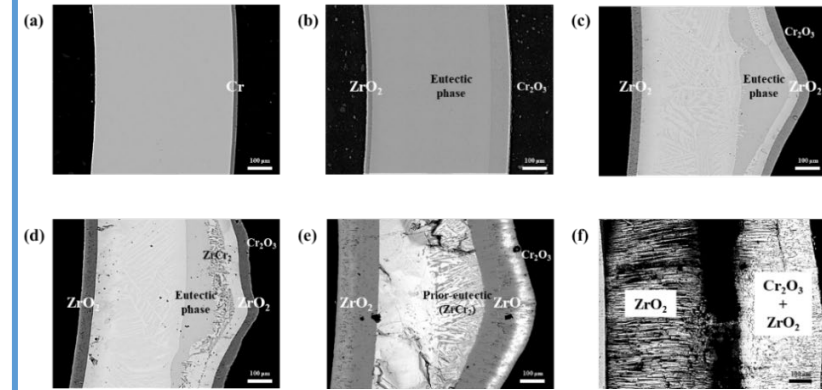
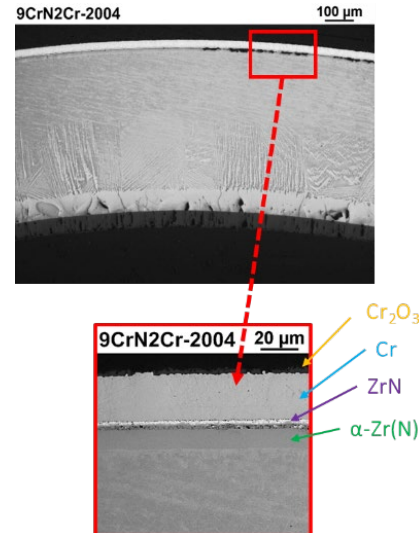
- Small scale SETs (test parameters according to internal methodologies):
  - CNPRI  – HT double-sided steam oxidation up to 1400 °C
  - CTU/ UJP  – double and single-sided steam oxidation + PQD evaluation
  - EK  – steam oxidation tests + RCTs
  - KAERI/ SNU  – LOCA testing; PQD evaluation
  - INCT  – Ar annealing test
  - CNPE  – steam oxidation test
- KIT , CRIEPI , KAERI/ SNU  – single rod tests – ramp/ isothermal



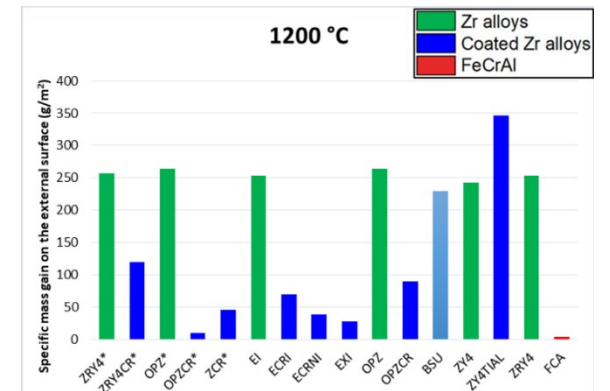
*Current ECR a PCT criteria are conservative and can be used for Cr/Zr evaluation. But the degradation mechanisms change significantly.*



*There are alternative materials/interlayers that can delay degradation observed for Cr/Zr.*



*Coating quality and defects are very important for evaluation. There's no generic Cr/Zr cladding.*



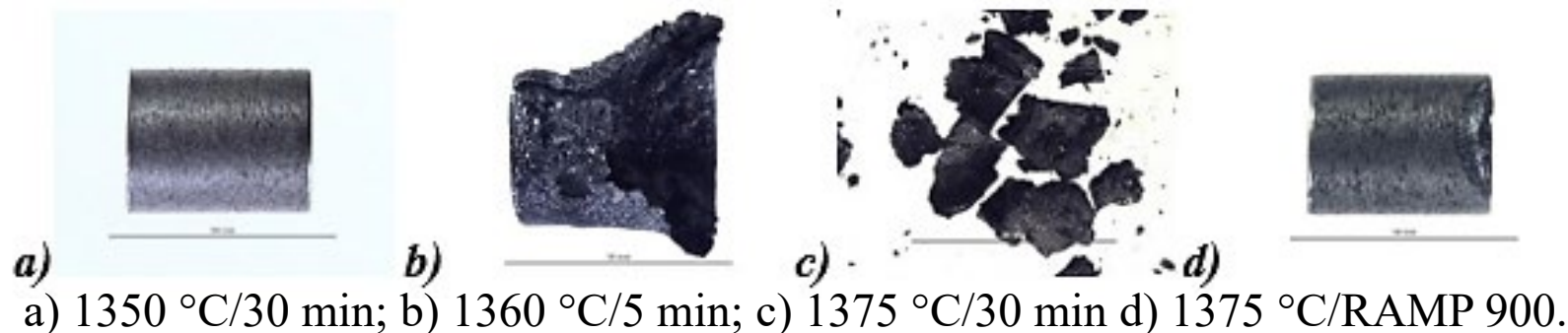
# HT oxidation – Main findings

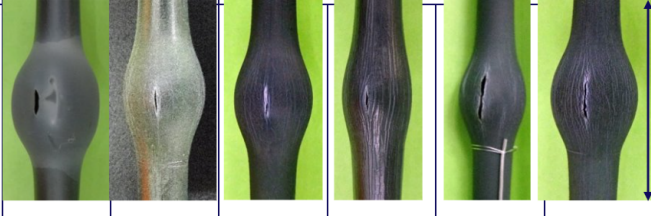
## Coated Zr:

- Eutectic Cr/ Zr – another degradation mechanism (e.g. secondary hydriding, oxygen embrittlement), not hard limit (melting point). Effect of coating thickness observed.
- ECR criteria for coated Zr – does not have physical meaning and should be replaced. But it's conservative and can be used by industry if needed.
- CrN/ Cr – benefits in BDBA conditions confirmed by CRIEPI, KIT. Open questions remain but it seems like a feasible way to further improve pure Cr coatings.

## FeCrAl:

- Focus on FeCrAl HT oxidation kinetics:



Item	S1'	S2	S3	S4	S5	S6
Coating thickness and materials	-	10 μm Cr	20 μm Cr	16/10 μm Cr/CrN	10 μm Cr	20 μm Cr
Max. Temp. (°C)	1350			1600		
Steam flow rate (g/s)	0.41	0.41	0.46	0.46	0.50	0.46
Heating rate (K/s)*	3.5-1.5	1.5	2.4-1.8	2.5-2.2	3.0-1.6	3.0-1.8
RIP at RT (MPa, He)	6.0					
Gas plenum volume (ml)	10	15	10			
Balloon & burst region						

## Conclusions and Summary

- Coordinated Research Project ATF -TS– organized by IAEA between 2019 and 2024.
- ATF-TS was divided into several work packages with strong interlinks – WPs 2, 3 and 4 relied on experimental results from WP1.
- Ten organizations fabricated and shared their ATF cladding materials, and 12 laboratories performed various experimental investigations. Variations in quantities, geometries and preferred partnerships.
- Optimization of fabrication parameters was out of the scope of the project – it was done previously by CRP participants = focus on higher TRLs. Material providers shared the materials based on their preferences and needs.
- Focus mostly on Cr coated Zr – but many different variations produced (substrates, deposition technologies, coating thicknesses, pre - and post -treatment).
- Alternative coating materials proposed and provided to eliminate the drawbacks of Cr/Zr ATF concept. Two types of FeCrAl and one type of SiC were also investigated.
- Detailed fabrication parameters are presented in the TECDOC. The material fabrication parameters should be linked to their performance.

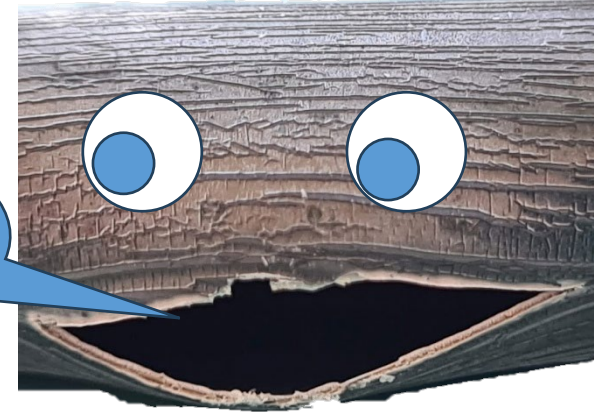
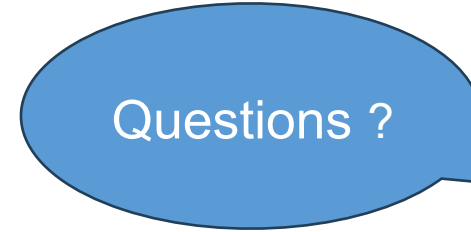


## Conclusions and Summary

- 14 laboratories performed various experimental investigations
  - Ballooning and burst – new failure criteria and creep correlations
  - HT steam oxidation – independent evaluation of all degradation mechanisms for all concepts
  - Autoclave corrosion – good performance confirmed even with low coating thicknesses and lower quality.
  - Mechanical performance – complex fracture mechanisms of different coating based on their microstructure (deposition parameters) which will further change with irradiation.
  - + many more tests documented in the TECDOC not covered here (hydrogen uptake, microstructure, thermal shock tests, thermophysical properties...)
- Despite many challenges, ATF -TS was the most successful and productive CRP in the Fuels&Materials area, especially in the experimental field.
- Hundreds of new open datasets, dozens of journal and conference publications, new material correlations and models, validation cases from both, separate effect and integral bundle tests... which provide a good foundation for the new CRP ATF -HBU.



**UJP PRAHA**



**Special thanks to all participants and partners within ATF -TS CRP.**

*We dedicate the CRP outcomes to the memory of Dr. Giovanni Pastore, who has made a significant contribution to this IAEA CRP and the fuel performance community in general.*



**Kinya Nakamura**

CRIEPI

## **Development Status of Accident-Tolerant Control Rods in Light Water Reactors at CRIEPI**

It is well known that during accident progression in current PWRs and BWRs, degradation of core structural materials such as control rod (CR), grid spacer (GS), and channel box (CB), precedes fuel rod failure (ex. P. Hofmann, 1999). The CR, in particular, is believed to trigger early core damage, as demonstrated by the CORA and QUENCH test series at KIT, the PHEBUS-FP test series at IRSN (now ASNR), and the LEISAN tests at JAEA. Fukushima Daiichi NPP accident enhanced efforts to improve the safety of light water reactors worldwide, and one of the activities is the development and deployment of Advanced Technology or Accident Tolerant Fuels (ATFs). In the near-term, it is envisaged that an ATF concept employing Cr-coated Zr alloy cladding will be practically used with the same core structural materials as currently in use.

PWR CRs using Ag-In-Cd alloys as a neutron absorber are susceptible to overpressure failure of the stainless steel (SS) cladding or damage caused by eutectic between the SS cladding and the Zr alloy guide tube during an accident, causing molten Ag-In-Cd alloy to chemically destroy the Zr alloy guide tube and neighboring fuel rods. BWR CRs using B<sub>4</sub>C or Hf as neutron absorbers are susceptible to B<sub>4</sub>C/SS eutectic damage to the SS blades and adjacent Zr alloy channel boxes. It has been suggested that the introduction of ATF technology with current CRs may not reduce the risk of early core damage. As one solution to this issue, CRIEPI has been proposing a concept of replacing the neutron absorbers in current PWR and BWR CRs with rare-earth sesqui-oxide-stabilized zirconia or hafnia, which is believed to simultaneously achieve longer life and improved accident tolerance. This concept of Accident Tolerant Control Rod (ATCR) involves replacing only the neutron absorbers while maintaining the current CR design and operating procedures.

This paper summarizes an overview of the current status of the ATCR in terms of neutronic reactivity worth, dimensional stability under thermal neutron irradiation, compatibility with primary coolant under PWR conditions, compatibility with steam and core structural materials at high temperatures, and coexistence with molten fuel at high temperatures leading to significantly reducing the re-criticality risk during accident progression, fuel debris retrieval, and mid- to long-term storage.

# Development Status of Accident-Tolerant Control Rods in Light Water Reactors at CRIEPI

Kinya Nakamura, Hirokazu Ohta, Naoki Tarumi

Central Research Institute of Electric Power Industry (CRIEPI)

*30th International QUENCH Workshop*

Karlsruhe Institute of Technology, Germany

16-18 December, 2025

# Outline

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1. Current Knowledge on Early Stage of Core Degradation
2. Accident Tolerant Control Rods
  - Concept
  - Roadmap
  - Current Status
3. Conclusion

# 1. Current Knowledge on Early Stage of Core Degradation

During a SA in LWRs, not only the fuel rods but also core component materials are degraded by high-temperature (HT) chemical reactions and decrease in mechanical strength, accelerating the progression of reactor core degradation.

## Control Rod (CR)

- At temperatures above 1200°C, CR cladding (SS) and neutron absorbers (Ag-In-Cd or B<sub>4</sub>C) may melt and fail before the fuel rods.
- The molten absorbers may relocate and damage neighboring fuel rods, increasing the risk of early FP release, reactor core degradation, and re-criticality.

## Grid Spacer (GS)

- Deformation and damage of GS, made of Zircaloy or Inconel, due to HT oxidation and liquefaction leads to a loss of its function of holding the fuel assemblies in place, accelerating core degradation.

- It has been suggested that the introduction of ATF technology with current core component materials may not reduce the risk of early core degradation.
- Along with the deployment of ATF claddings, it is also crucial to improve the accident tolerance of core component materials.

\*1: Z. Hozer, et al., IAEA TM on ATF, IAEA HQ, Oct. 28-31, 2025.

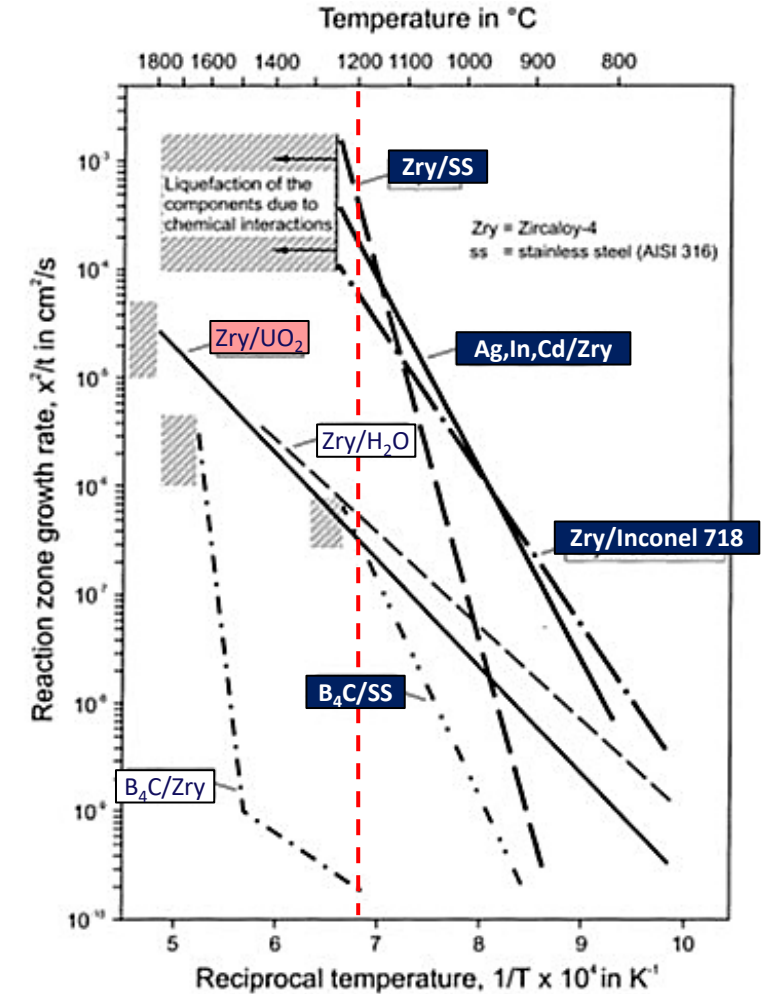


Fig. 10. Total reaction zone growth rates of various reaction couples of fuel element components. In most cases liquefaction of the materials occurs below their melting points.

P. Hofmann, JNM, 1999.

Zry: Zr alloy

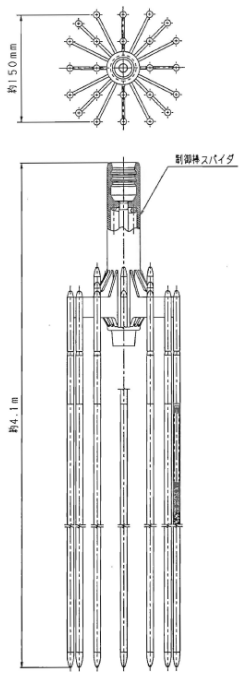
# 1. Current Knowledge on Early Stage of Core Degradation **Control Rods**

## PWR

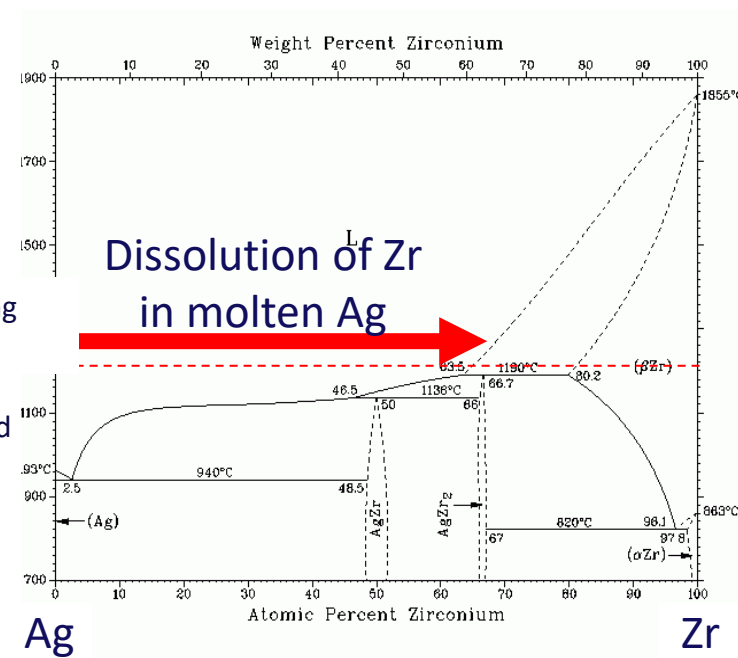
- Degradation of CR, Ag-In-Cd/SS system, at **1200-1400°C**
  - Overpressure failure due to Cd vaporization
  - Eutectic of SS cladding/Zircaloy guide tube
- Molten alloy including Ag may chemically destroy the local fuel rods.

## BWR

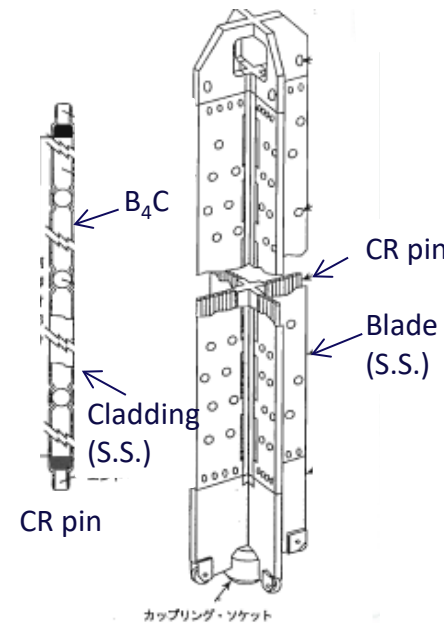
- Degradation of CR, B<sub>4</sub>C/SS system, at **1200-1400°C**
  - Eutectic of B<sub>4</sub>C/SS cladding and/or blades, leading to interaction with Zircaloy channel box and local fuel rods



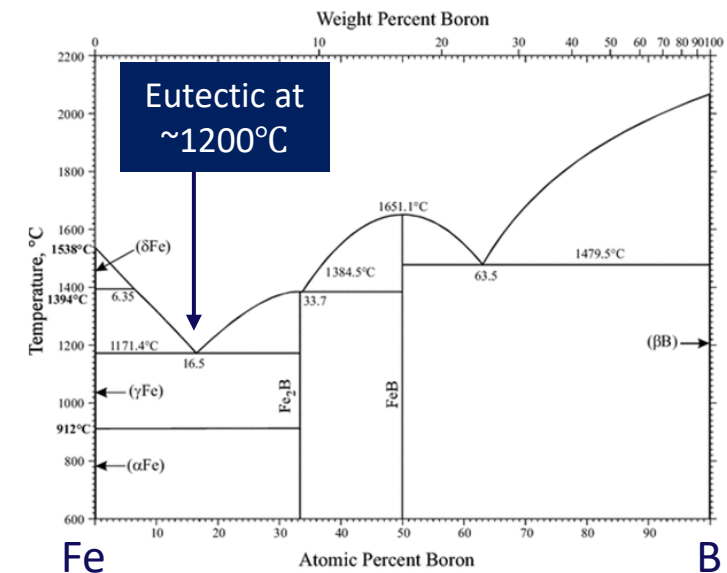
CR pin



Phase diagram of Ag-Zr binary system



Control blade



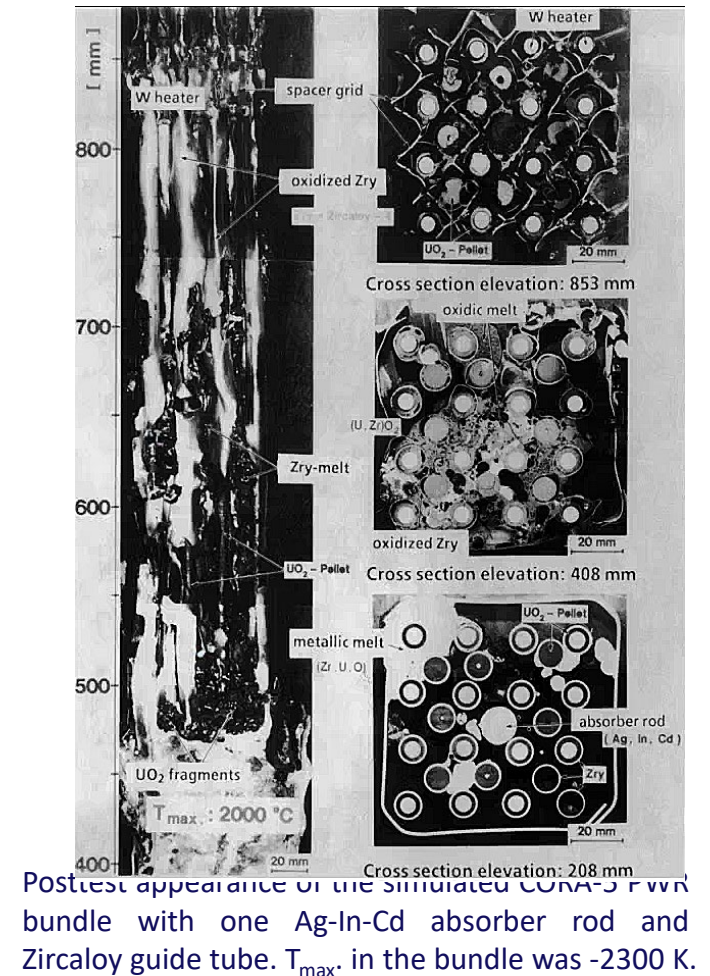
Phase diagram of Fe-B binary system

# 1. Current Knowledge on Early Stage of Core Degradation **Control Rods**

To investigate the impact of CR failure on early stage of core degradation, series of integral tests have been carried out by CORA, Phebus-FP, CODEX, QUENCH, and LEISAN etc.

## Common knowledge

- CR failure before the fuel rods
- HT reactions between CR and core component materials:  
Ex. SS/Zr, Ag/Zr, and B<sub>4</sub>C/SS
- Acceleration of local core degradation due to melt relocation
- Increase of the risk of early FP release (such as I and Cs) and re-criticality



P. Hofmann, NT, 1997.

These knowledge have deepened understanding of core degradation processes and provided an essential foundation for the improvement of SA analysis codes and current ATCR development.



# 2. ATCR: Concept

## Requirements

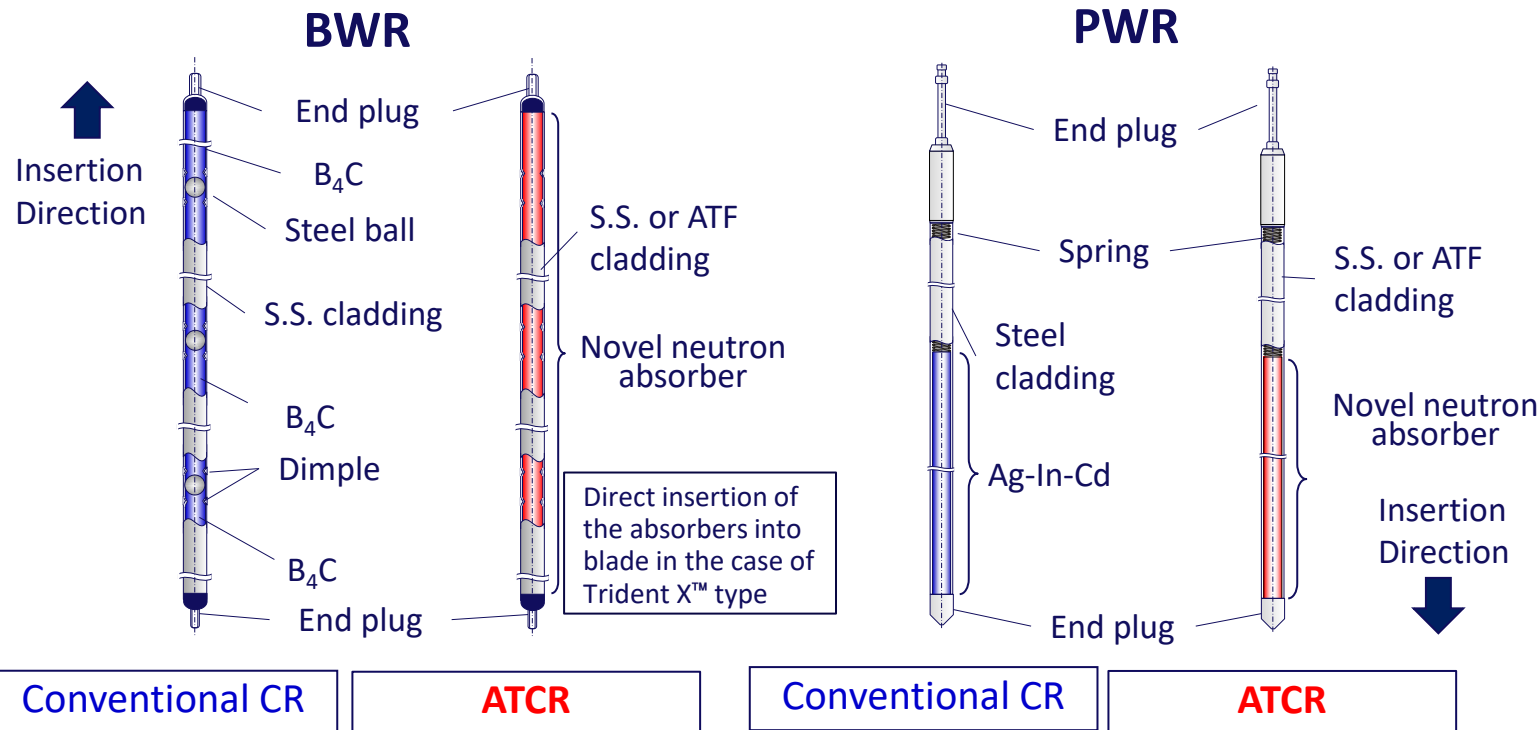
ATCR should have

- Sufficient neutron absorption effect equivalent to or higher than conventional CRs,
- Higher failure temperature than that of conventional CRs (~ 1200 - 1400 °C),
- Favorable compatibility with core component materials (SS, Zircaloy or ATF),
- High melting points comparable to fuel failure temperatures (~2300°C), and
- Favorable miscibility with molten corium and fuel debris.

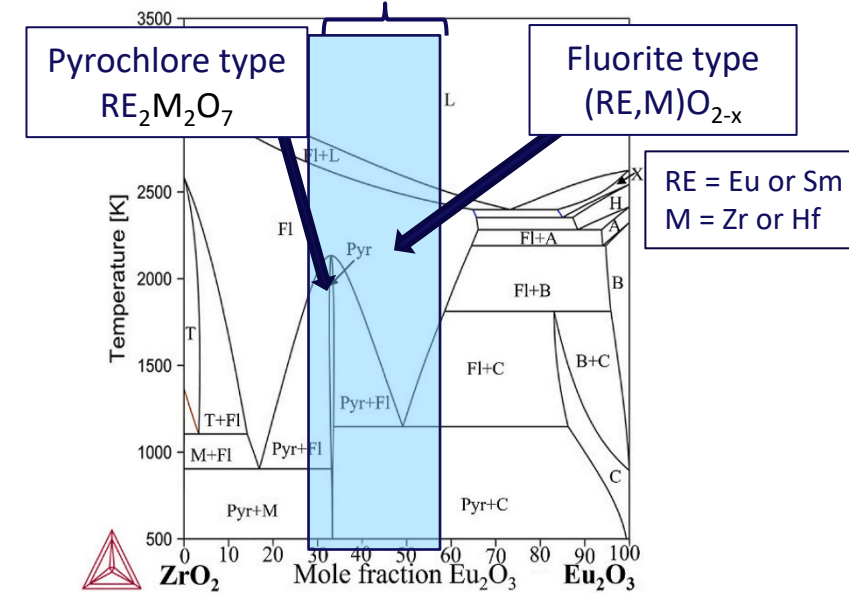
## Candidate Materials

For both PWR & BWR,

- Absorber: RE<sub>2</sub>O<sub>3</sub> stabilized ZrO<sub>2</sub> or HfO<sub>2</sub>, RE (Rare Earth) =Eu or Sm
- Cladding and/or blade: SS, Cr-coated Zircaloy or SiC<sub>f</sub>-SiC



## Composition range

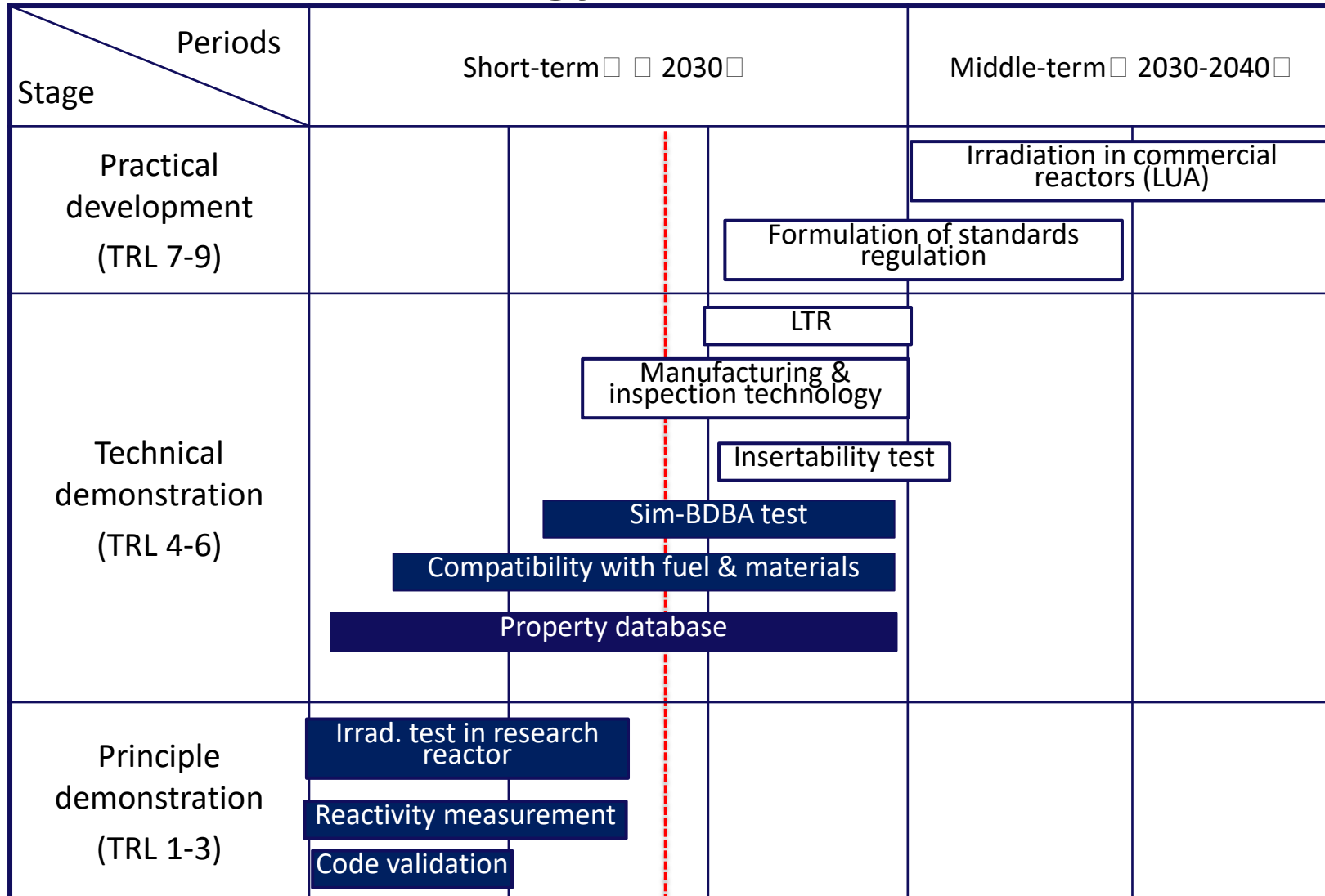


Phase diagram of ZrO<sub>2</sub>-Eu<sub>2</sub>O<sub>3</sub> system

Qu, Gang, et al., Ceramics International 50.14 (2024): 24948-24959.

# 2. ATCR: Roadmap

## Technology Readiness Levels



## 2. Current Status: Neutronic Properties

- Enough neutronic reactivity worth comparable to or higher than the conventional absorbers
- Applicable to conventional CR assemblies without significant change in design and reactor operation
- Extended neutronic lifetime by 2 - 5 times, resulting in reduction of the storage space of used CRs

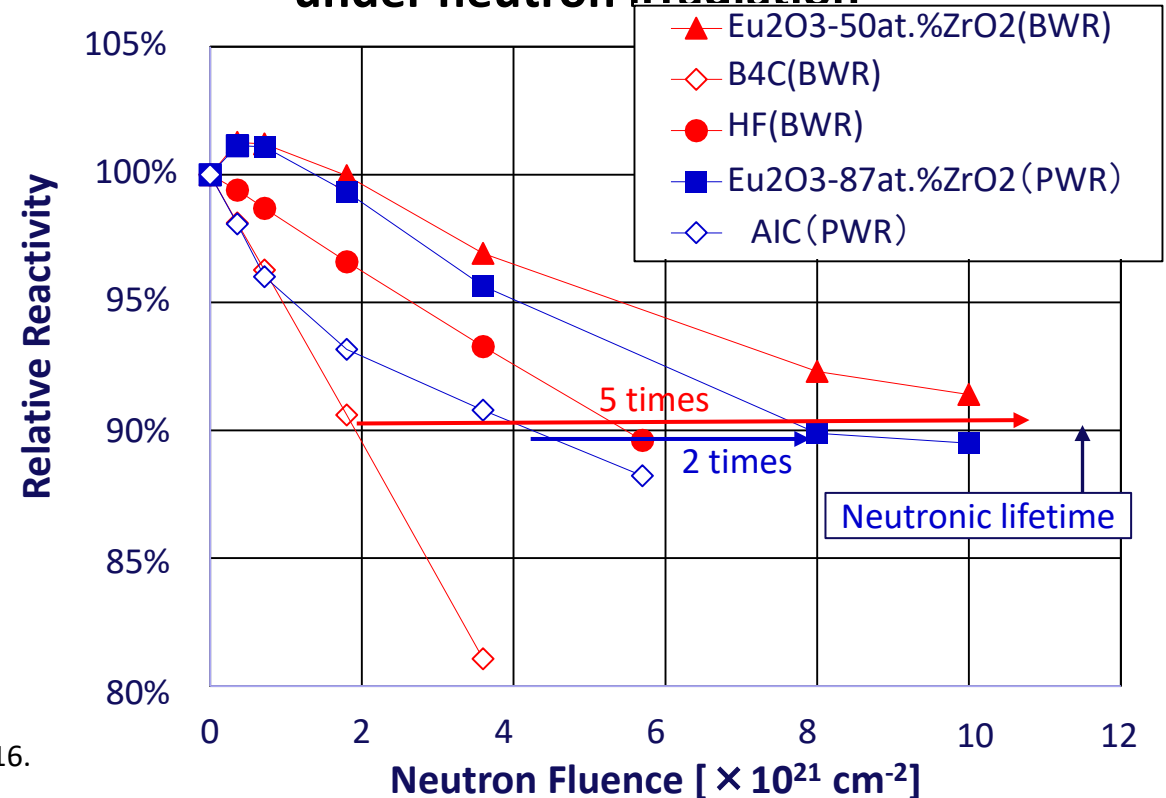
CR reactivity worth in LWRs  
(Continuous-energy Monte Carlo code: MVP)

Materials	Reactivity Worth [%Δk/k']	
	BWR	PWR
Sm <sub>2</sub> O <sub>3</sub> -HfO <sub>2</sub>	-15.9	-5.4
Sm <sub>2</sub> O <sub>3</sub> -ZrO <sub>2</sub>	(-14.5 ~ -14.7)*	-4.9
Eu <sub>2</sub> O <sub>3</sub> -HfO <sub>2</sub>	-19.2	-6.4
Eu <sub>2</sub> O <sub>3</sub> -ZrO <sub>2</sub>	-18.5	-6.2
B <sub>4</sub> C	-18.6	
Ag-In-Cd		-5.2
Composition equivalent worth to B <sub>4</sub> C or AIC	Eu <sub>2</sub> O <sub>3</sub> -50 at% ZrO <sub>2</sub>	Eu <sub>2</sub> O <sub>3</sub> -87 at% ZrO <sub>2</sub>

\* Estimated value

H. Ohta, et al., *Top Fuel 2016*, Boise, Idaho, USA, 11-15 Sep. 2016.  
H. Ohta, et al., *AESJ Annual Meeting*, 8 Sep. 2016.

Change in neutronic reactivity worth under neutron irradiation



## 2. Current Status: Neutron Irradiation Stability

- RE isotopes do not generate gases by neutron absorption due to (n,γ) reaction.
- Neutron capture product with the same element and higher mass numbers without change in composition
- Expected lower irradiation swelling than conventional absorbers
- Neutron irradiation test results in research reactor KUR indicated negligible change in weight and dimension under low neutron fluence condition.
- The feasibility of LTR or LUA irradiation tests in a commercial LWR is being investigated.

**Neutron capture products have also high neutron capture cross-sections.**

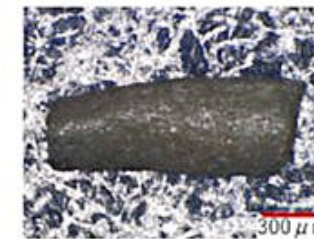
- $^{151}\text{Eu} \rightarrow ^{152}\text{Eu} \rightarrow \underline{^{153}\text{Eu}} \rightarrow ^{154}\text{Eu} \rightarrow ^{155}\text{Eu} \rightarrow ^{156}\text{Eu} \rightarrow \dots$
- $^{146}\text{Sm} \rightarrow ^{147}\text{Sm} \rightarrow ^{148}\text{Sm} \rightarrow ^{149}\text{Sm} \rightarrow ^{150}\text{Sm} \rightarrow ^{151}\text{Sm} \rightarrow \underline{^{152}\text{Sm}} \rightarrow ^{153}\text{Sm} \rightarrow ^{154}\text{Sm} \rightarrow \dots$

Red: Natural isotopes, underline: most abundance

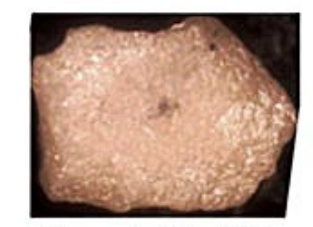
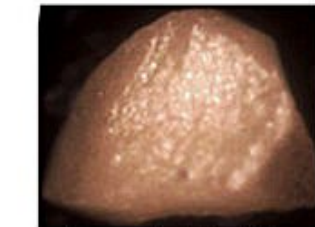
Weight change of  $\text{Sm}_2\text{O}_3$ -50 mol%  $\text{ZrO}_2$  sintered samples after irradiation in Kyoto University Reactor (KUR)

Sample No.	Neutron fluences (n/cm <sup>2</sup> )	(1)	(2)	(3)
Pre-irrad.		1.95 mg	6.21 mg	5.15 mg
1 <sup>st</sup> post-irrad.	$2.39 \times 10^{19}$	1.97 mg	6.15 mg	5.11 mg
2 <sup>nd</sup> post-irrad.	$2.13 \times 10^{19}$	1.91 mg	6.24 mg	5.16 mg

Before Irradiation



After 2<sup>nd</sup> Irradiation



Sample No.(1)

Sample No.(2)

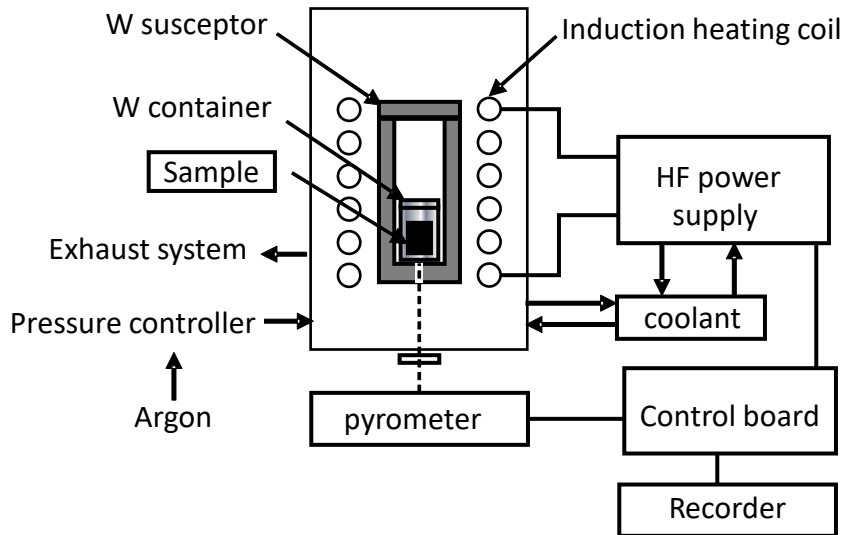
Sample No.(3)

H. Ohta, et al., *NuMat 2022*, Ghent, Belgium, October 24-28, 2022.

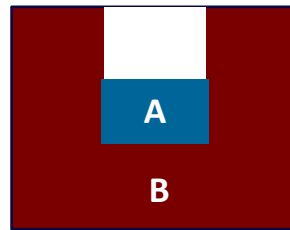
## 2. Current Status: Compatibility with core component materials

- Favorable compatibility with core component materials, such as SS, Zircaloy, B<sub>4</sub>C, Ag-In alloy, and a mixture of two of these materials, in the temperature range of 1600-2000 °C
- Limited corrosion rate with Cr-coated Zircaloy, FeCrAl, and SiC up to 2000 °C
- Good coexistence with (U,Zr)O<sub>2</sub> as corium or fuel debris simulat at 2200-2600 °C

### Experimental Set-up



### Sample



- Temperature: 1600-2000 °C
- Holding time: 10-60 min.
- Atmosphere: Argon

### Test grid

Concept	A: core component materials 5mm in diameter, 3mm height	B: Neutron absorbers ID 5.5 mm, IH 7 mm, 5 mm height
SS clad ATCR	<ul style="list-style-type: none"> <li>➤ Fe</li> <li>➤ SS</li> <li>➤ SS+Zircaloy-4</li> <li>➤ B<sub>4</sub>C</li> <li>➤ SS+B<sub>4</sub>C</li> <li>➤ Ag-In alloy</li> </ul>	<ul style="list-style-type: none"> <li>➤ fluorite (Eu,Hf)O<sub>2-x</sub></li> <li>➤ fluorite (Eu,Zr)O<sub>2-x</sub></li> <li>➤ pyrochlore Eu<sub>2</sub>Hf<sub>2</sub>O<sub>7</sub></li> </ul>
ATF clad ATCR	<ul style="list-style-type: none"> <li>➤ Zircaloy-4<sup>*1</sup></li> <li>➤ FeCrAl<sup>*1,2</sup></li> <li>➤ SiC<sup>*1</sup></li> </ul>	<ul style="list-style-type: none"> <li>➤ fluorite (Eu,Zr)O<sub>2-x</sub></li> <li>➤ fluorite (Sm,Zr)O<sub>2-x</sub></li> </ul>
Molten fuel	➤ (U,Zr)O <sub>2</sub>	➤ fluorite (Eu,Hf)O <sub>2-x</sub>

K. Nakamura, et al, 11th EPRI/DOE/INL Joint Workshop on Accident Tolerant Fuel, 28–29 Mar 2022.

K. Nakamura, et al, 27th International QUENCH Workshop 27 - 29 Sep. 2022

<sup>\*1</sup> Assumption that unpressurized ATCR cladding tubes will not burst up to 2000°C

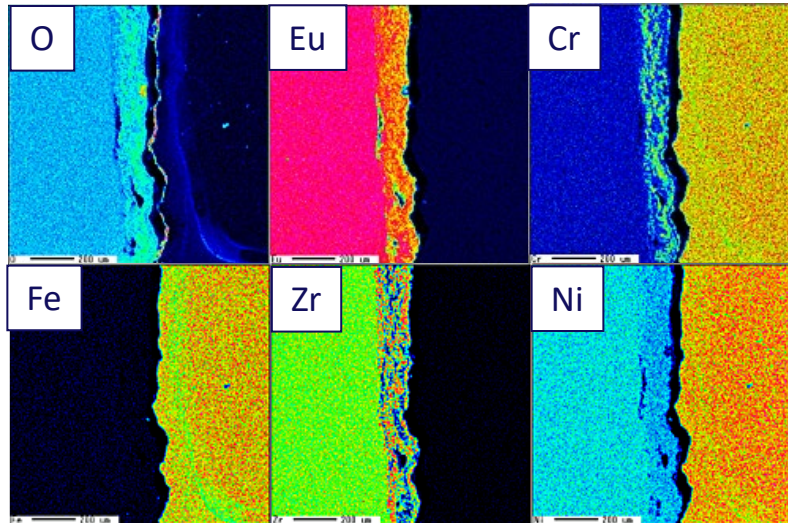
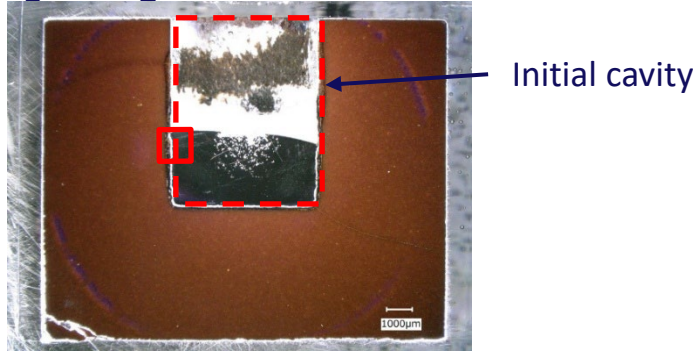
<sup>\*2</sup> Fe<sub>0.777</sub>Cr<sub>0.13</sub>Al<sub>0.07</sub>Mo<sub>0.02</sub>Si<sub>0.002</sub>Y<sub>0.0005</sub> in wt. fraction

## 2. Current Status: Compatibility with core component materials

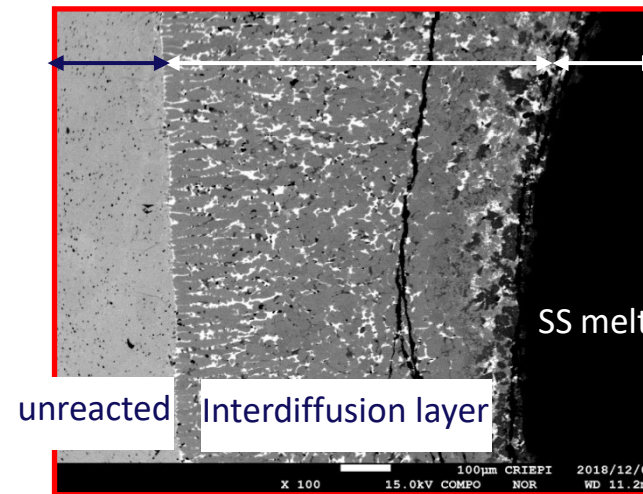
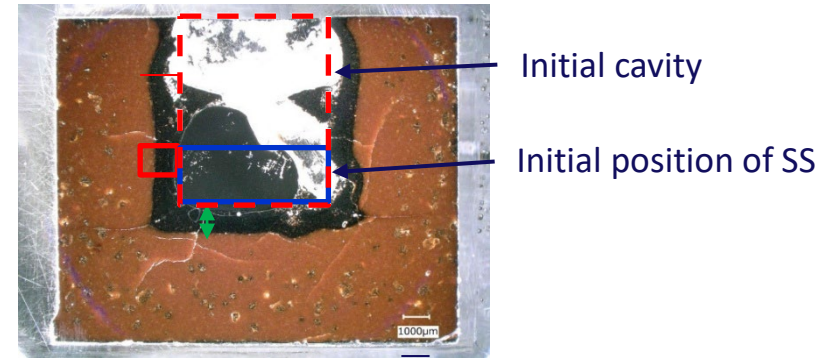
### SS clad ATCR

\* Simulating of ATCR with SS cladding

SS /  $\text{Eu}_2\text{O}_3\text{-ZrO}_2$  at 1600°C held for 60 min.



SS /  $\text{Eu}_2\text{O}_3\text{-ZrO}_2$  at 2000°C held for 10 min.



SEI: Secondary electron image,  
BEI: Backscattered electron image

➤ Interdiffusion layer thickness: 140 µm at 1600°C for 60 min, and 1500 µm at 2000°C for 10 min

## 2. Current Status: Compatibility with core component materials

### ATF\* clad ATCR

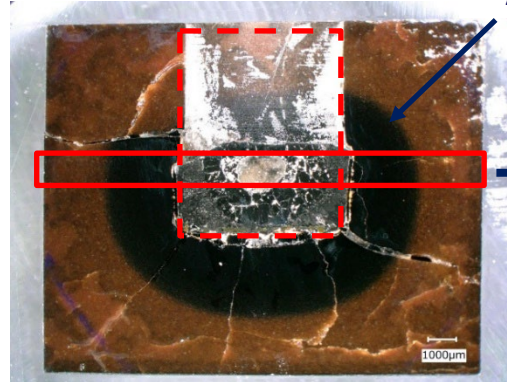
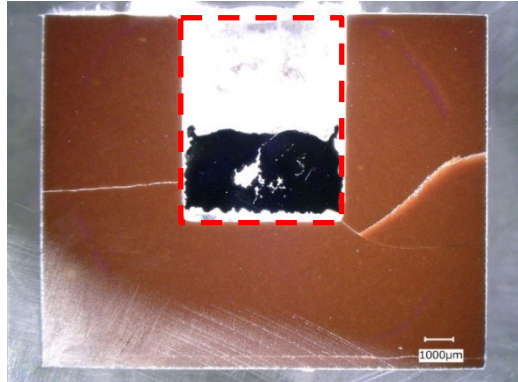
\* Simulating of Cr coated Zircaloy cladding

1800°C for 30 min

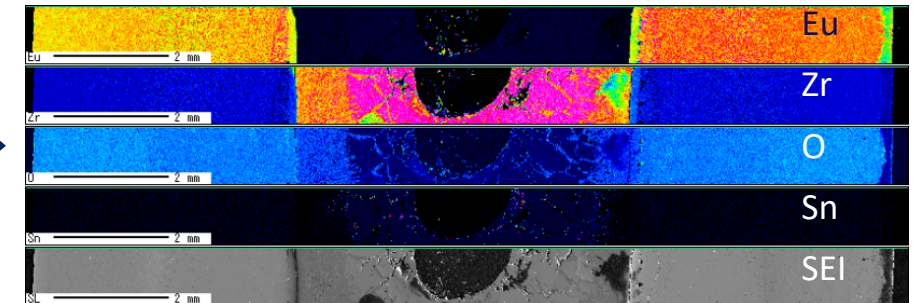
2000°C for 10 min

Zircaloy-4

Fluorite  
(Eu,Zr)O<sub>2-x</sub>



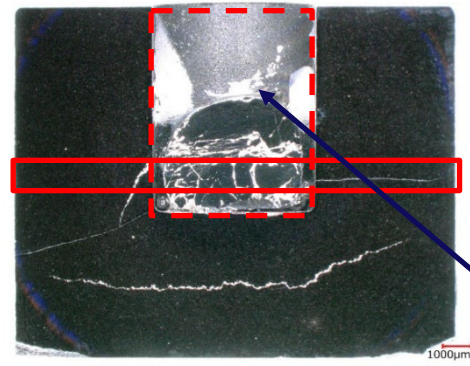
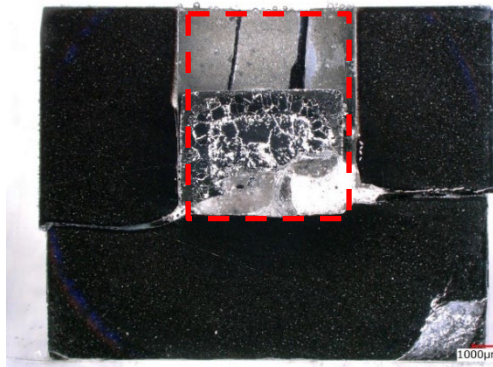
Hypo-stoichiometric composition region



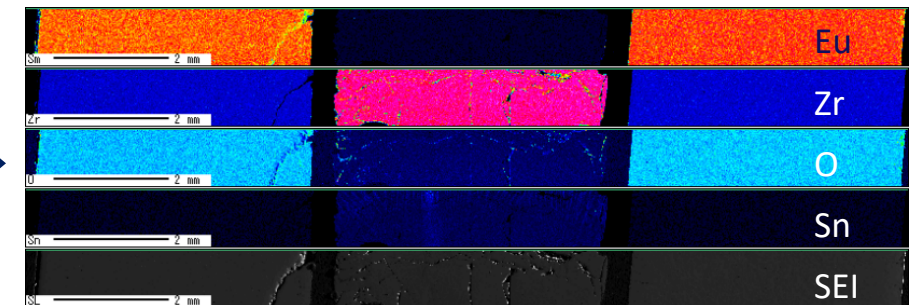
Interdiffusion layer thickness 230µm

Zircaloy-4

Fluorite  
(Sm,Zr)O<sub>2-x</sub>



Oxygen stabilized α-Zr as solid

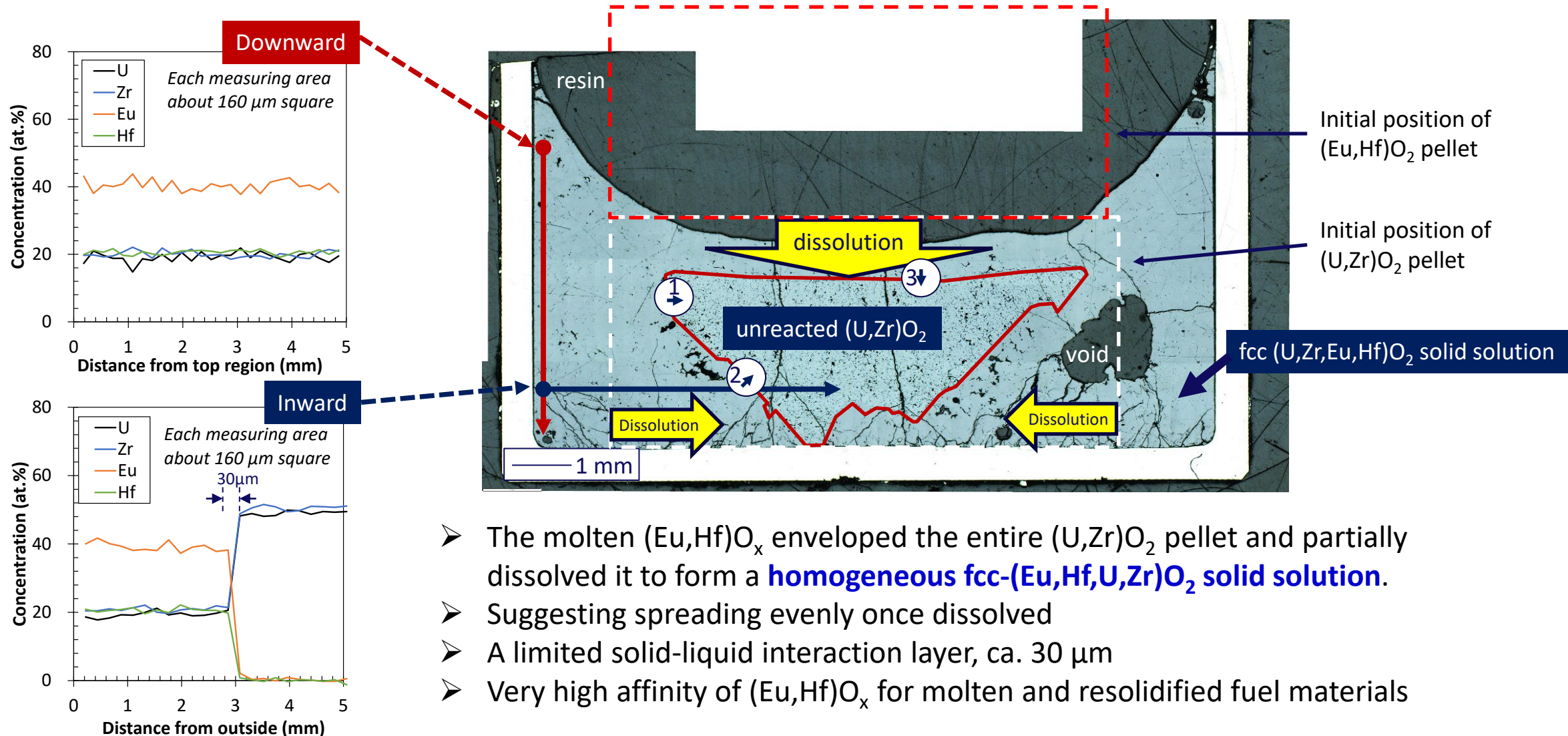


Interdiffusion layer thickness 30µm

- Limited interdiffusion layer formation with oxygen dissolved Zircaloy at both 1800 °C and 2000 °C.
- Diffusion of oxygen in the absorber into the Zircaloy-4 resulted in the formation of hypo-stoichiometric regions in the absorber and the formation of solid α-Zr (O) in Zircaloy-4.

## 2. Current Status: Late phase severe accident phenomena

### Miscibility of $(\text{Eu,Hf})\text{O}_2$ and Corium $(\text{U,Zr})\text{O}_2$ at $2600^\circ\text{C}$ for 3 min.





## 2. Current Status: Stability in Primary Coolant

- RE<sub>2</sub>O<sub>3</sub> has a high melting point but is highly hygroscopic when in contact with water or moisture even at room temperature, producing powdered RE(OH)<sub>3</sub>.
- Mixing with ZrO<sub>2</sub> or HfO<sub>2</sub> as a stabilizer significantly reduce the hygroscopicity.
- Long-term stability of RE<sub>2</sub>O<sub>3</sub> - MO<sub>2</sub> sintered pellets in PWR primary coolant water condition was confirmed.

### Autoclave tests in PWR primary loop system

- Water volume: 350 L
- Temperature : ~300 °C
- Pressure : ~16 MPa
- Water chemistry:
  - B 1248 – 1310 wt ppm
  - Li 6.8 - 7.0 wt ppm
  - H<sub>2</sub> ≤ 2.7 wt ppm
  - O<sub>2</sub> ≤ 0.5 wt ppb
- Period : ~63 days (15, 16, and 32 days)

Samples	Weight change ratio
Sm <sub>2</sub> O <sub>3</sub> -HfO <sub>2</sub>	No data*
Sm <sub>2</sub> O <sub>3</sub> -ZrO <sub>2</sub>	-0.0822% ~ -0.0075%
Eu <sub>2</sub> O <sub>3</sub> -HfO <sub>2</sub>	-0.0246% ~ +0.0339%
Eu <sub>2</sub> O <sub>3</sub> -ZrO <sub>2</sub>	+0.0253% ~ +0.0798%

\* Complete powderization due to non-uniform mixing during the manufacturing process



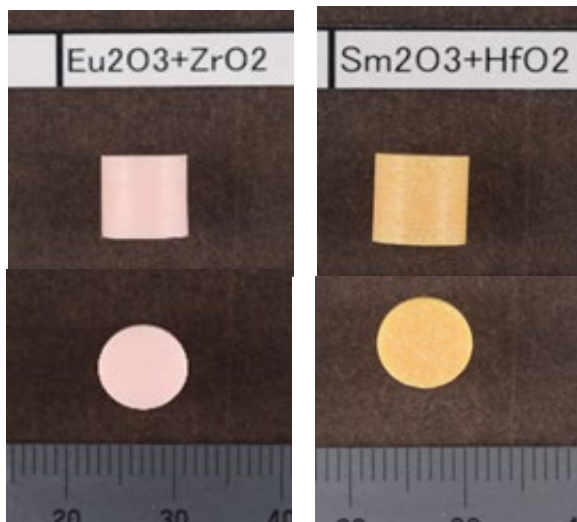
Eu<sub>2</sub>O<sub>3</sub>-50 mol% ZrO<sub>2</sub> sintered pellets

H. Ohta, et al., *NuMat 2022*, Ghent, Belgium, October 24-28, 2022.

## 2. Current Status: **Manufacturability**

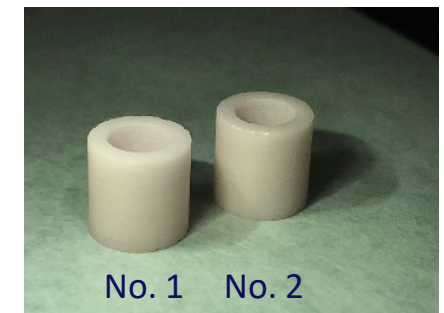
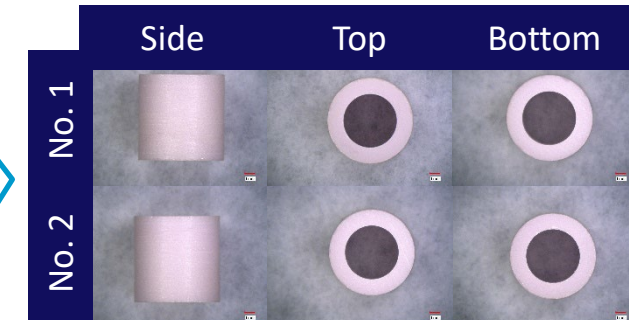
- Depending on the CR design, it may be possible to manufacture high-density neutron absorbers such as solid or annular pellets, rods, plates, or granules using conventional manufacturing techniques, such as
- Powder compaction,
  - Slip casting, and
  - Hot Isostatic Press.

Solid pellets



Annular pellets

items	Preliminary specifications	No. 1	No. 2
Chemical composition	$\text{Eu}_2\text{O}_3$ -50mol% $\text{ZrO}_2$		
Crystal structure	Fluorite-(Eu,Zr) $\text{O}_2$		
Outer diameter (mm)	$8.0 \pm 0.05$	7.998	7.983
Inner diameter (mm)	$5.0 \pm 0.05$	5.016	5.020
Height (mm)	$8.0 \pm 0.05$	8.033	8.035
Chamfering	-		
Purity of oxide raw materials	$\text{ZrO}_2$ >99.9%, $\text{Eu}_2\text{O}_3$ >99.9%		



# 3. Conclusion

- To improve nuclear safety in LWRs, CRIEPI has been developing a concept of ATCR, which replace the neutron absorbers in current PWR and BWR with rare-earth sesquioxide-stabilized zirconia or hafnia, which is believed to simultaneously achieve extension of lifetime and improved accident tolerance.
- Overview of the current developments of the ATCR was summarized:
  - Neutronic Properties
  - Neutron Irradiation Stability
  - Compatibility with core component materials
  - Late phase severe accident phenomena
  - Stability in Primary Coolant
  - Manufacturability
- ATCRs with extended neutronic lifetime, will not be damaged before fuel failure in accidents, which is expected to reduce the risk of early core damage, early release of FPs, and re-criticality.

Why not add these to your wish list in 2026?



**NUTHOS-15**

Kashiwa-no-ha, JAPAN

**September 28 - October 1, 2026.**

**Kashiwa-no-ha, Chiba, JAPAN**

*1 hour by train or bus from Narita Airport*

**Abstract Deadline: Dec. 31, 2025 Extended**

**Topics:**

- General Thermal-Hydraulics
- Advanced Thermal-Hydraulics
- Plant Operations
- Regulation, Accident Analysis and Source Term
- Thermal Hydraulics and Safety of Advanced Reactors
- Machine Learning and Artificial Intelligence
- Big Data Applications
- Advanced-Technology Fuels

**Technical Tour: Fukushima-Daiichi NPP**

# FDR2026

**October 02-05, 2026**

**J-Village, Naraha, Fukushima, JAPAN**

*4+ hours by train from Haneda Airport*

**Abstract Deadline: April 30, 2026**

**Tracks:**

- Accident Analysis, Fuel Debris Retrieval
- Robot Technology, Remote Control System
- Radiation Measurement and Analysis
- Waste Management

**Technical Tour: Fukushima-Daiichi NPP**



**October 12 - 15, 2026**

**Shinagawa, Tokyo, JAPAN**

*30 min by train from Hanada Airport*

**Abstract Deadline: Jan 16, 2026**

**Tracks:**

- Operation and Experience
- Advances in Designs, Materials, and Manufacturing
- Evolutionary and Innovative Advanced Technology Fuels (ATF)
- Modeling, Analysis, and Methods
- Transient Fuel Behavior and Safety Related Issues
- Used Fuel Storage, Transportation, and Re-Use
- Advanced Reactor Fuel Designs and Performance

Thank you for your attention!





**Robert Farkas**

HUN-REN EK

## **Post-test examination of the integral air ingress experiment CODEX-ATF-AIT**

The CODEX-ATF-AIT integral air ingress test was successfully performed at the HUN-REN Centre for Energy Research (EK), Budapest. The test section included an electrically heated seven-rod bundle composed of Cr coated optZIRLO™ cladding tubes provided by the Czech Technical University in Prague (CTU). The design of the test section was similar to the previous CODEX tests [1][2][3]. The fuel rods were filled with zirconia pellets. The rods were pressurized by krypton. The bundle was fixed by Cr coated Zr spacer grids. Electrical heating with two tungsten heaters in each rod was used. External heating was also applied to the test section. The bundle was covered by a Cr-coated Zr shroud and several thermal insulation layers. The proposed scenario focused on covering several phenomena of fuel behavior during accidents (burst, oxidation, nitriding, eutectic formation).

In the preparatory phase the facility was heated up to 600 °C in steam – argon flow using both external heaters and fuel rod heaters. The pre-oxidation phase continued with the same flow rates and with stepwise increased heating power on the rods. During the heat-up phase the rods were pressurized and cladding burst took place between 750-800 °C on most of the rods. The opening allowed the coolant to enter the rods and start chemical reactions on both sides of the cladding. In the intermediate cool-down phase the temperatures were reduced below 750 °C. In the steam-air phase the temperature increase was very smooth compared to the reference experiment CODEX-AIT-3 [2]. The reason of the slower temperature increase was the protective effect of the Cr coating. The duration of air ingress phase in the reference experiment was 1 hour with 1600 °C maximum cladding temperature, and it was 1.5 hour in the CODEX-ATF-AIT with 1545 °C maximum cladding temperature. The temperature profile significantly changed during the air ingress phase similar to the reference experiment: the maximum temperature moved from the upper section of the bundle to lower elevations due to the intense chemical interactions in the less oxidized and/or melted lower part. The maximum shroud temperature was similarly around 1470 °C at 300, 500 and 700 mm elevations.

The outlet gas composition showed that during the air ingress phase steam and oxygen starvation conditions were established. The partial consumption of nitrogen indicated the formation of nitrides as well. The total of 1.4 g hydrogen was produced during the pre-oxidation phase and 3.3 g of hydrogen during the air ingress phase. Slow cool-down of the bundle was performed in argon flow in order to avoid interactions that might take place during water quench.

Post-test examinations (endoscopy, LOM, SEM, EDX) focused on the identification of cladding degradation mechanisms. At the lower half of the bundle (between about 200 and 500 mm) the rods did not suffer any ballooning and the Cr coating remained intact and could prevent the zirconium oxidation in the pre-oxidation phase. The main degradation mechanism of rods at these elevations was the Cr-Zr eutectic melt formation (Cr diffused into the Zr cladding wall to a large extent) and its fast oxidation/nitriding in the last phase of the experiment. From 600 mm upwards, all the pressurized rods were ballooned and the Cr coating became cracked on their surfaces. The zirconium oxidation started locally through the cracks of the Cr layer in the pre-oxidation phase and continued in the air ingress phase. These rods were strongly oxidized and nitrided. The oxygen penetrated into the zirconium metal prohibited the Cr diffusion into the cladding wall. The cladding tube walls often cracked through where the local oxidation started. In the case of the non-pressurized rod, the Cr coating remained intact and could prevent the zirconium oxidation both in the pre-oxidation phase and air ingress phase because of the not too high (lower than the Cr-Zr eutectic formation) temperatures at these elevations of the bundle.

The CODEX-ATF-AIT test showed that under high-temperature air ingress accident conditions, the bundle with Cr-coated components exhibited a longer coping time compared to bundles with conventional fuel materials. The observed fuel degradation phenomena were similar in both cases; however, the presence of the Cr coating led to eutectic formation and localized melting.

- [1] Farkas, R., Hózer, Z., Nagy, I., Vér, N., Szabó, P., Horváth, M., Kostka, P., Lajtha, G. (2023). Experimental simulation of selected design extension condition scenarios without core meltdown in the CODEX facility. *Progress in Nuclear Energy*, 161, 104720.
- [2] Farkas, R., Hozer, Z., Nagy, I., Ver, N., Horvath, M., Steinbrück, M., Stuckert, J., Grosse, M. (2022). Effect of steam and oxygen starvation on severe accident progression with air ingress. *Nuclear Engineering and Design*, 396, 111884.
- [3] Hózer, Z., Windberg, P., Nagy, I., Maróti, L., Matus, L., Horváth, M., Csordás, A., P., Balaskó, M., Jani, P. (2003). Interaction of failed fuel rods under air ingress conditions. *Nuclear Technology*, 141(3), 244-256.



# Post-test examination of the integral air ingress experiment CODEX-ATF-AIT

Róbert Farkas, Nóra Vér, Berta Bürger, Zoltán Hózer, Anna Pintér-Csordás

*30th International QUENCH Workshop*

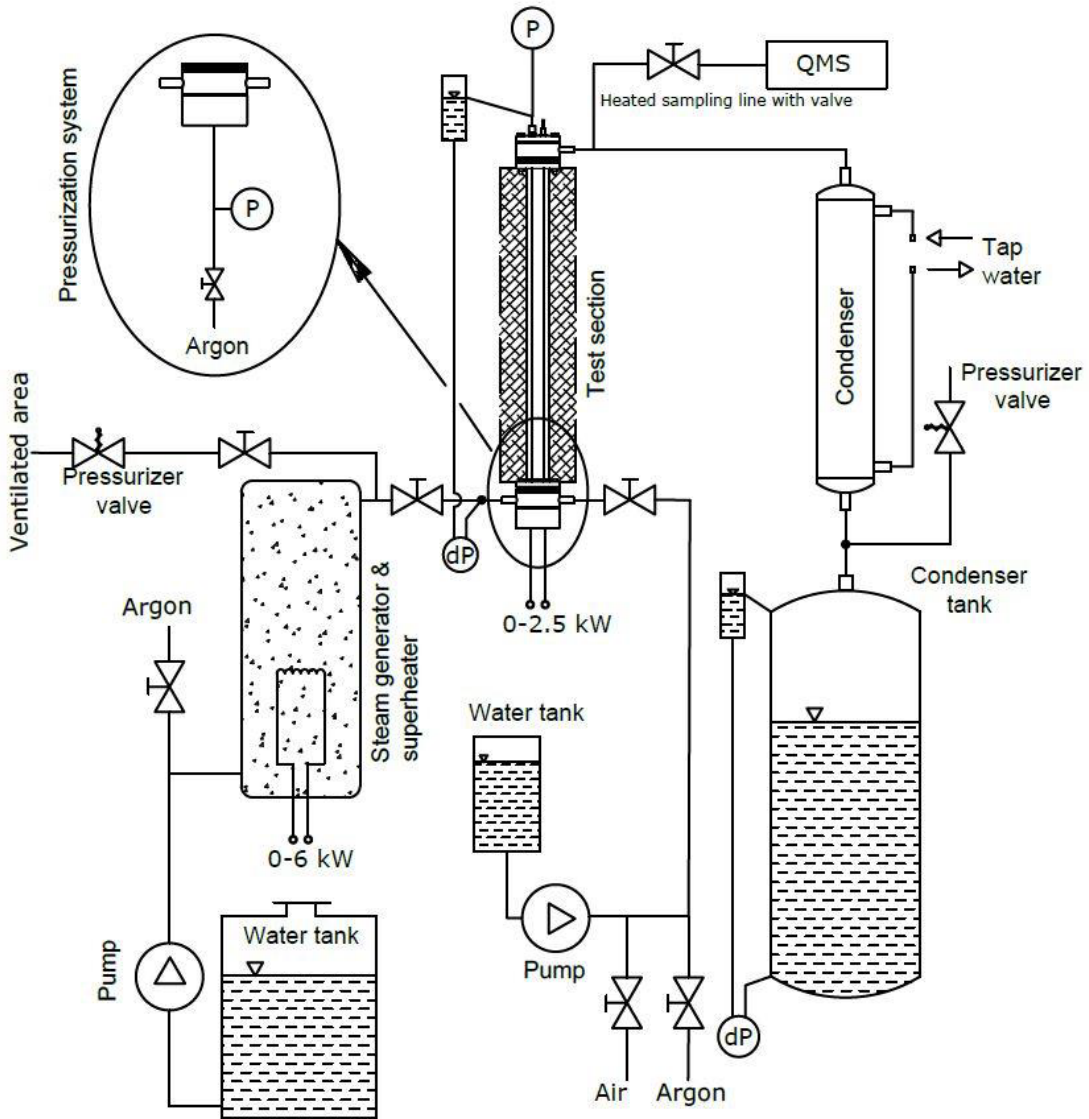
*Karlsruhe Institute of Technology, Campus North, H.-von-Helmholtz-Platz 1, 76344 Egg.-Leopoldshafen, Germany*

*16-18 December 2025*

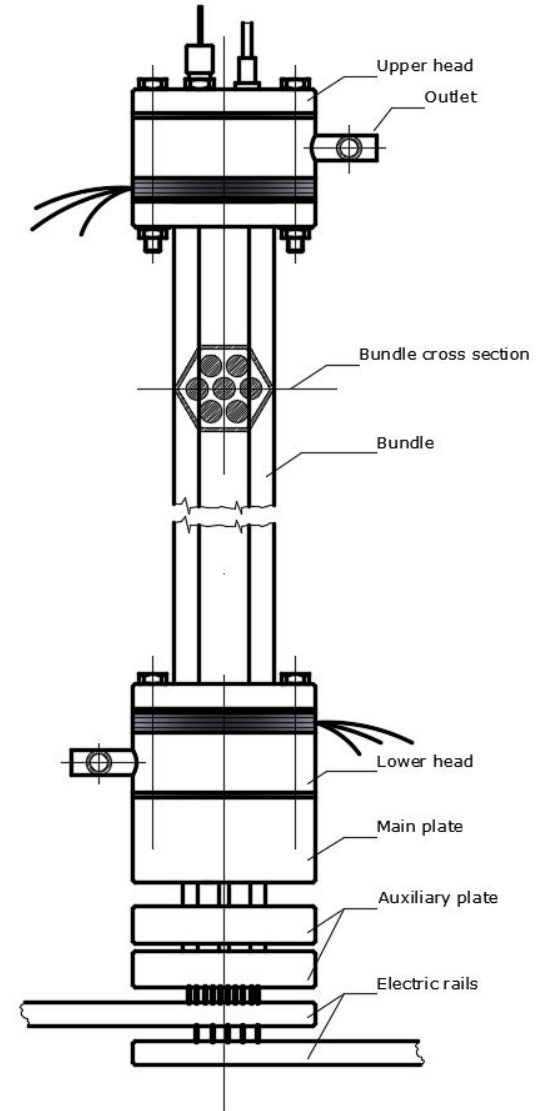


## Integral testing of accident tolerant fuel design under air ingress conditions (CODEX-ATF-AIT)

- The CODEX-ATF-AIT experiment was performed in the framework of the EU OFFERR project.
- The main objective of the proposed test was to check if Cr coating would have a protective role in case of NPP accidents with air ingress.
- The proposed scenario was focused on covering several phenomena of fuel behavior during accidents
  - burst,
  - oxidation,
  - nitriding,
  - eutectic formation.
- CODEX-AIT-3 experiment was chosen for reference test which was an air ingress test conducted with traditional Zr materials.

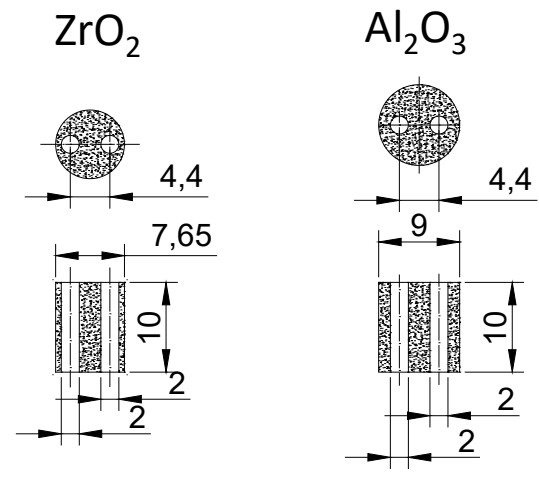
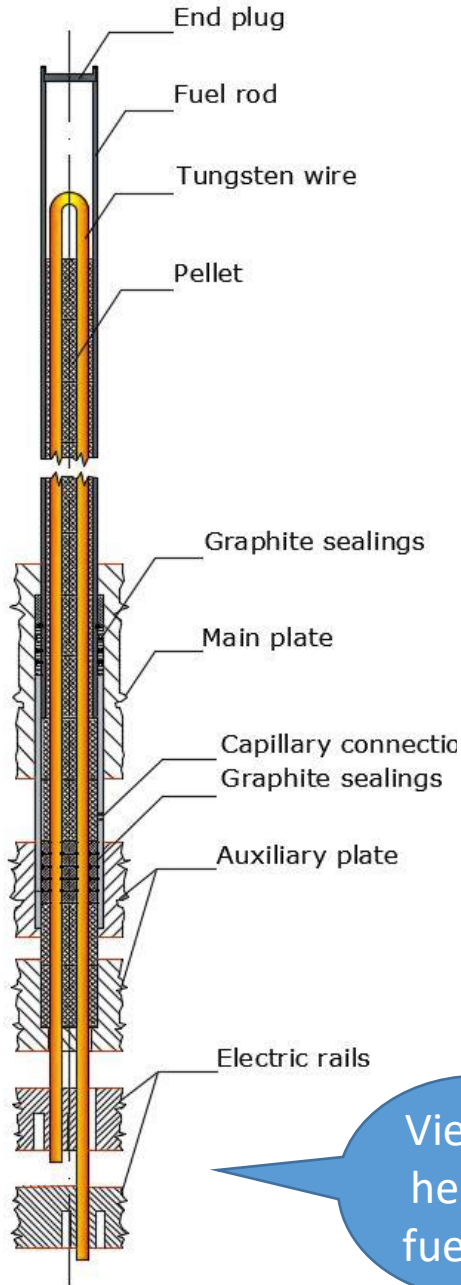


Schematic view of the CODEX facility



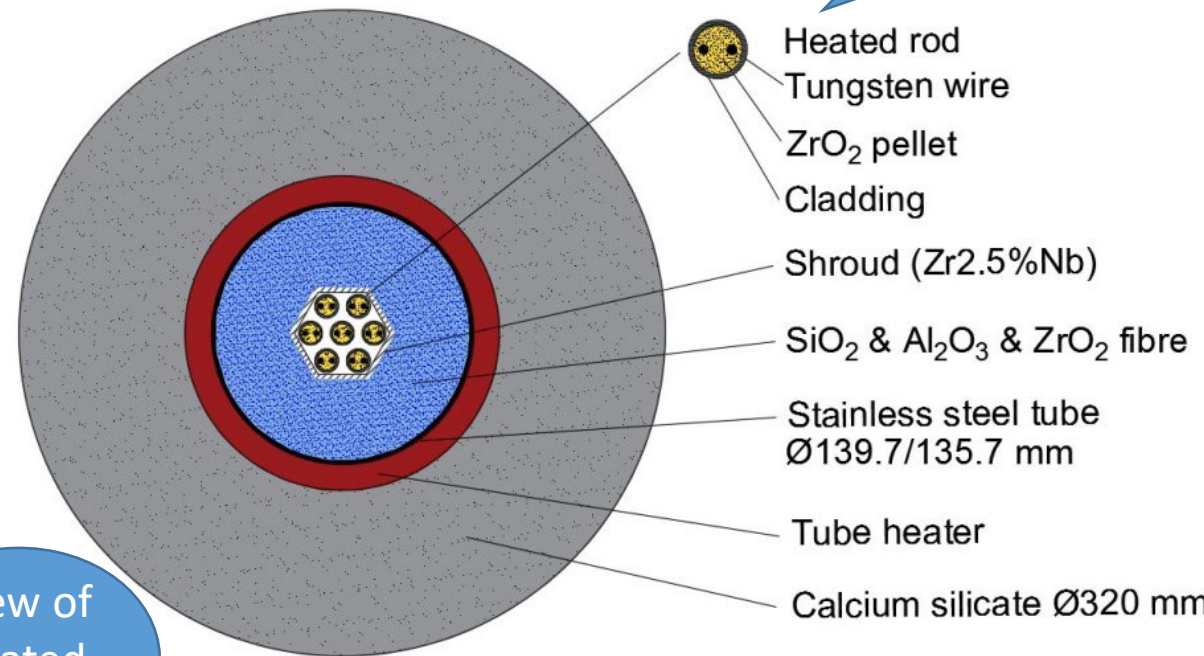
View of the test section with seven-rod bundle

- VVER bundle type: hexagonal arrangement of 7 rods
- 6 rods electrically heated with tungsten heaters
  - CODEX-AIT-3: rod No. 1. (in the center)
  - CODEX-ATF-AIT: rod No. 7. (periphery)
- Rods pressurized
  - CODEX-AIT-3: rod No. 1. (in the center) pressurized with Ar
  - CODEX-ATF-AIT: all rods pressurized with Kr except rod No. 6.
- ZrO<sub>2</sub> ceramic pellets
- 3 spacer grids
- Hexagonal shroud



View of ceramic pellets

Cross section of the test section



View of heated fuel rod



## CODEX-AIT-3

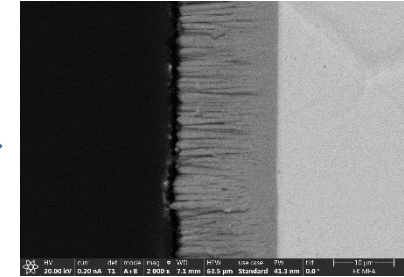
Reference test

Number of fuel rods	7
Cladding of fuel rods	<b>E110G</b>
Length of fuel rods	<b>1000 mm</b>
External diameter of fuel rods	9.1 mm
Cladding wall thickness	0.69 mm
Pellet material	ZrO <sub>2</sub>
Pellet material in the bottom of the rods	Al <sub>2</sub> O <sub>3</sub>
Height of pellet	10 mm
Diameter of pellet	7.65 mm
Hole diameter in the pellet	2 mm
Spacer grid material	<b>Zr1%Nb</b>
Height of spacer grid	10 mm
Thickness of spacer grid	0.4 mm
Number of spacer grids	3
Shroud material	<b>Zr2.5%Nb</b>
Shroud thickness	2 mm
Length of shroud	1000 mm

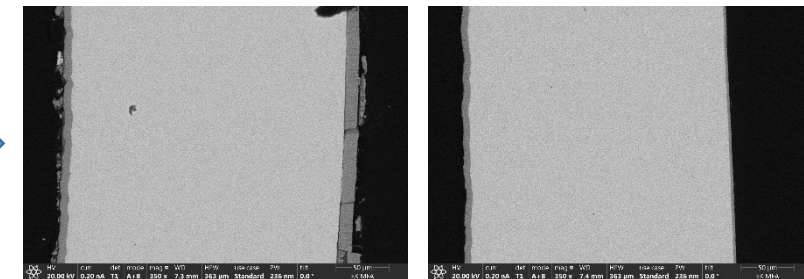
## CODEX-ATF-AIT

Number of fuel rods	7
Cladding of fuel rods	<b>Cr-coated optZIRLO™</b>
Length of fuel rods	<b>900 mm</b>
External diameter of fuel rods	9.1 mm
Cladding wall thickness	0.57 mm
Pellet material	ZrO <sub>2</sub>
Pellet material in the bottom of the rods	Al <sub>2</sub> O <sub>3</sub>
Height of pellet	10 mm
Diameter of pellet	7.65 mm
Hole diameter in the pellet	2 mm
Spacer grid material	<b>Cr-coated Zr1%Nb</b>
Height of spacer grid	10 mm
Thickness of spacer grid	0.4 mm
Number of spacer grids	3
Shroud material	<b>Cr-coated Zr2.5%Nb</b>
Shroud thickness	2 mm
Length of shroud	1000 mm

**Cr coating:** Czech Technical University in Prague, PVD technique



Uniform Cr coating layer around the circumference of the cladding **~15.5 μm**



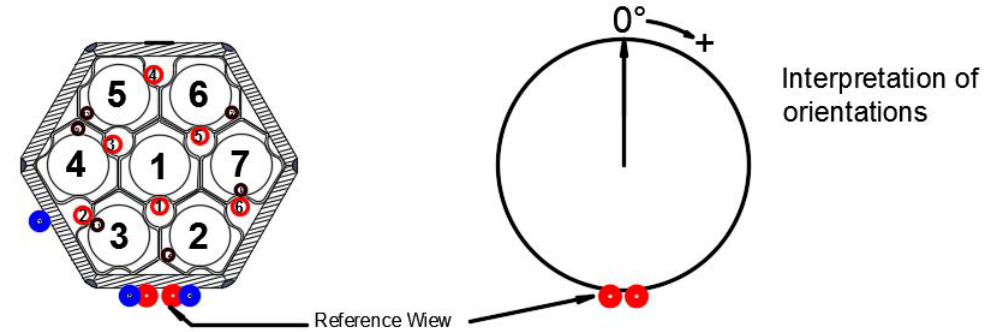
Thickness of the Cr layer on spacer grid

- at the straight sections almost uniform **~10 – 12 μm**
- at the curved parts **~2 – 3 μm**

## On-line measurements and data acquisition:

- **temperatures** (rod surfaces, others: shroud, stainless steel tube, coolant, off-gas, ...)
- **pressures** (system and rods),
- **flowrates** (argon, air),
- **power**,
- **outlet gas composition.**

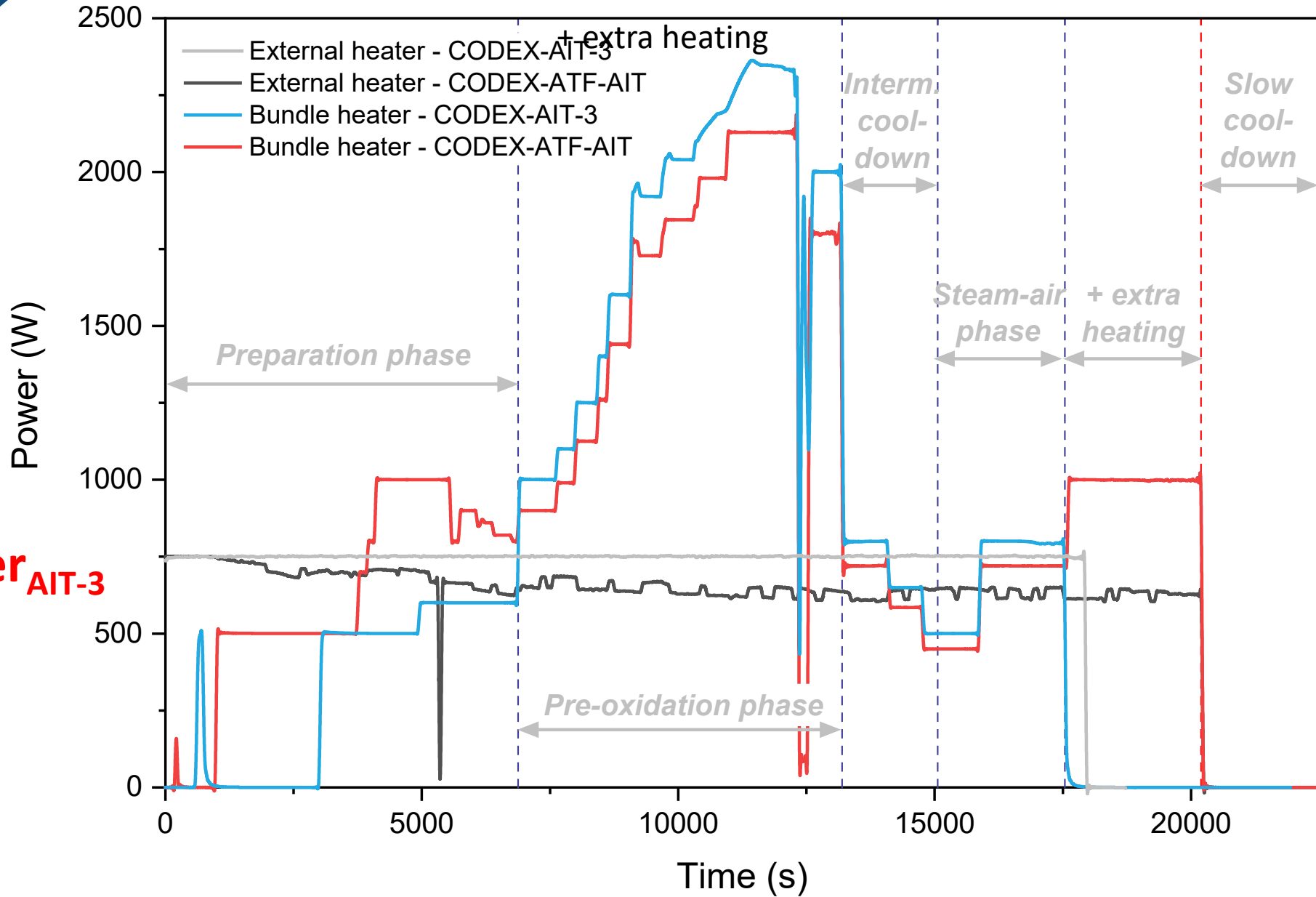
## Thermocouple positions



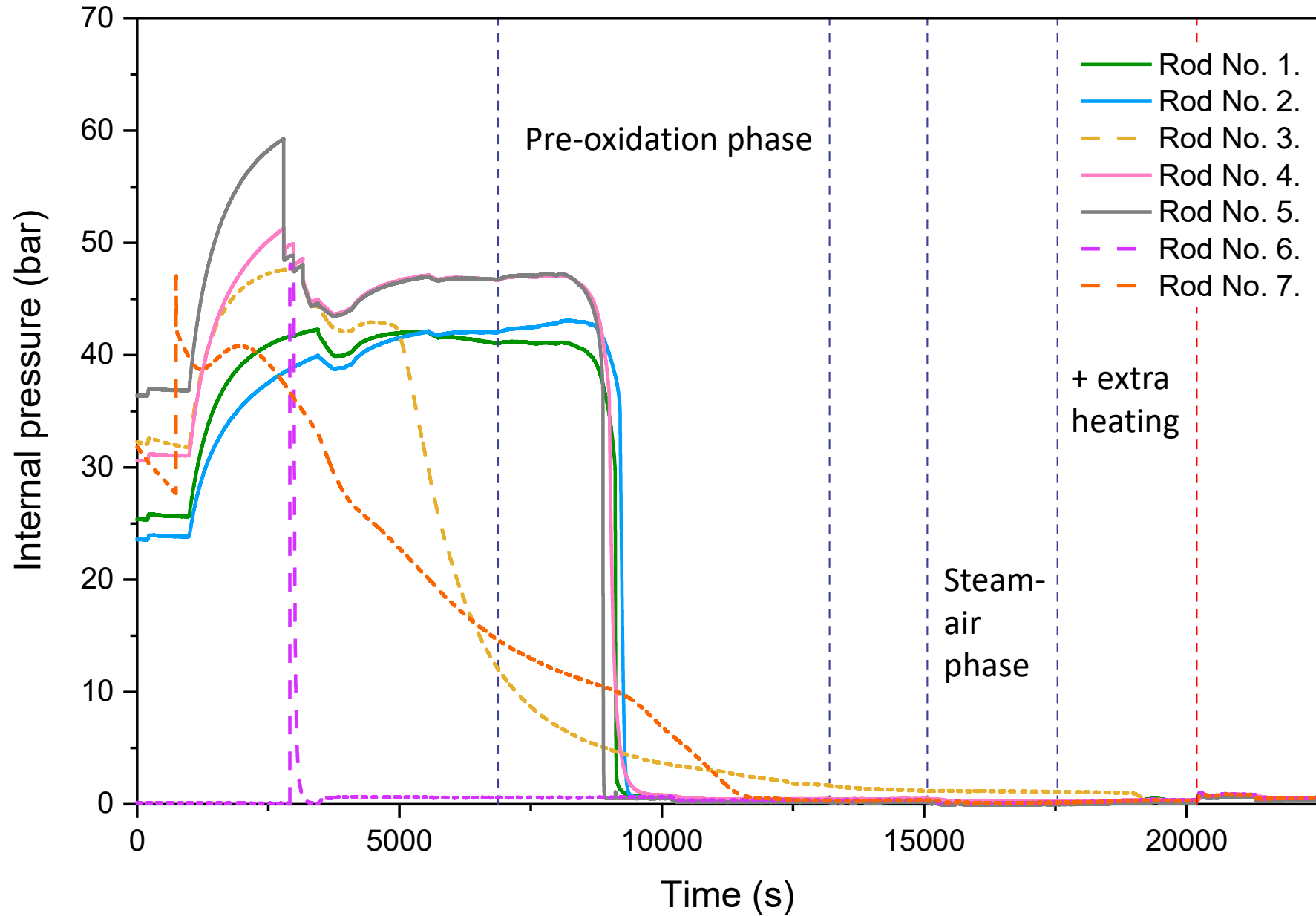
- ① W5Re/W26Re at elevation 850 mm with orientation of 180°
- ② W5Re/W26Re at elevation 650 mm with orientation of 300°
- ③ W5Re/W26Re at elevation 750 mm with orientation of 60°
- ④ W5Re/W26Re at elevation 650 mm with orientation of 60°
- ⑤ W5Re/W26Re at elevation 750 mm with orientation of 180°
- ⑥ W5Re/W26Re at elevation 500 mm with orientation of 180°
- ⑧ "K" type at elevation 50 mm with orientation of 0°
- ⑩ "K" type at elevation 50 mm with orientation of 180°
- ⑪ "K" type at elevation 150 mm with orientation of 300°
- ⑫ "K" type at elevation 150 mm with orientation of 120°
- ⑬ "K" type at elevation 500 mm with orientation of 240°
- ⑭ "K" type at elevation 200 mm with orientation of 240°
- ⑮ "K" type at elevation 750 mm
- ⑯ "K" type at elevation 650 mm
- ⑰ "K" type at elevation 500 mm

**High  
temperature  
thermocouples  
(6 pieces)**

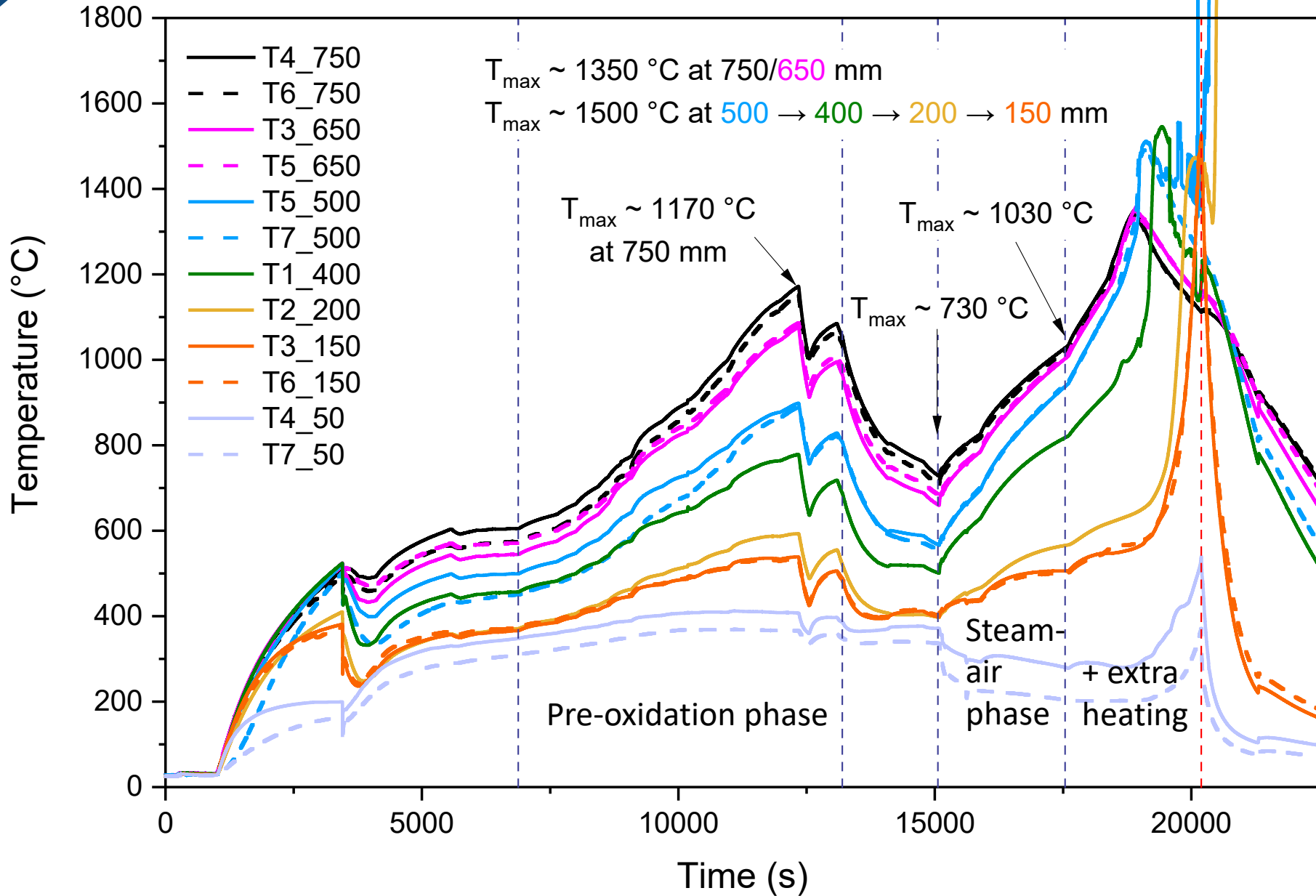
**K-type  
thermocouples  
(26 pieces)**

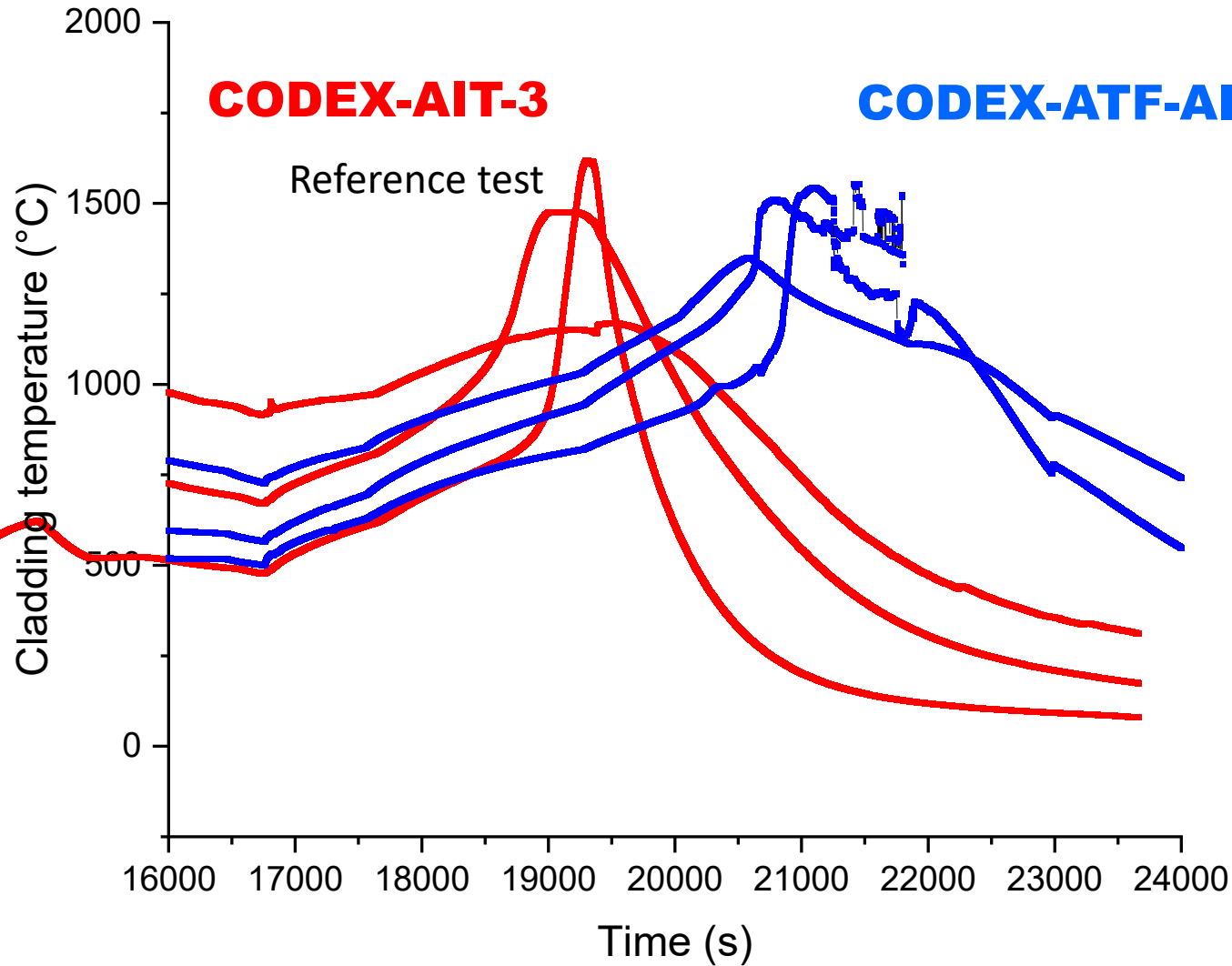


# Rod pressures





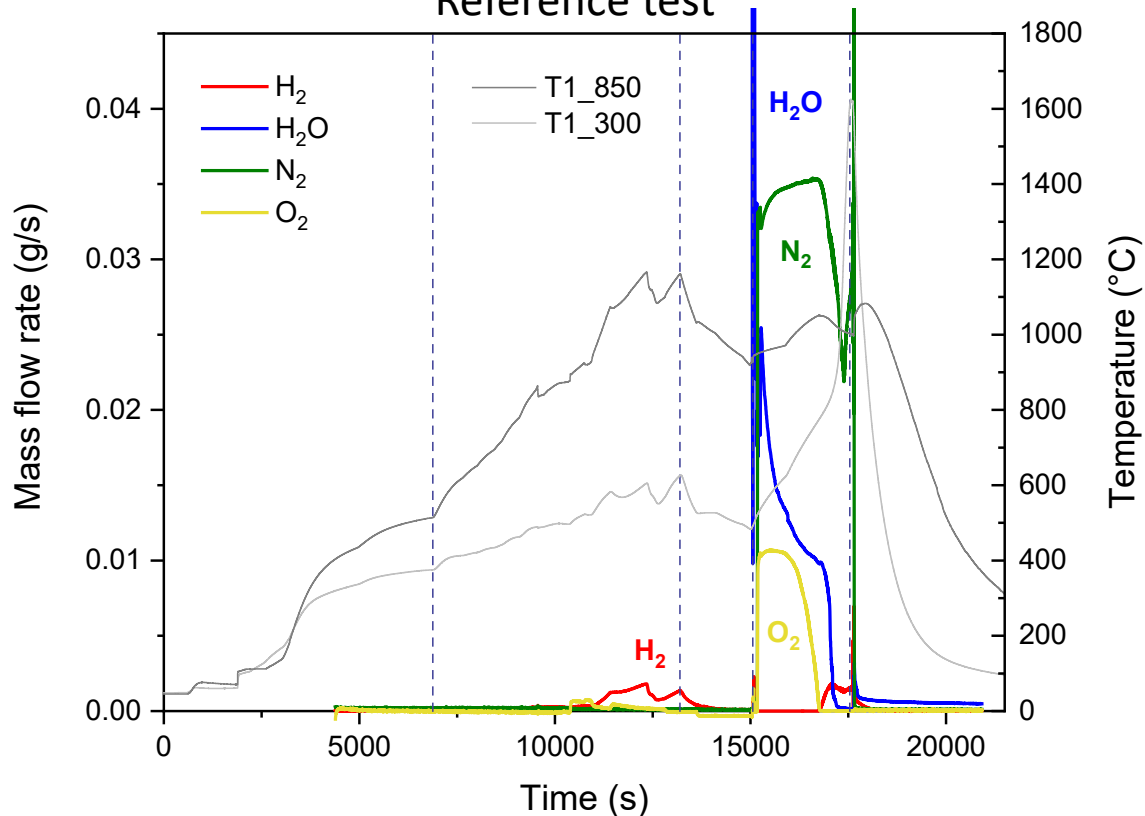




- Extra power was needed with Cr coating to accelerate temperature increase, thanks to the protection of the Cr coating
- Half hour delay in escalation

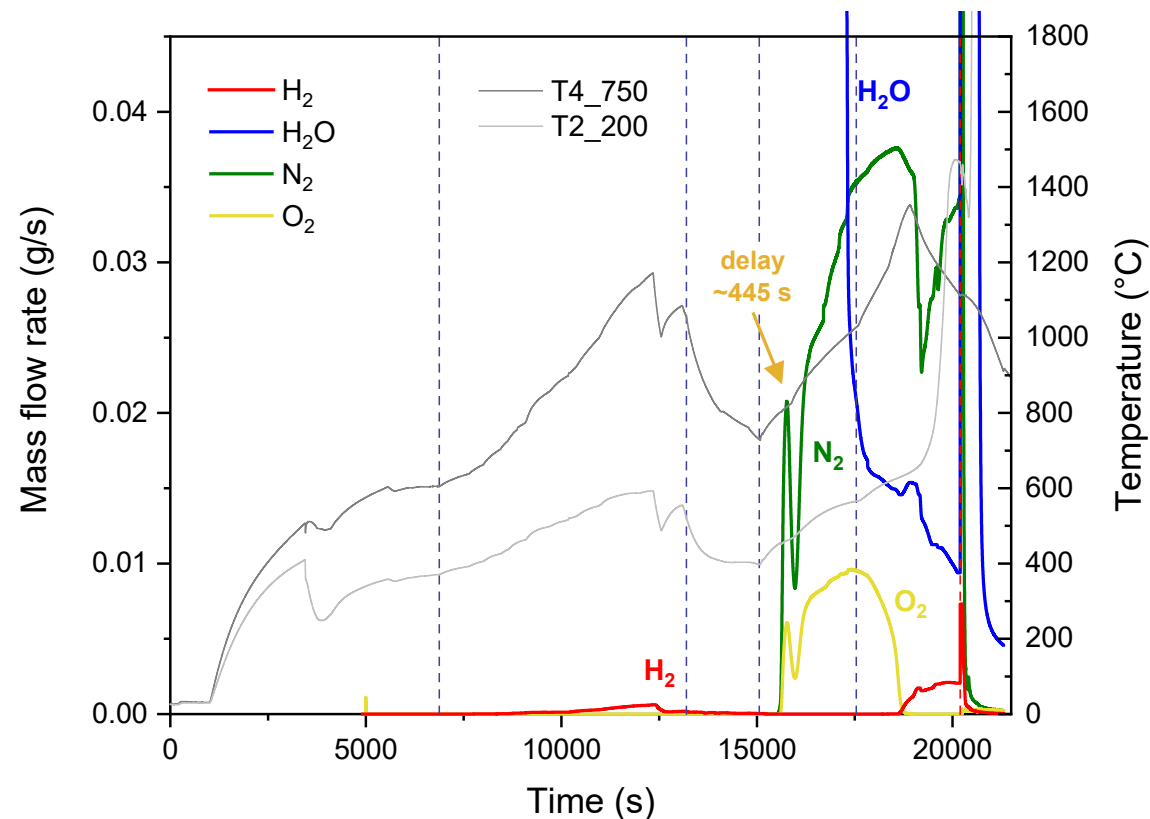
## CODEX-AIT-3

Reference test



CODEX-AIT-3		
Total	Pre-oxidation phase	Air-ingress phase
H <sub>2</sub> release (g)	3,8	1,4
O <sub>2</sub> uptake (g)		12
N <sub>2</sub> uptake (g)		3

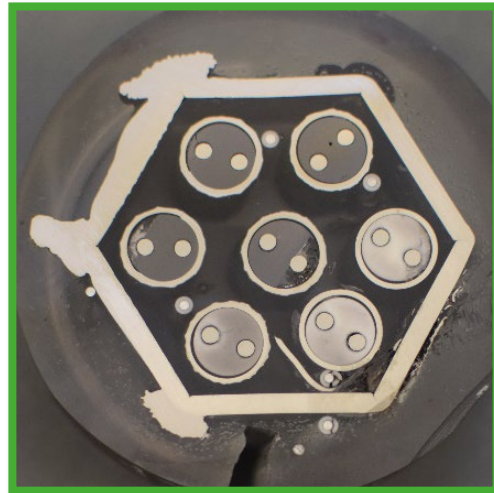
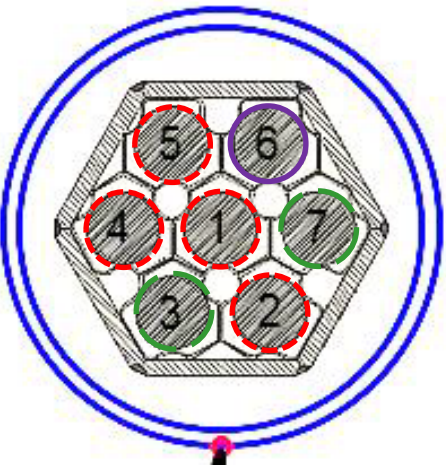
## CODEX-ATF-AIT



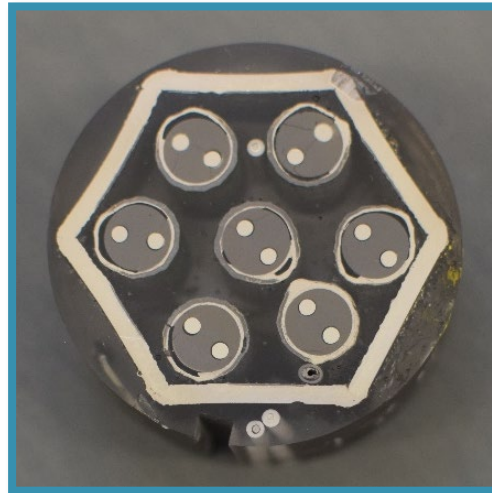
CODEX-ATF-AIT			
Total	Pre-oxidation phase	Air-ingress phase	Extra air-ingress phase
H <sub>2</sub> release (g)	1,4	-	3,3
O <sub>2</sub> uptake (g)		-	17
N <sub>2</sub> uptake (g)		-	9

# Cross sections of the CODEX-ATF-AIT bundle

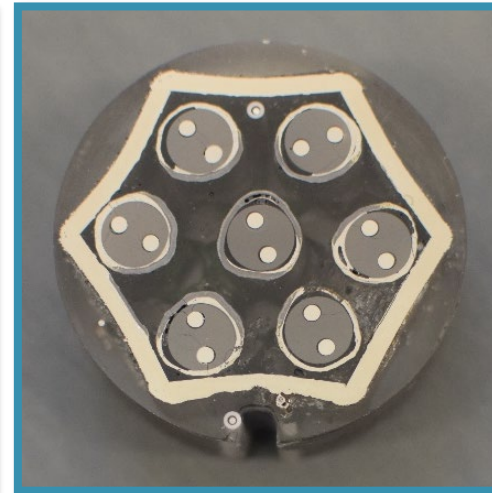
PRE-OXIDATION PHASE: NO BALLONING, NO OXIDATION → EXTENDED AIR INGRESS PHASE: EUTECTIC MELT FORMATION



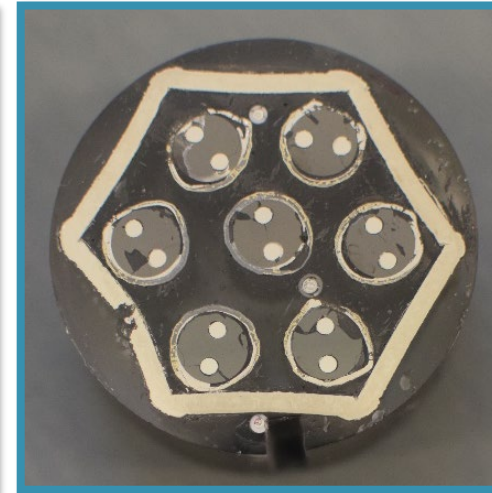
125 mm



200 mm




300 mm



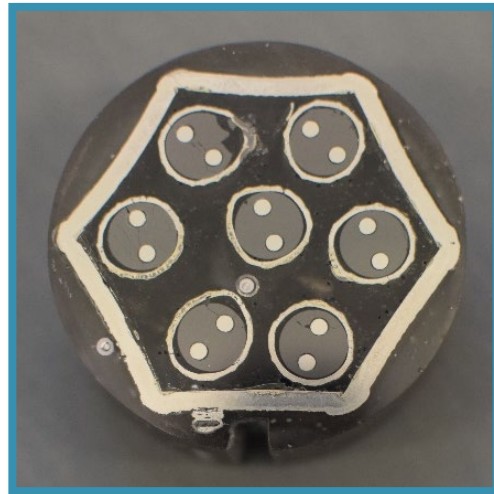
400 mm

 non-ballooned

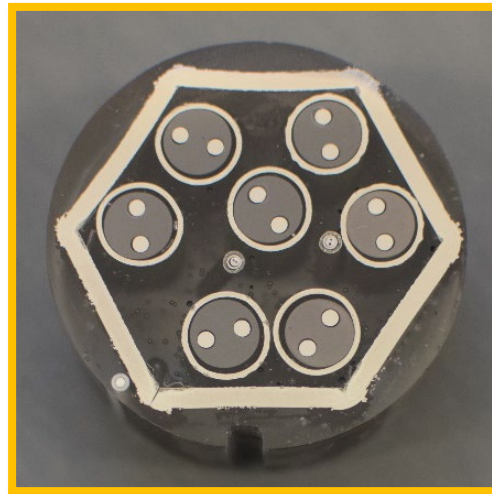
 ballooned and non-burst

 ballooned and burst

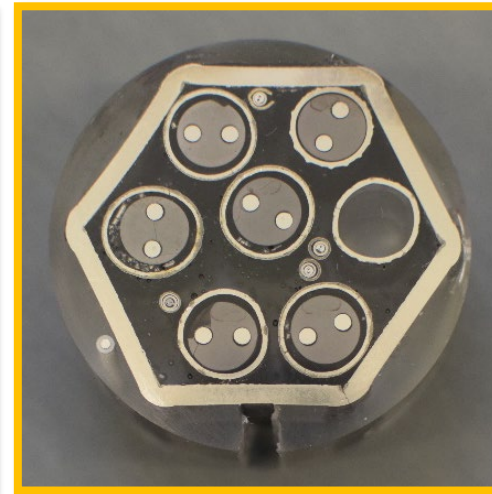
PRE-OXIDATION PHASE: BALLONING, OXIDATION → EXTENDED AIR INGRESS PHASE: (NO) EUTECTIC MELT FORMATION



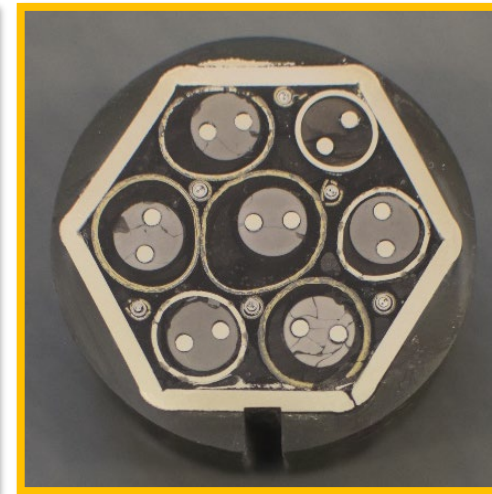
500 mm



600 mm



700 mm



800 mm

# Cross section of rods at 125 mm

**PRE-OXIDATION PHASE:** no balloning, no oxidation ( $T < 600\text{ }^{\circ}\text{C}$ )

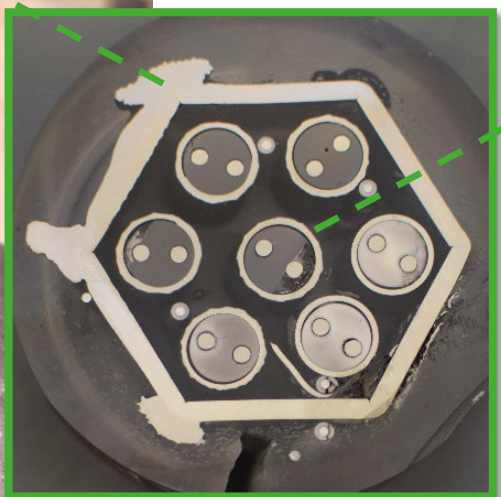
**EXTENDED AIR INGRESS PHASE:** eutectic melt formation ( $T_{\text{max}} \approx 1400\text{ }^{\circ}\text{C}$ )



$\alpha$ -Zr(O) (60-80 at. % Zr – 15-30 at. % O) and thin Cr-rich features (2-5 at. % Cr)

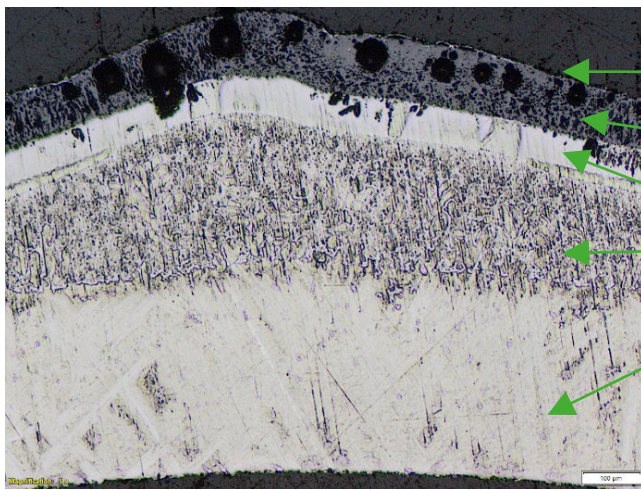
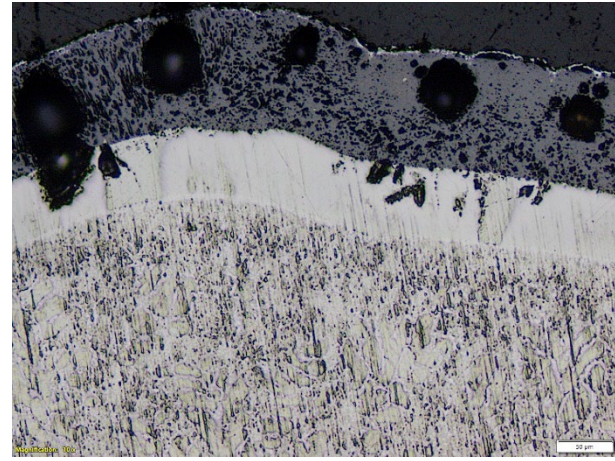
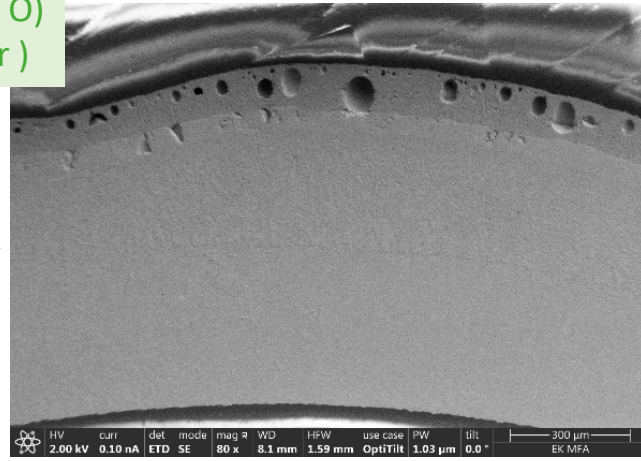
96 at. % Zr  
2 at. % Cr  
2 at. % Fe

64 at. % Cr  
30 at. % Zr  
3 at. % Fe



125 mm

Cr diffused into the Zr



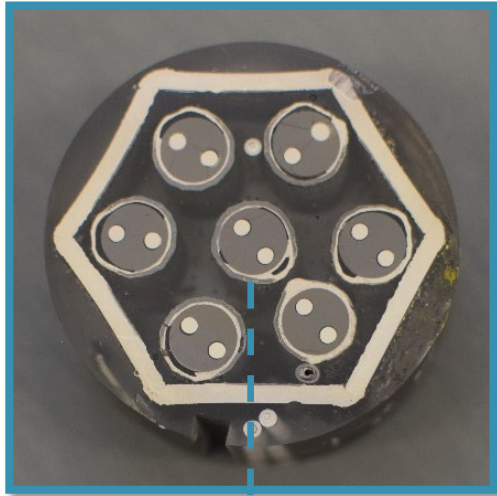
1. Cr coating
2.  $\approx 100\text{ }\mu\text{m}$   $\text{ZrO}_2$  layer
3.  $50\text{-}60\text{ }\mu\text{m}$   $\alpha$ -Zr(O) layer
4.  $150\text{-}250\text{ }\mu\text{m}$  eutectic region
5.  $\approx 350\text{ }\mu\text{m}$   $\beta$ -Zr layer

**PRE-OXIDATION PHASE:** no ballooning, no oxidation ( $T < 900\text{ }^{\circ}\text{C}$ )

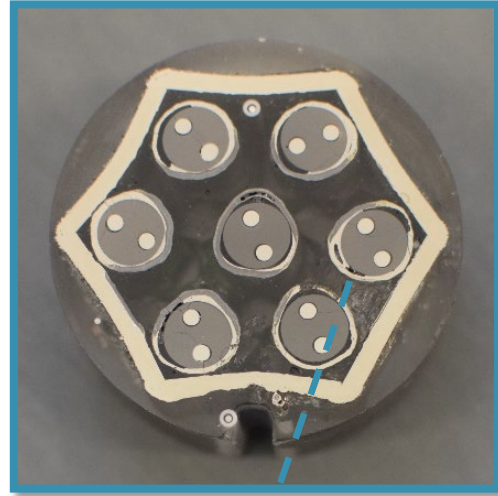
**EXTENDED AIR INGRESS PHASE:** eutectic melt formation ( $T_{\text{max}} \approx 1400\text{ }^{\circ}\text{C}$ )

Rods were strongly degraded- main degradation mechanism was the Cr-Zr eutectic melt formation and its fast oxidation/nitriding in the last phase.

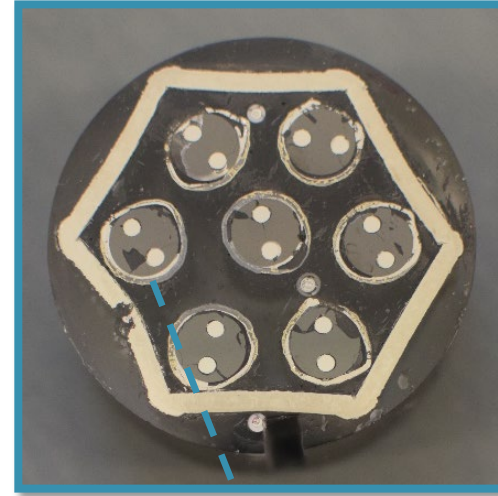
200 mm



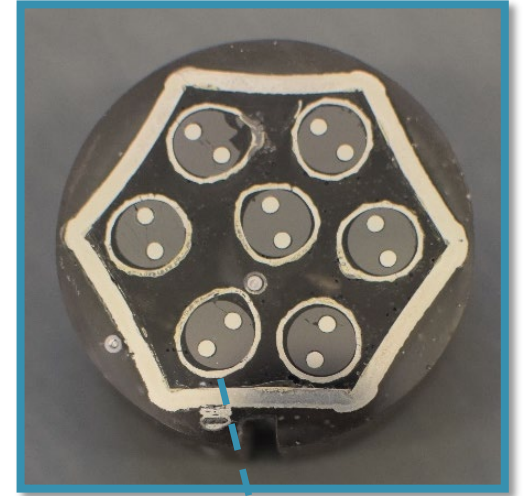
300 mm



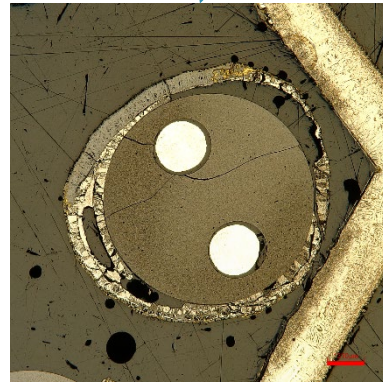
400 mm



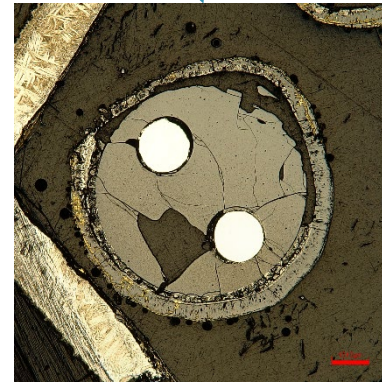
500 mm



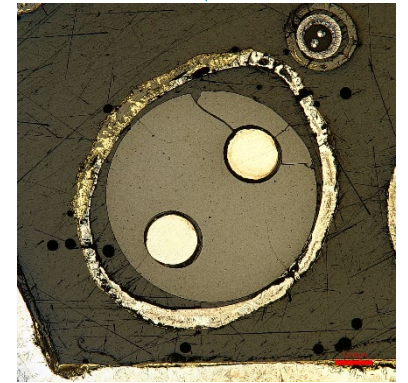
Rod No. 1.



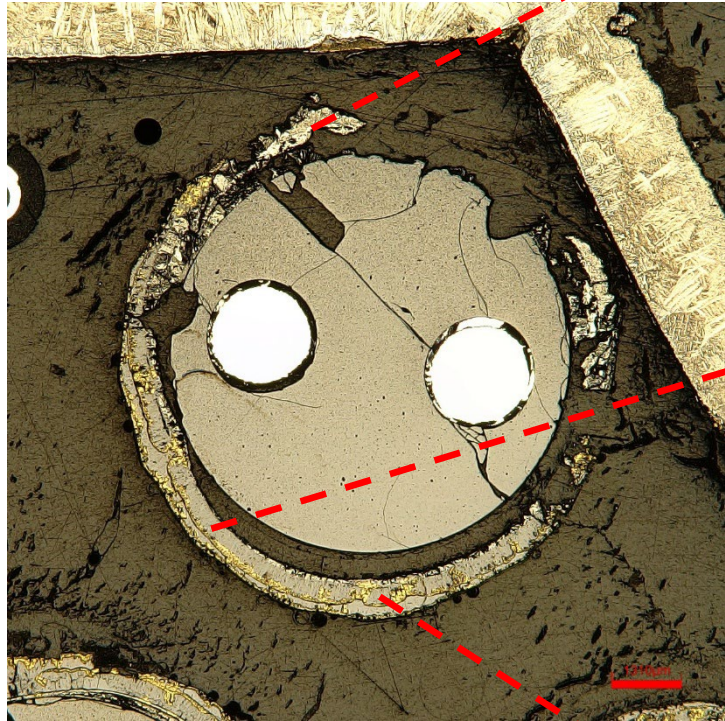
Rod No. 7.



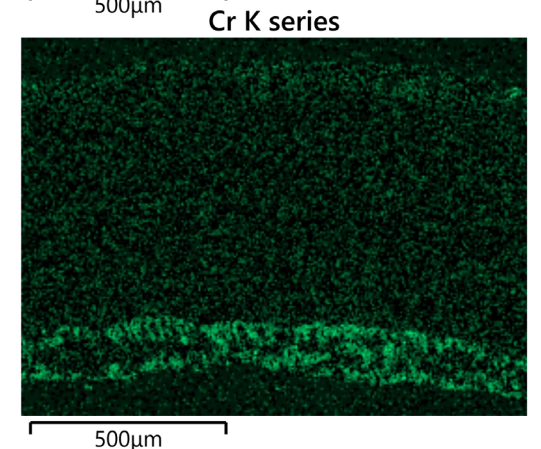
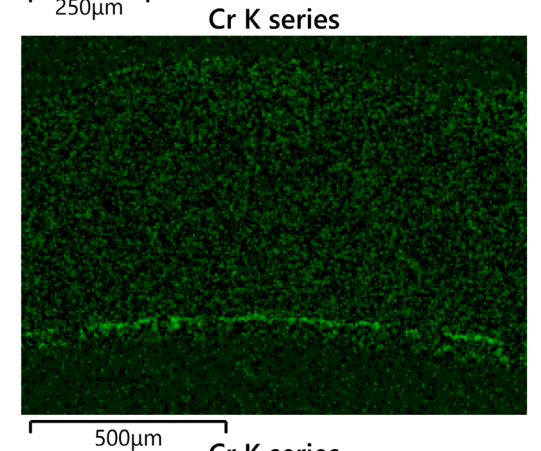
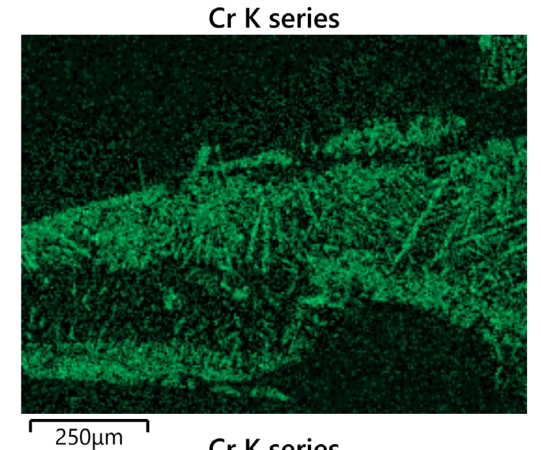
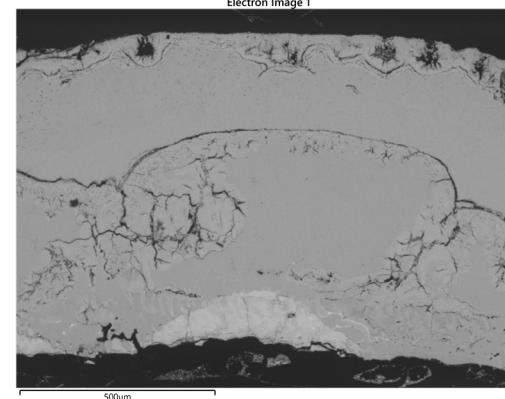
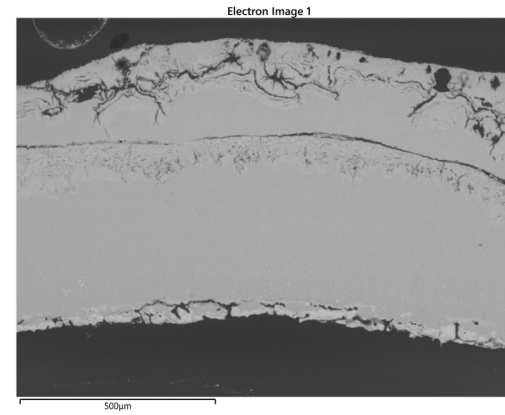
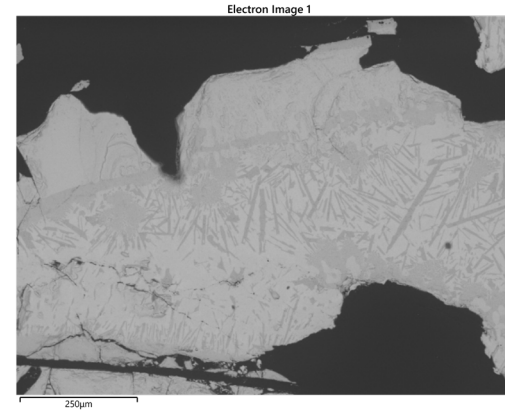
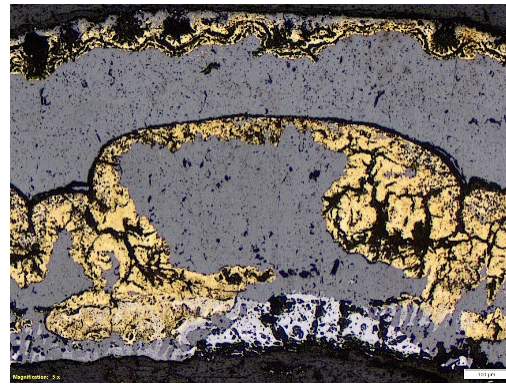
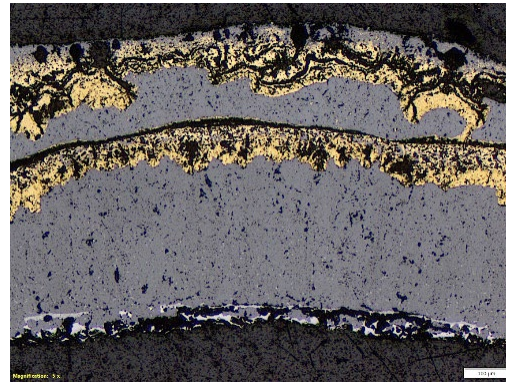
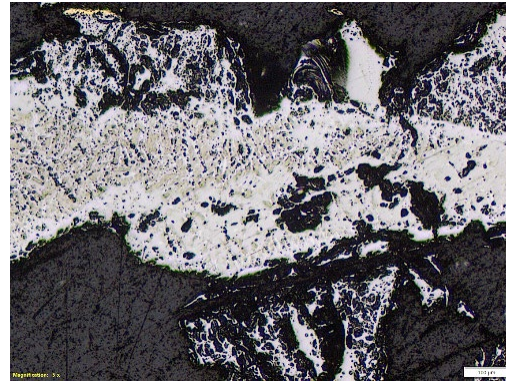
Rod No. 4.



Rod No. 3.



No Cr layer- Cr diffused into the Zr cladding wall-extensive Cr-Zr eutectic region



# Cross sections of rods at 600 - 800 mm

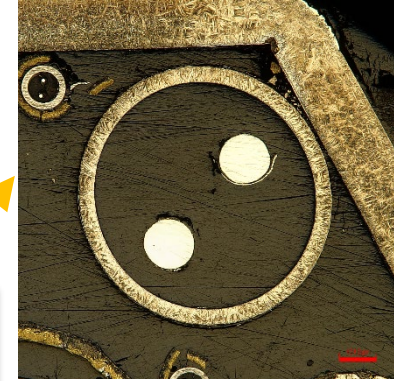
**PRE-OXIDATION PHASE:** ballooning, oxidation ( $T_{max} < 1000 - 1150 \text{ } ^\circ\text{C}$ )

**EXTENDED AIR INGRESS PHASE:** eutectic melt formation at 600 and 700 mm,  
no eutectic melt formation at 800 mm

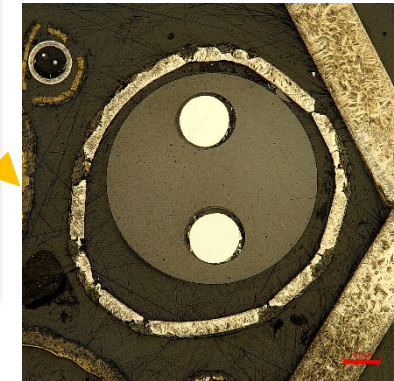
600 mm

700 mm

800 mm

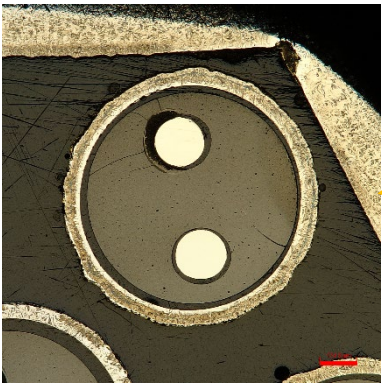
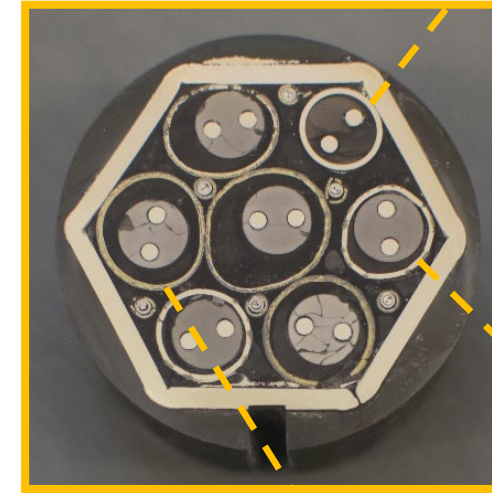
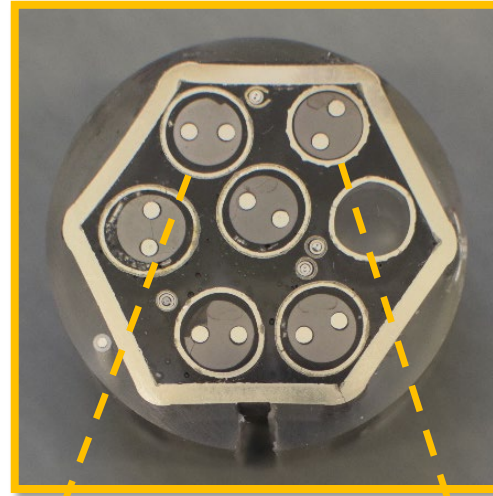
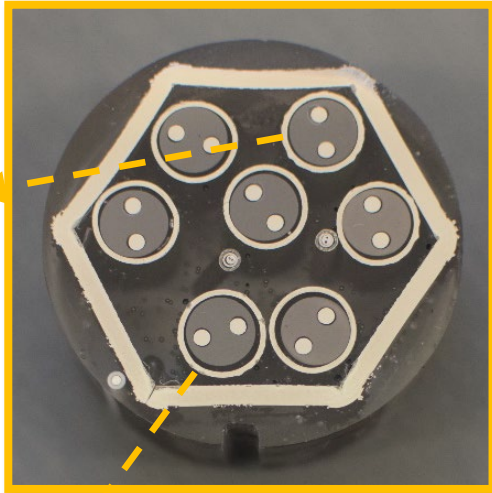


Rod No. 6.



Rod No. 7.

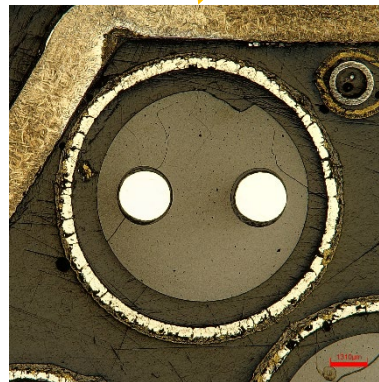
Cracked Cr-layer



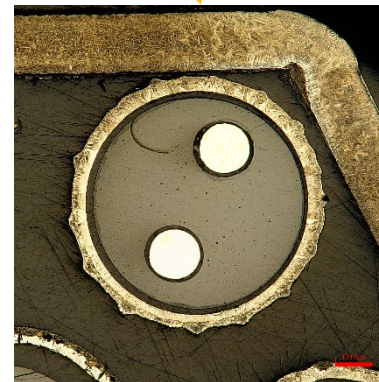
Rod No. 6.



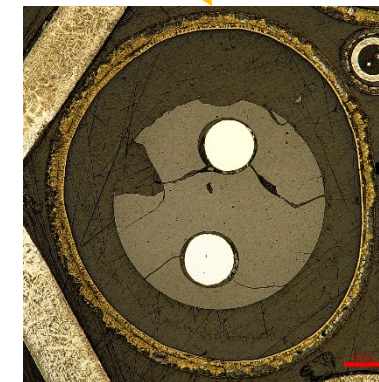
Rod No. 3.



Rod No. 5.



Rod No. 6.



Rod No. 4.

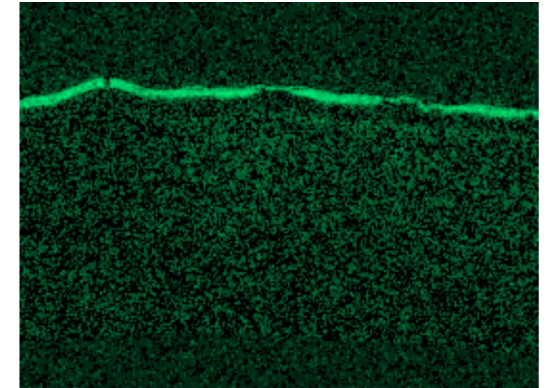
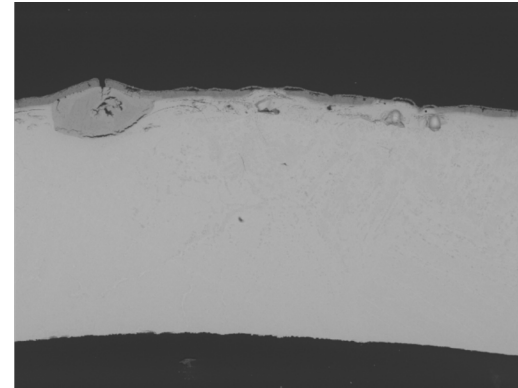
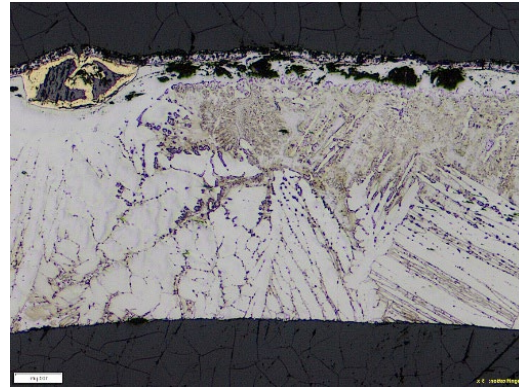
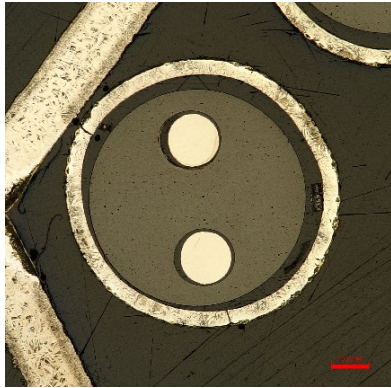


# Cross sections of rods at 600 mm

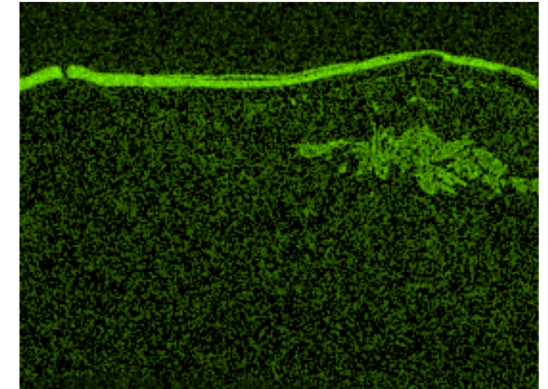
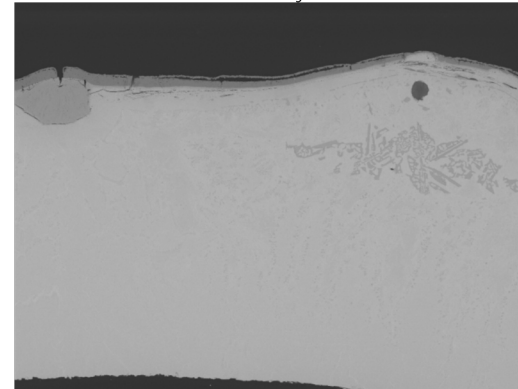
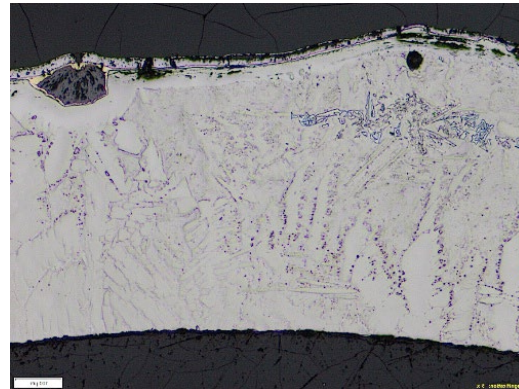
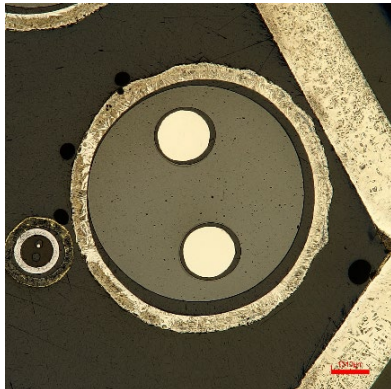
Zr oxidation locally through the cracks of the Cr-layer in the pre-oxidation phase

O penetrated through the cracks of the Cr-layer into the zirconium metal and prohibited the Cr diffusion into the cladding wall

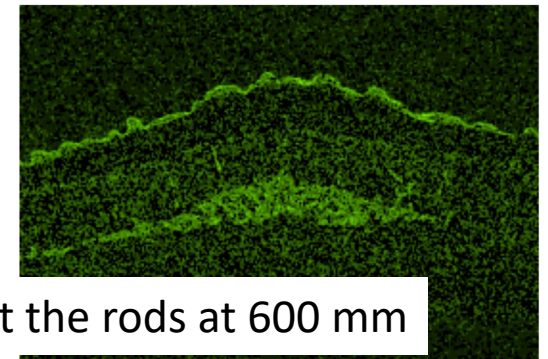
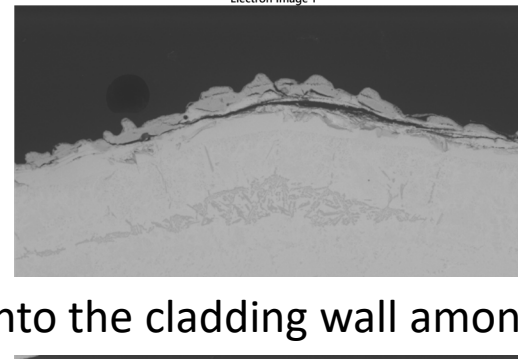
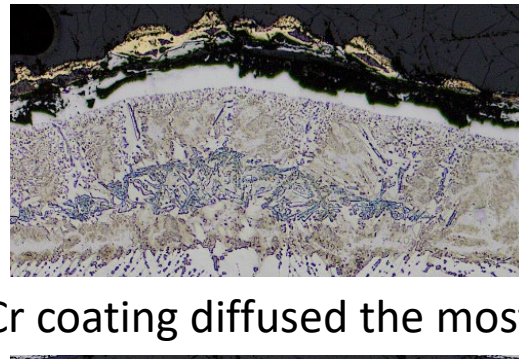
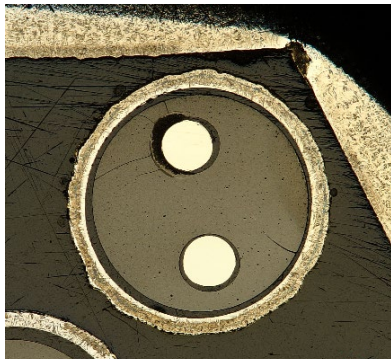
**No. 4.**  
ballooned  
and burst



**No. 7.**  
ballooned and  
non-burst



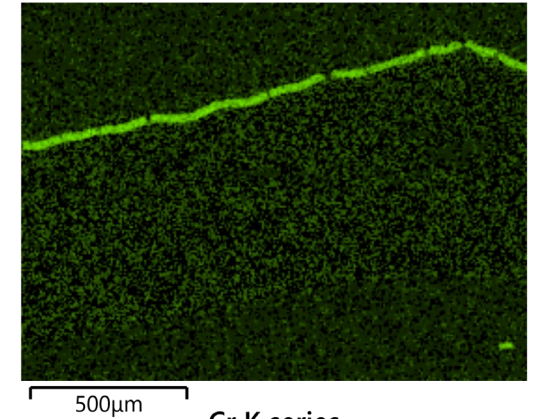
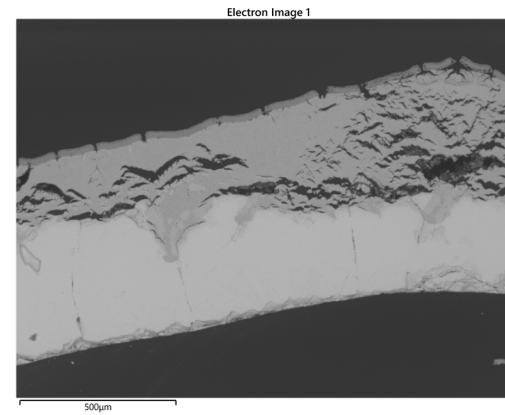
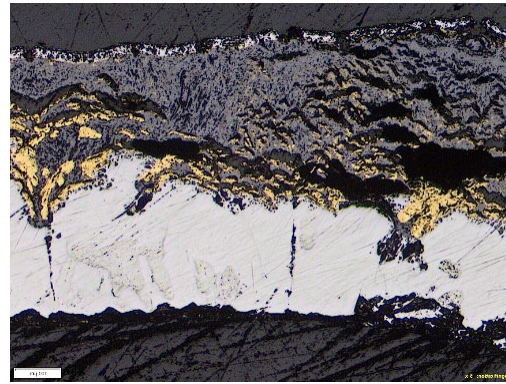
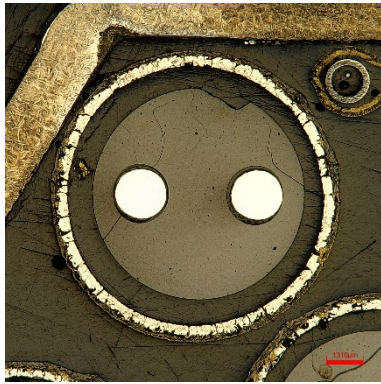
**No. 6.**  
non-ballooned



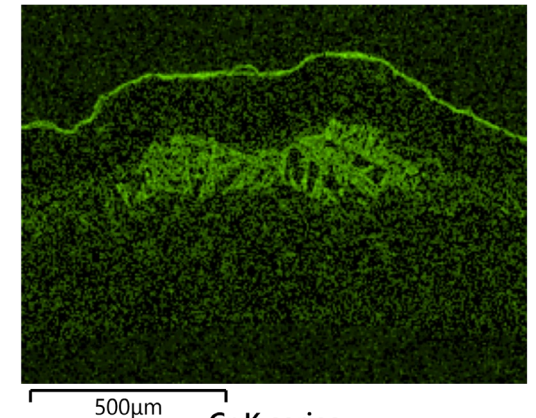
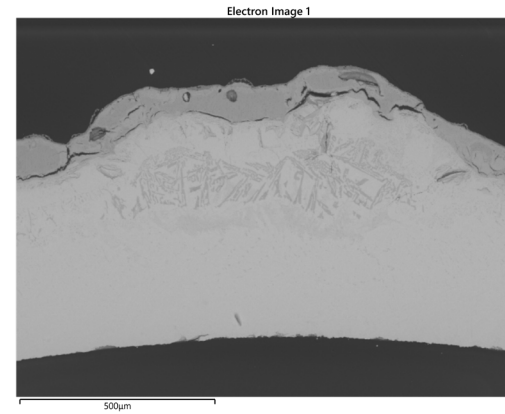
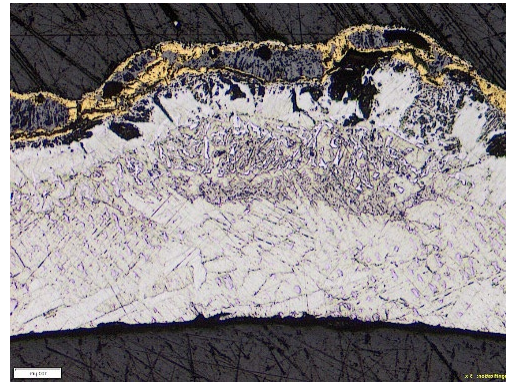
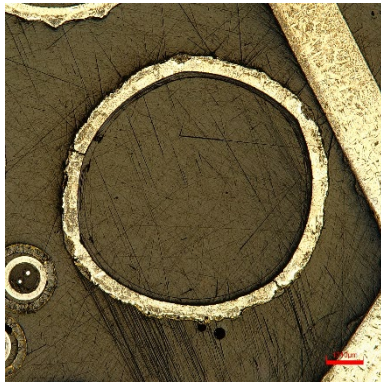
Cr coating diffused the most into the cladding wall amongst the rods at 600 mm

Ballooning- Cr coating became cracked. The Cr layer lost its protective role and these rods oxidised and nitrided the most

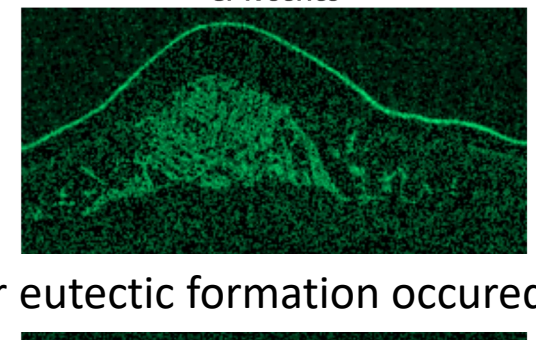
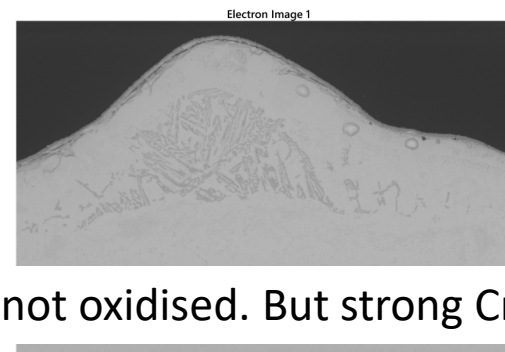
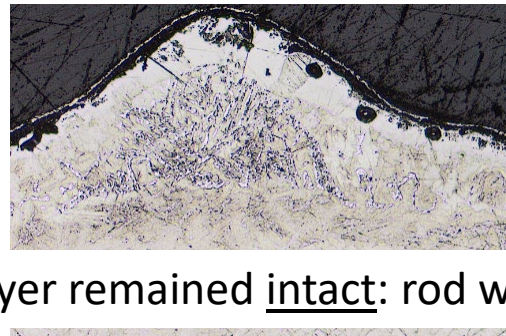
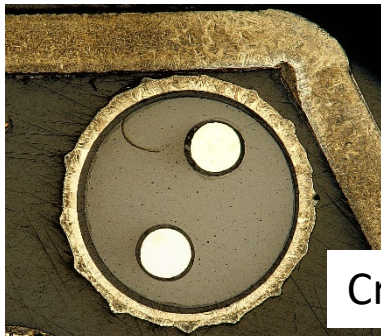
**No. 5.**  
ballooned  
and burst



**No. 7.**  
ballooned  
and non-burst



**No. 6.**  
non-ballooned

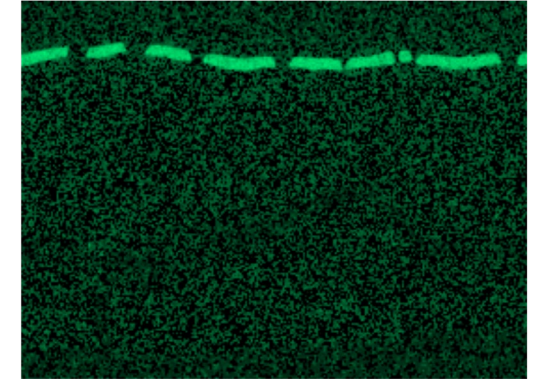
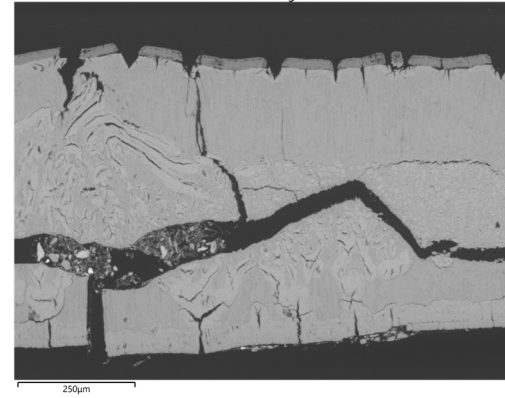
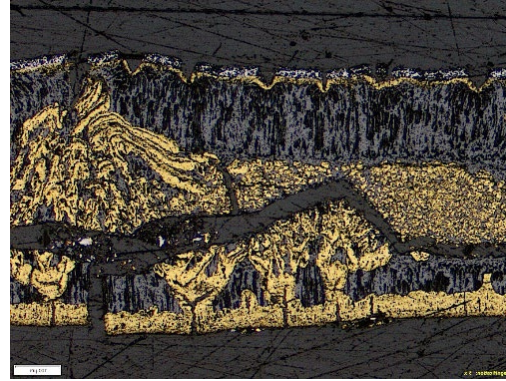
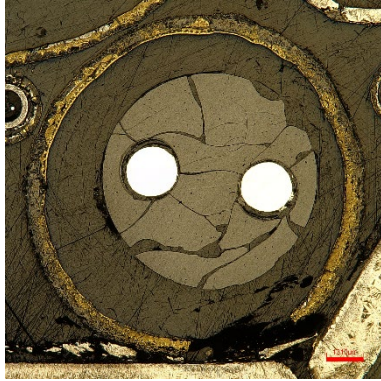


Cr layer remained intact: rod was not oxidised. But strong Cr-Zr eutectic formation occurred

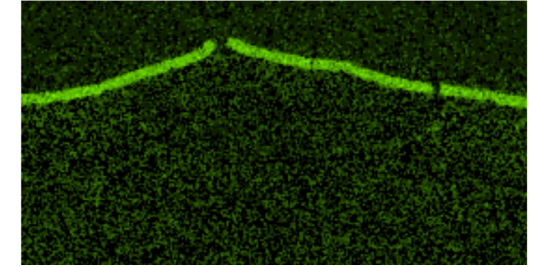
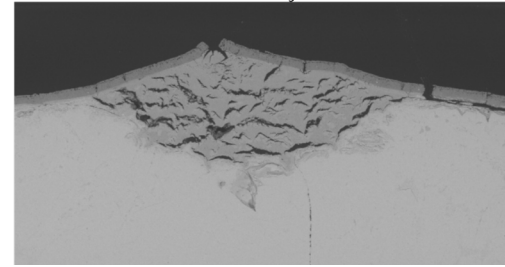
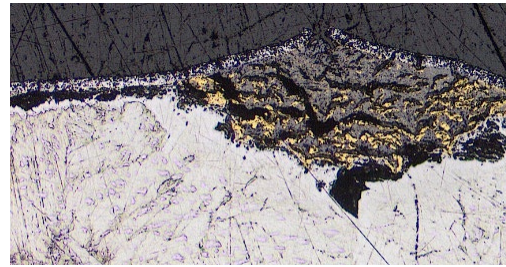
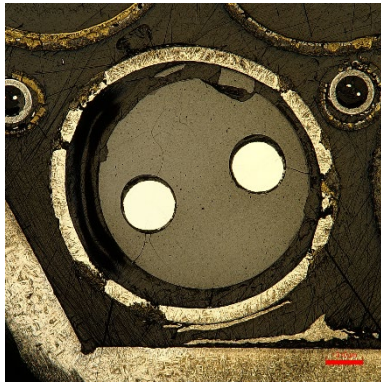
# Cross sections of rods at 800 mm

Strong ballooning, burst: oxidised and nitrided the most.  
 Burst location were near to this position: inner oxidation/nitriding

**No. 2.**  
 ballooned  
 and burst

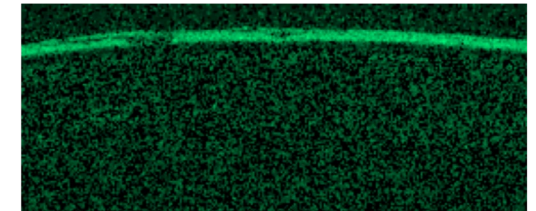
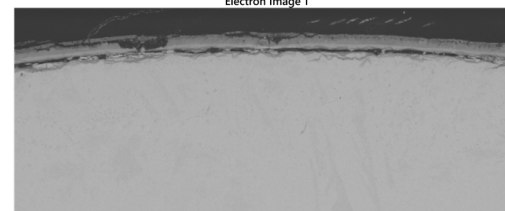
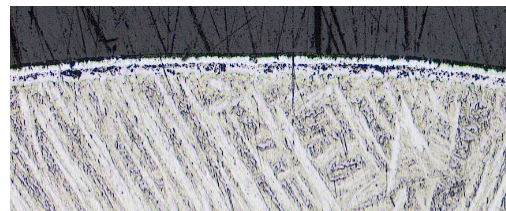


**No. 3.**  
 ballooned  
 and non-burst



Oxidation occurred locally and the tube wall often cracked through where the local oxidation started.

**No. 6.**  
 non-ballooned



Cr layer remained intact: no oxidation. No eutectic formation: low T

- The comparison of results from the CODEX-AIT-3 and CODEX-ATF-AIT tests suggests that ATF materials can increase the coping time in the event of air ingress type reactor accidents.
- The ATF cladding reacted significantly less with high-temperature steam below 1200 °C than traditional Zr cladding material.
- In the reference test, air ingress led to a temperature excursion, with cladding temperatures reaching 1625 °C within 40 minutes. Under the same conditions in the CODEX-ATF-AIT test, the cladding temperature increased only to 1030 °C over the same period.

- The Cr coating provided significant protection against oxidation in both steam and air atmospheres as long as the coating remained intact.
  - Effect of ballooning: after cracking of the Cr layer, local oxidation of Zr began. The local oxidation spots could facilitate full cross-sectional fracture of the cladding tube wall.
  - Cr-Zr eutectic melt formation: can take place if Cr diffuses into the Zr cladding wall to a large extent and the temperature reach the Cr-Zr eutectic melt formation temperature. Fast oxidation/nitriding of the metallic Cr-Zr eutectic melt could start.
- The degradation of the ATF fuel occurred more slowly in the integral tests compared to traditional fuel.

Many thanks to Martin Steinbrück, Juri Stuckert, Mirco Grosse (KIT), Tadas Kaliatka (LEI), Martin Ševeček (CTU), Liviusz Lovász (GRS)

**CODEX-ATF-AIT 29/OCT/2024**



Thank you for your  
attention!

The CODEX-ATF-AIT experiment was supported by OFFERR.



**Katerina Frederick**

WEC LLC

### **Accident Tolerant Fuel: Cr Coated Cladding Development at Westinghouse**

In response to the nuclear industry's desire for improved fuel performance in accident conditions following the Fukushima accident in Japan in 2011, Westinghouse's **EnCore**<sup>®</sup> accident tolerant fuel (ATF) program is developing and commercializing advanced fuel cladding and fuel pellet products with the main goals of improving safety and economic performance through power uprates and increased burnups. The program includes a near-term high energy **EnCore** ATF product, comprised of chromium-coated zirconium-alloy fuel cladding and doped fuel pellets with potential enrichments greater than 5% <sup>235</sup>U. The chromium-coated cladding has undergone testing in various environments and facilities to provide valuable results to validate the design and specification of the chrome coating. Lead test rod (LTR) and lead test assembly (LTA) campaigns with utility partners provide real-world data on the irradiation performance of the coated cladding. LTR post-irradiation examination (PIE) data will be presented and discussed. Additionally, out-of-pile testing highlighting coating differences from development will be presented.

# Accident Tolerant Fuel: Cr Coated Cladding Development at Westinghouse

Katerina Frederick

30<sup>th</sup> International QUENCH Workshop

December 16-18, 2025





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# Outline

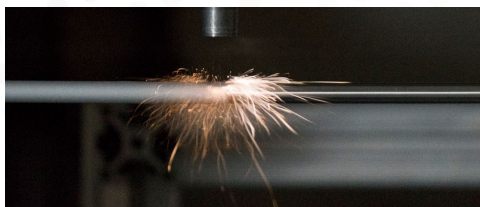
- Westinghouse **EnCore**<sup>®</sup> High Energy Fuel Program
  - LTA and LTR Status
  - Operating Experience
- Hydrogen Absorption Testing
- SiC Update

ADOPT, EnCore, AXIOM, ZIRLO, Optimized ZIRLO are trademarks or registered trademarks of Westinghouse Electric Company LLC, its affiliates and/or its subsidiaries in the United States of America and may be registered in other countries throughout the world. SiGA is a registered trademark of General Atomics, its affiliates and/or its subsidiaries in the United States of America and may be registered in other countries throughout the world. All rights reserved. Unauthorized use is strictly prohibited. Other names may be trademarks of their respective owners.

# EnCore<sup>®</sup> High Energy Fuel Program

Utilities are striving for maximum electricity generation and reduced operating costs while enhancing safety with Accident Tolerant Fuel (ATF) technologies

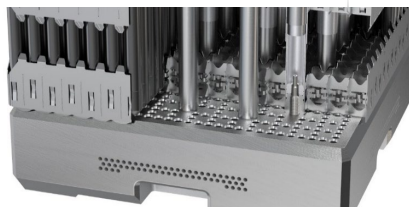
The EnCore High Energy Fuel (HEF) Program combines near-term and future advancements to support these critical nuclear industry drivers



**Chromium Coated Cladding**



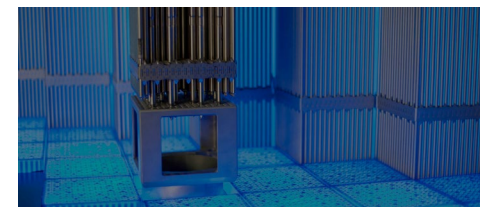
**ADOPT<sup>™</sup> Fuel Pellets**



**PRIME<sup>™</sup> Fuel Features**



**AXIOM<sup>®</sup> High Performance Cladding**



**LEU+ and Higher Burnup**  
(>5 w/o & >62 GWd/MTU)

## Applications



Enhanced Safety



Optimization of Fuel Cycle Costs



24-Month Cycle Operations

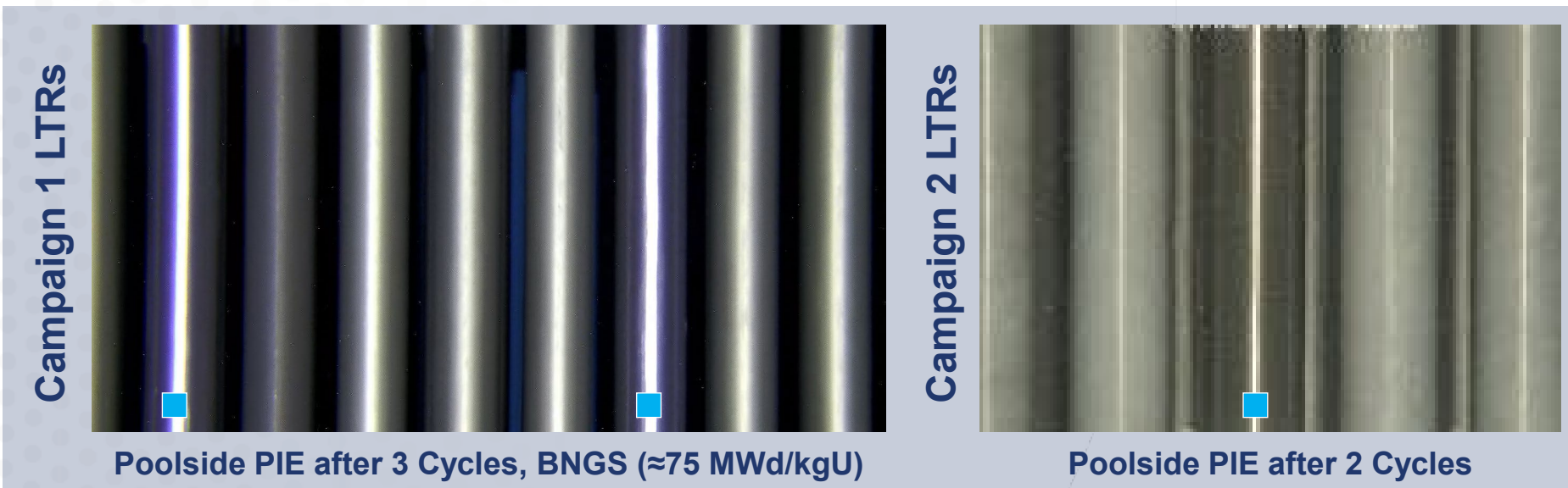


Power Uprating

# EnCore<sup>®</sup> HEF Irradiation Campaigns

- Lead Test Rod (LTR) campaigns with Utility Partners provide data for fuel qualification
- Campaigns 1 and 2 complete
  - Poolside PIE throughout irradiation to 54-month high burnup complete. Hot cell PIE underway.
- Campaign 3 started Spring 2025 (contains LEU+)
- Additional programs in planning stages

	Cr Coated Cladding	ADOPT Pellets	LEU+ Pellets
Campaign 1 (2019)	✓	✓	
Campaign 2 (2020)	✓		
Campaign 3 (2025)	✓	✓	✓



**Cr coated cladding appears "pristine" with excellent adherence and little indication of crud**

■ Cr Coated Rods

# ATF and HEF: Ongoing Operating Experience

**Reduced Normal Operation Corrosion**

~55 MWd/kgU

**Reduced Hydrogen Pickup**

Coating

Hydride

~55 MWd/kgU

Burnup (MWd/kgU)	Average H-Content (ppm)
~31	< 50
~55	
~75	<b>Coming soon!</b>

**Improved Accident Performance**

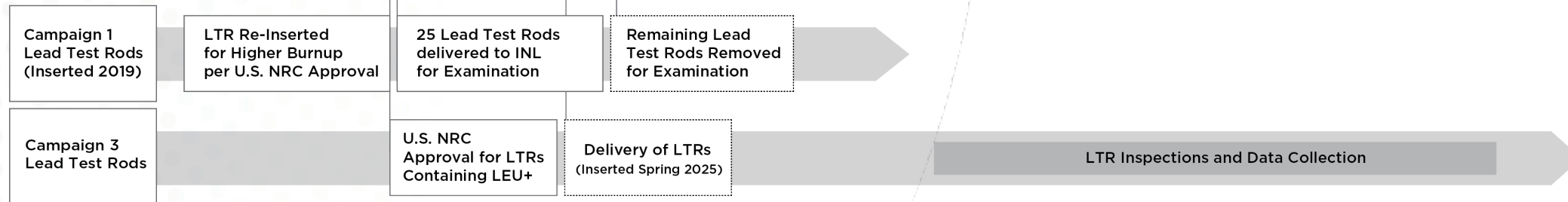
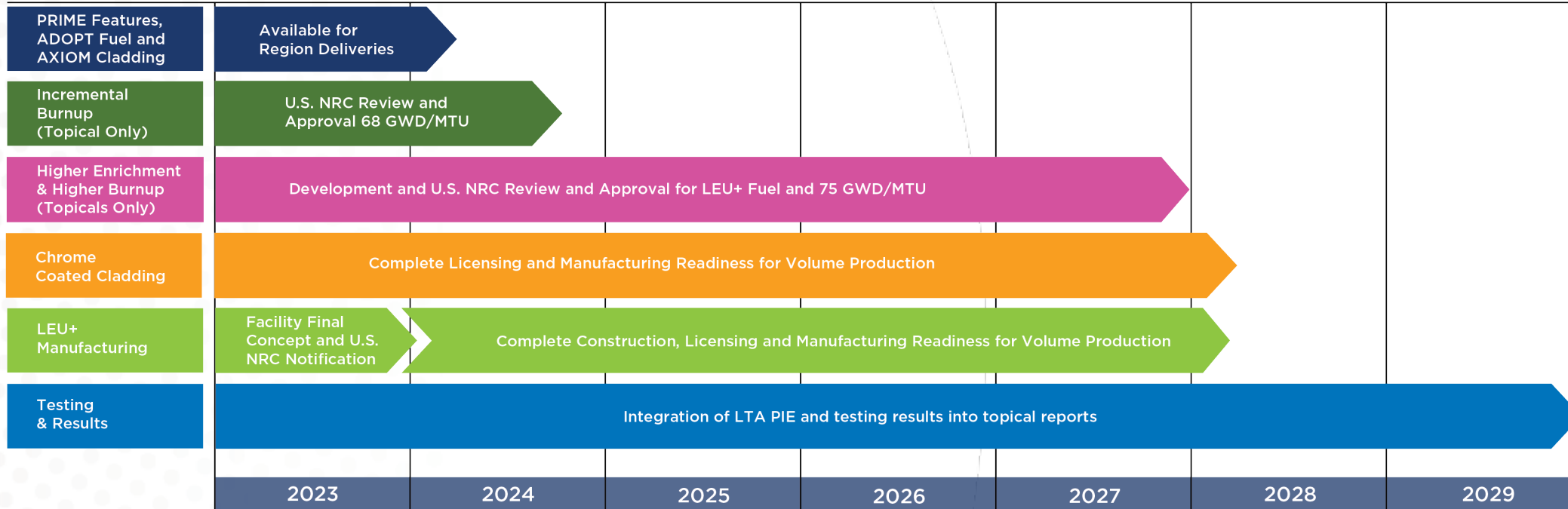
Cr Coated

Uncoated

*LOCA Burst Test Results (Irradiated)*

# EnCore<sup>®</sup> High Energy Fuel Program

## Integrated Timeline for LEU+ Fuel Deployment



**Engaging U.S. NRC early for multiple licensing actions to support 2028 reloads**

# Hydrogen Absorption as Coating Quality Indicator

## Test Conditions

$$P_{RT}V_{net} = nRT_{RT}$$

$V_{net}$  = net quartz tube volume

$n$  = moles H<sub>2</sub> gas to increase H concentration by C<sub>H</sub> (ppm)

$M_s$  = mass of cladding exposed to H<sub>2</sub>

$R$  = gas constant

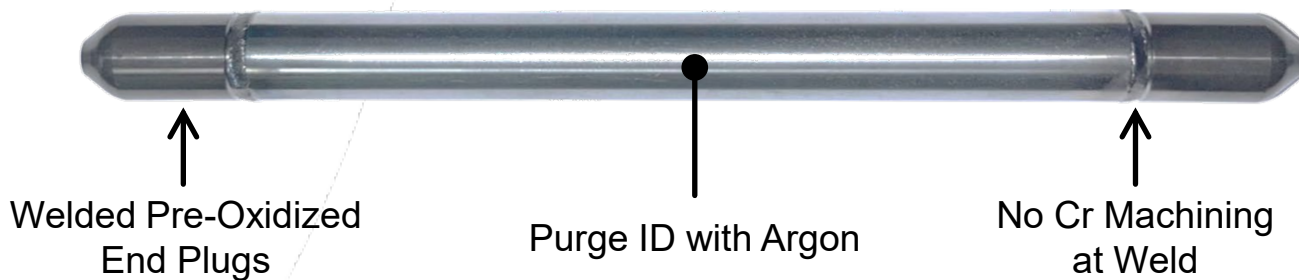
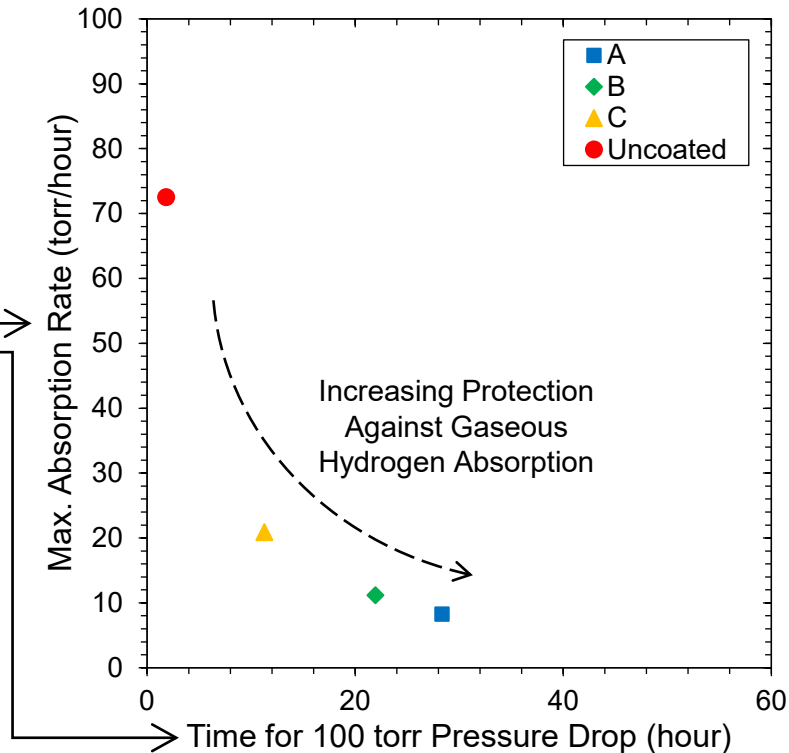
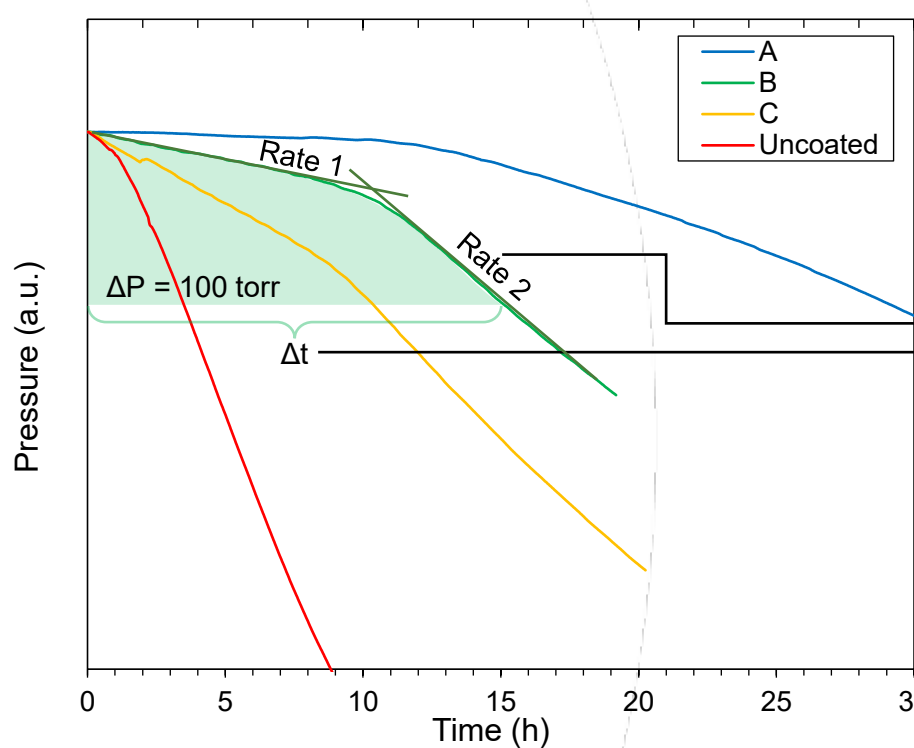
$T_{RT}$  = room temperature (293 K)

$$P_{RT} = \frac{0.0091C_H M_s}{V_{net}}$$

Parameter	Value
$V_{net}$ (L)	0.45
$M_s$ (g)	7.6
$C_H$ (ppm)	2186
$P_{293K}$ (torr)	336
$T_{charging}$ (°C)	430
$P_{703K}$ (torr)	504

## Final Test Parameters

Duration:  
Maximum 48 hours or a pressure drop of 100 torr

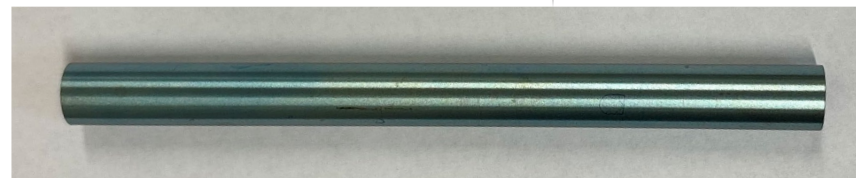
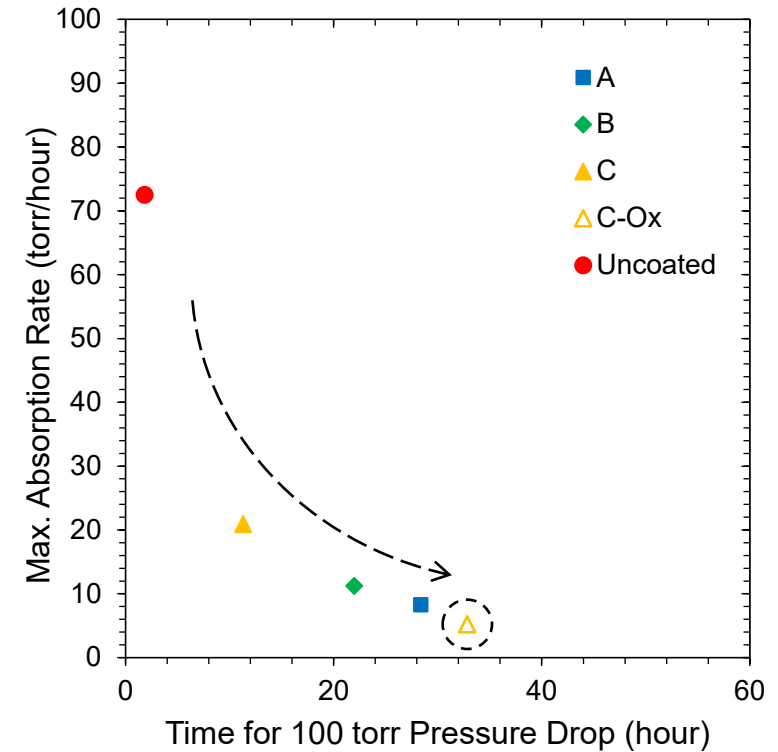
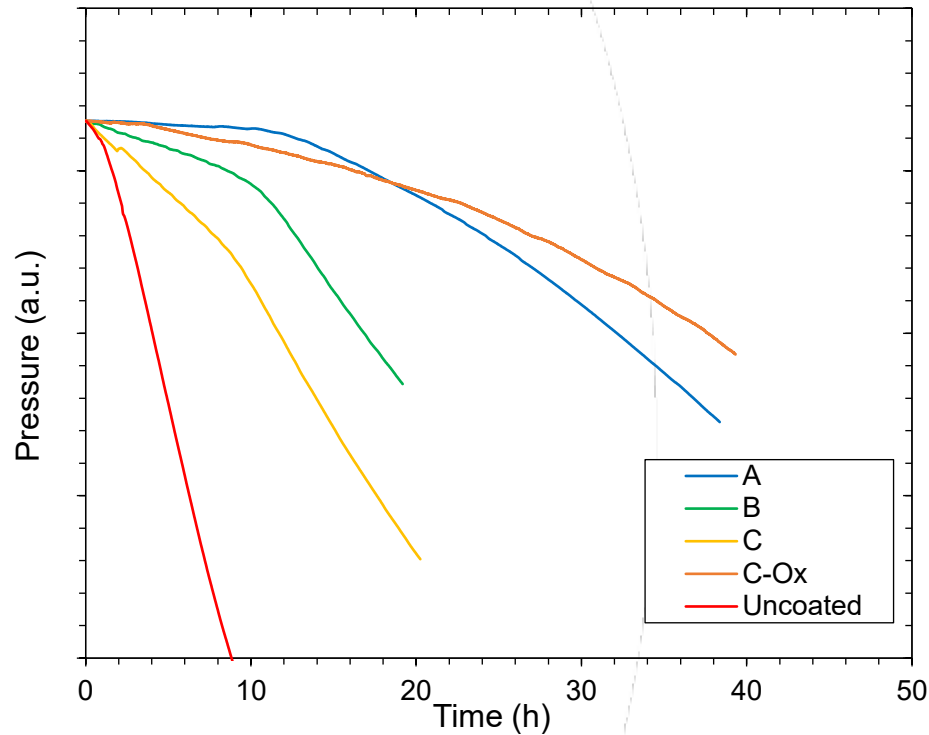


# Effect of Oxidation on Hydrogen Absorption

## Simulating Materials In-Reactor

- Normal operation is in an oxidizing environment
- Assumption: 1  $\mu\text{m}$   $\text{ZrO}_2$  is impermeable to  $\text{H}_2$
- Open tube samples oxidized in steam autoclave environment
- Pre-oxidized samples were tested for better comparison of coating protection after initial oxidation occurs

**Note:** Gaseous hydrogen is not representative of real-world H pickup mechanisms, therefore data is *only* used to assess coating integrity



Pre-Oxidized Open Tube

Oxidation occurring on coatings in-reactor provides added protection



# Next Generation Fuels: SiC and SiC Reinforced Cladding

- Continued autoclave and high temperature testing of General Atomics SiGA® and Ceramic Tubular Products fully ceramic SiC cladding
- Potential additional operating margin (fuel temperatures) and safety margin (response time)
- Next steps in 2026
  - Fabricate cladding test samples with fiber holding mechanism
  - High temperature burst testing and hermeticity testing

## SiC Reinforced Zr Alloy Cladding

- Exploratory work with the University of Wisconsin and Free Form Fibers
- Minimal increase in cost over Zr only cladding due to short manufacturing time and minimal SiC fiber use
- Hybrid SiC/Zr Cladding Shows Significant Performance Gains (Ramp Rate: 833 °C/min)

Sample	Burst Temperature (°C)
Control Zr-Alloy	750
Thin Layer (0.25 mm)	975
Thick Layer (0.50 mm)	1100



# Thank You



Westinghouse  
Electric Company



@WECNuclear



Westinghouse  
Electric Company



wecchinanuclear

[westinghousenuclear.com](http://westinghousenuclear.com)



Westinghouse



**Martin Steinbrück**

KIT

## **Oxidation and degradation of Cr-coated zirconium alloy: Effect of Cr thickness**

This presentation examines the influence of chromium (Cr) coating thickness on the oxidation and degradation behavior of zirconium alloys under high-temperature conditions relevant to severe nuclear accidents. Using magnetron-sputtered Cr coatings of 5–25  $\mu\text{m}$  on Zry-4 substrates, isothermal tests (1000–1400°C in steam) and transient tests up to 1500°C were performed. Results show that all coatings provide effective protection at 1000°C, while at 1200°C only coatings  $\geq 15 \mu\text{m}$  maintain integrity for one hour; thinner coatings fail due to rapid consumption by oxidation and diffusion. Above the Zr-Cr eutectic temperature (1330°C), protective effects vanish regardless of thickness, and eutectic melt formation accelerates degradation. Post-test analyses revealed a four-layer structure ( $\text{Cr}_2\text{O}_3/\text{Cr}/\text{ZrCr}_2/\text{Zry}$ ) and edge effects influencing oxidation kinetics. Optimal coating thickness was identified as 15–20  $\mu\text{m}$ , balancing durability and thermomechanical stability, whereas excessive thickness may induce cracking. These findings provide critical input for Accident Tolerant Fuel (ATF) design and modeling, highlighting the limitations of Cr coatings under extreme conditions and their role in improving severe accident management strategies.

# Oxidation and degradation of Cr-coated zirconium alloy: Effect of Cr thickness

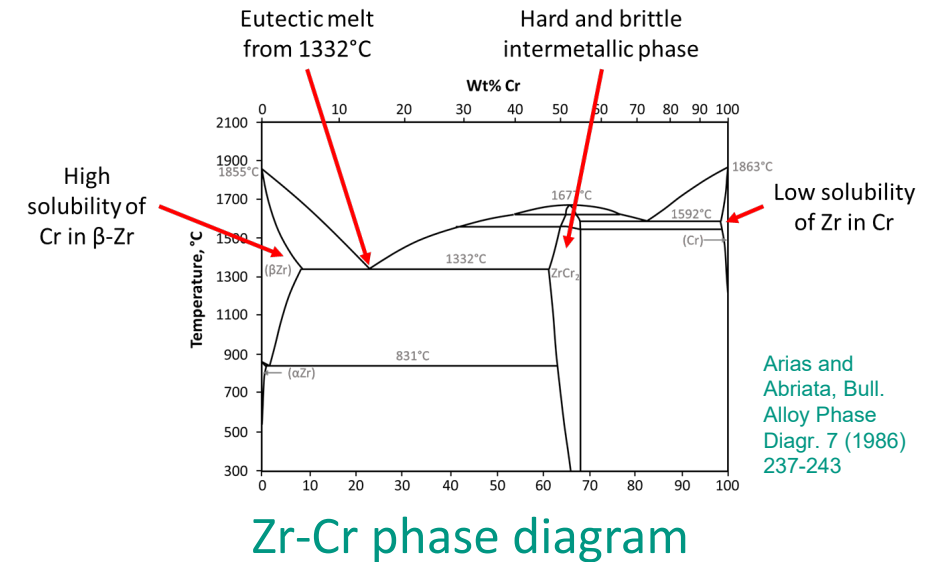
**M. Steinbrueck, I. Lee, U. Stegmaier, C. Tang**

30<sup>th</sup> International QUENCH Workshop, Karlsruhe, Germany, 16-18 Dez 2025

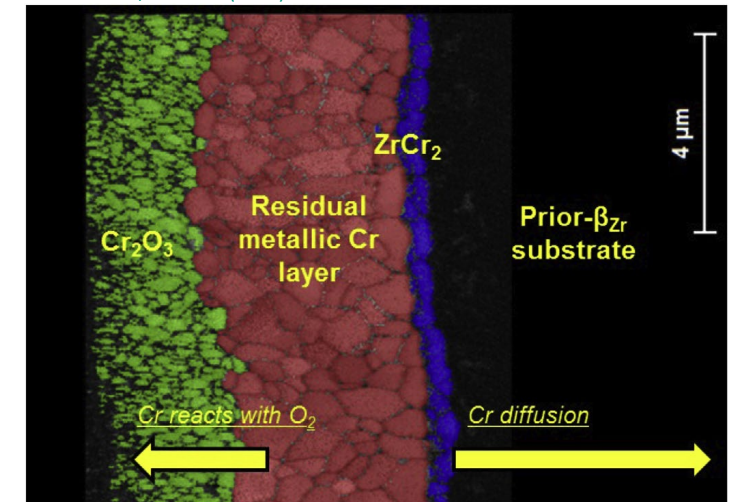


# Oxidation and degradation of Cr/Zry at high temperatures

- $2 \text{Cr} + 3 \text{H}_2\text{O} \rightarrow \text{Cr}_2\text{O}_3 + 3 \text{H}_2$ 
  - ➔ Adherent and well protective oxide scale
  - ➔ Consumption of Cr layer
- $\text{Zr} + 2 \text{Cr} \rightarrow \text{ZrCr}_2$ 
  - ➔ Consumption of Cr coating by formation of an intermetallic layer
- Solubility of Cr in Zry bulk (and vice versa)
  - ➔ Consumption of Cr coating by diffusion into Zry bulk
- Zr-Cr eutectic melt formation at  $1332^\circ\text{C}$ 
  - ➔ Ultimate upper limit of application



Brachet et al., JNM 517 (2019) 268-285



4-layer structure of protective coating

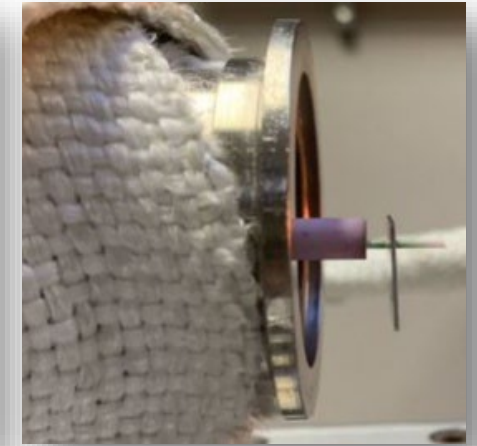
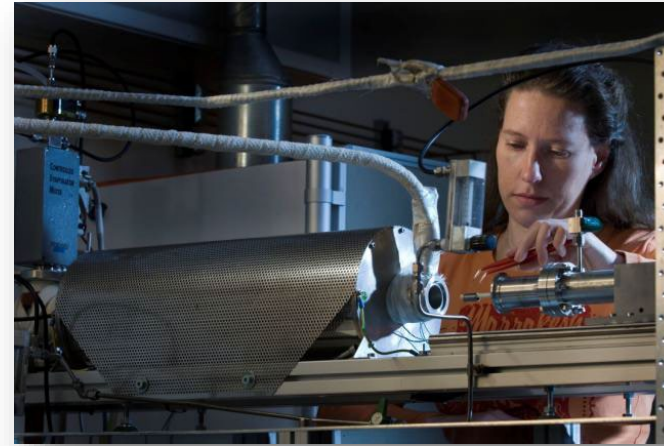
# Test facilities

## Thermal balance Netzsch STA449



- Max. temperature in dry atmosphere 1600°C
- Max. temperature in steam 1250°C
- Coupled with steam supply system (inlet) and mass spectrometer (outlet)
- Applied for isothermal tests at 1000 and 1200°C in steam, and for transient test in O<sub>2</sub>

## BOX tube furnace



- Max. temperature in steam 1600°C
- Coupled with sample lock, steam supply system (inlet) and mass spectrometer (outlet)
- Applied for isothermal tests at 1400°C and transient tests up to 1500°C

# Samples and test conduct

## Samples

- Zry-4 plates 15 x 10 x 0.65 mm<sup>3</sup>
- PVD Cr coating produced in-house by magnetron sputtering

## Test series

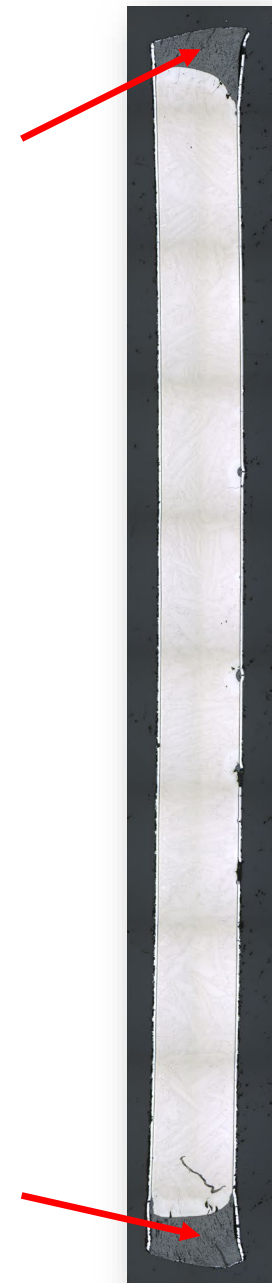
- 2 hours at 1000°C in steam
  - 1 hour at 1200°C in steam
  - 10 min at 1400°C in steam
- } **5-25 μm Cr**
- Transient tests with 17-μm samples in oxygen from 500 to 1380°C with **2-50 K/min** heating rate



As-coated sample

# Edge effect

- $\text{ZrO}_2$  formation at the poorly coated edges of the samples
- Correction methods:
  - Subtraction of the mass gain by Zr oxidation at the edges ✓
  - Calculation of the mass gain based on  $\text{Cr}_2\text{O}_3$ ,  $\text{ZrO}_2$  and  $\alpha\text{-Zr(O)}$  ✓
    - Shown in this presentation by colored dots
  - Subtraction of the mass gain by Zr oxidation using C/P correlation

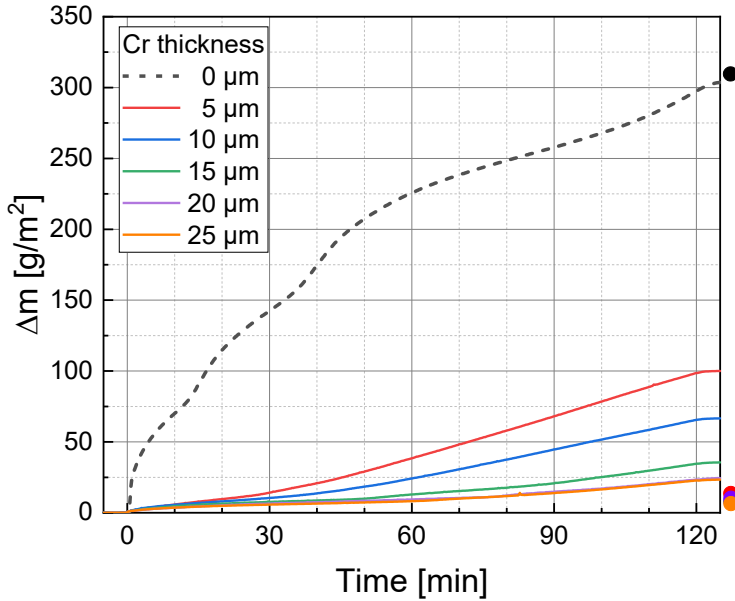




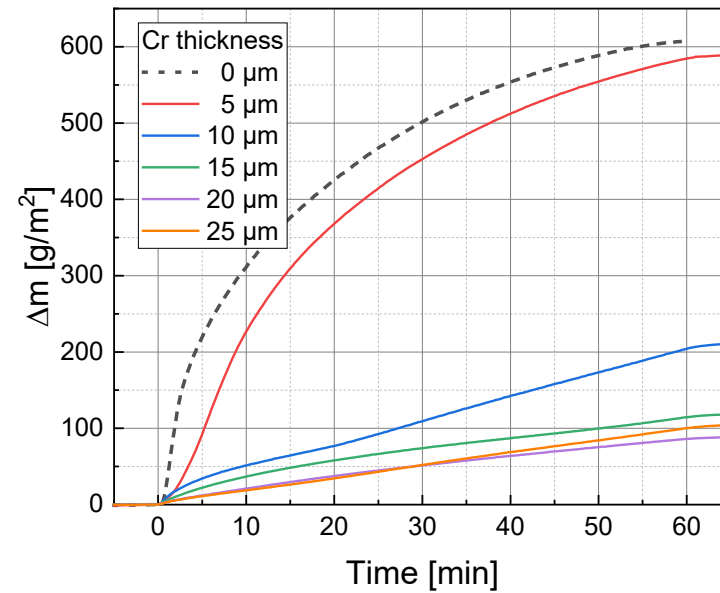
# Isothermal tests

# Mass gain in dependence on temperature and Cr thickness

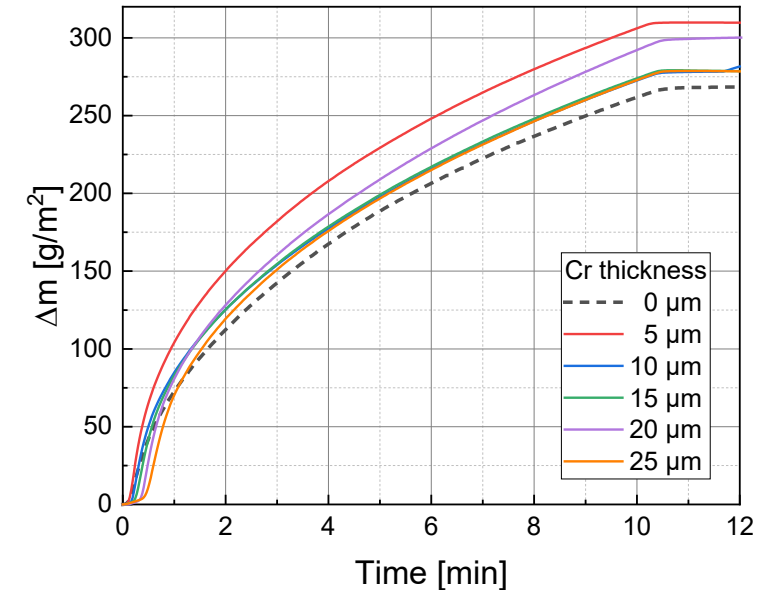
1000°C



1200°C



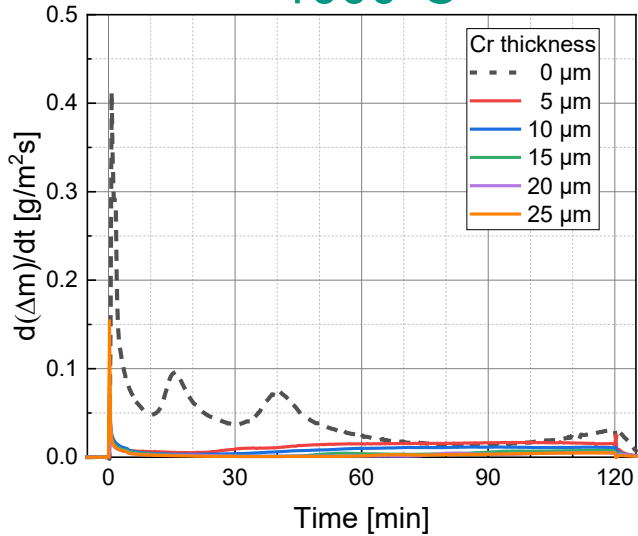
1400°C



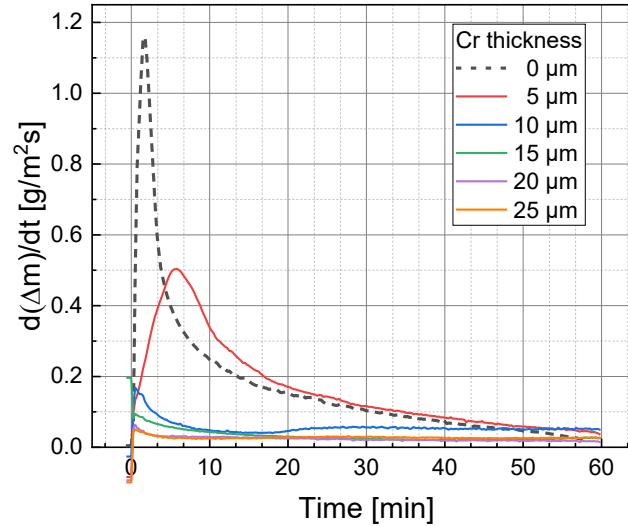
- 1000°C: All coatings provide protection for two hours
- 1200°C: Almost no protective effect of 5- $\mu\text{m}$  Cr coating, slow degradation of the 10- $\mu\text{m}$  coating, and protection for one hours from 15 to 25  $\mu\text{m}$  Cr thickness
- 1400°C: No protective effect independent on Cr thickness  $\rightarrow$  comparable oxidation kinetics of coated and uncoated samples

# Mass gain rates and integral values

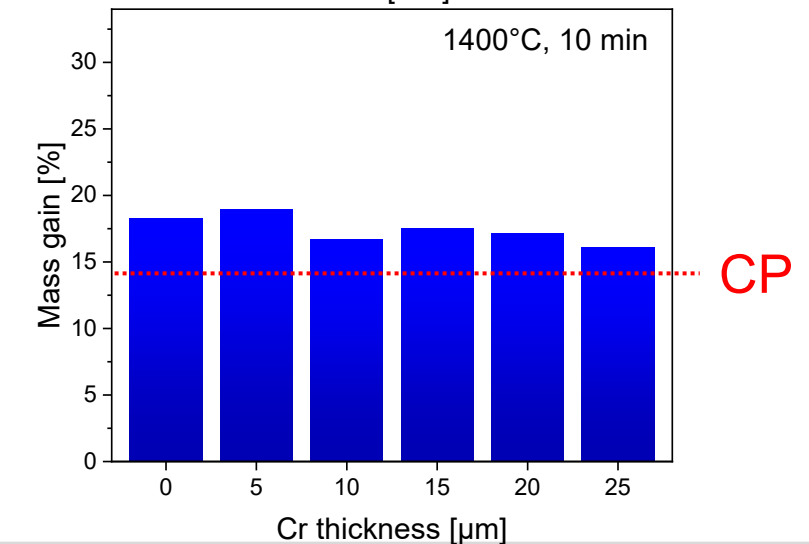
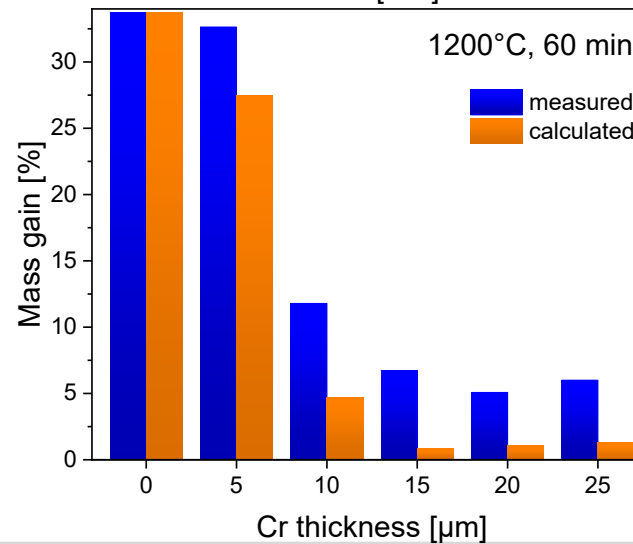
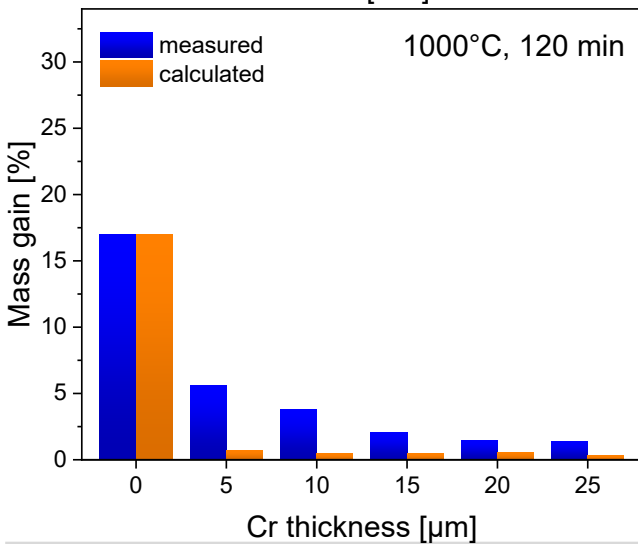
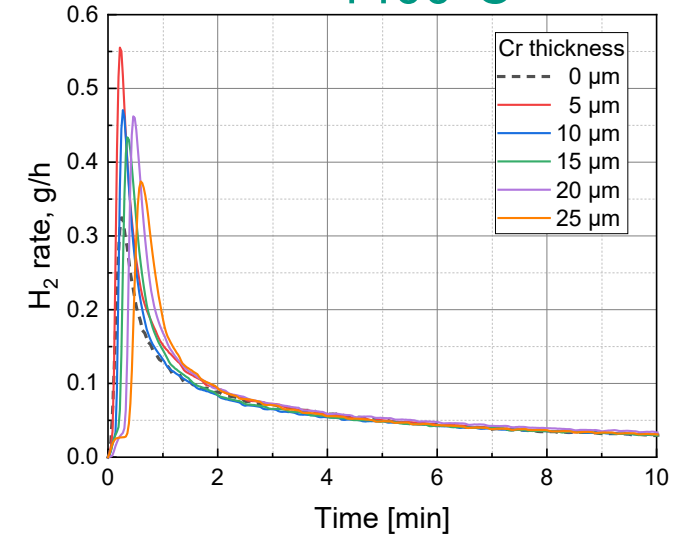
1000°C



1200°C

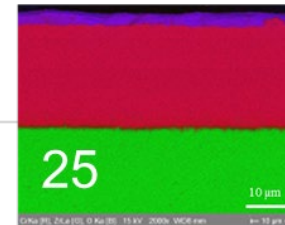
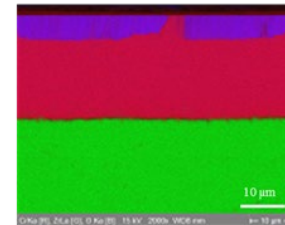
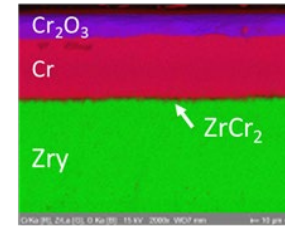
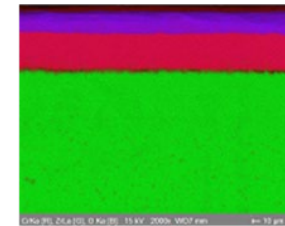
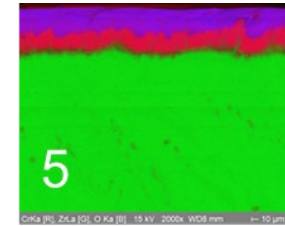
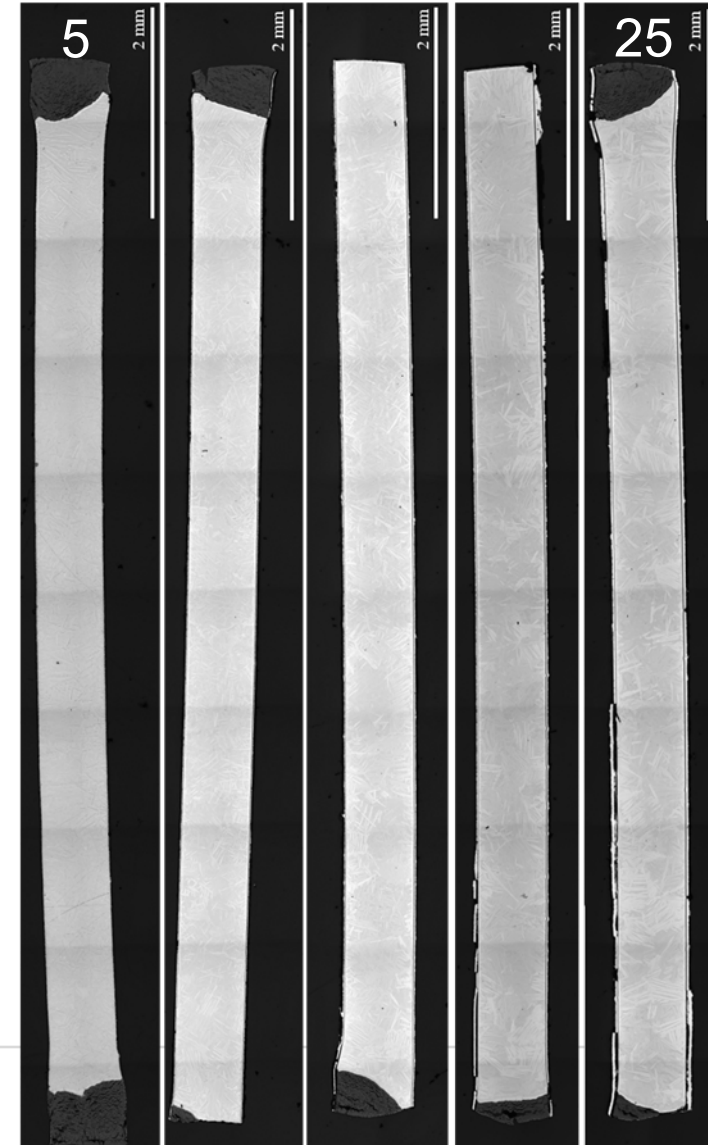
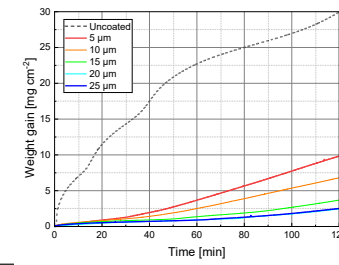


1400°C

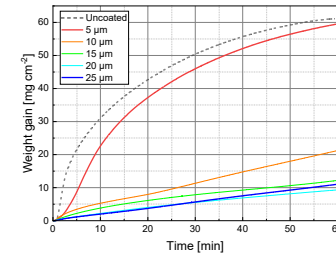


# Post-test examination of 1000°C samples

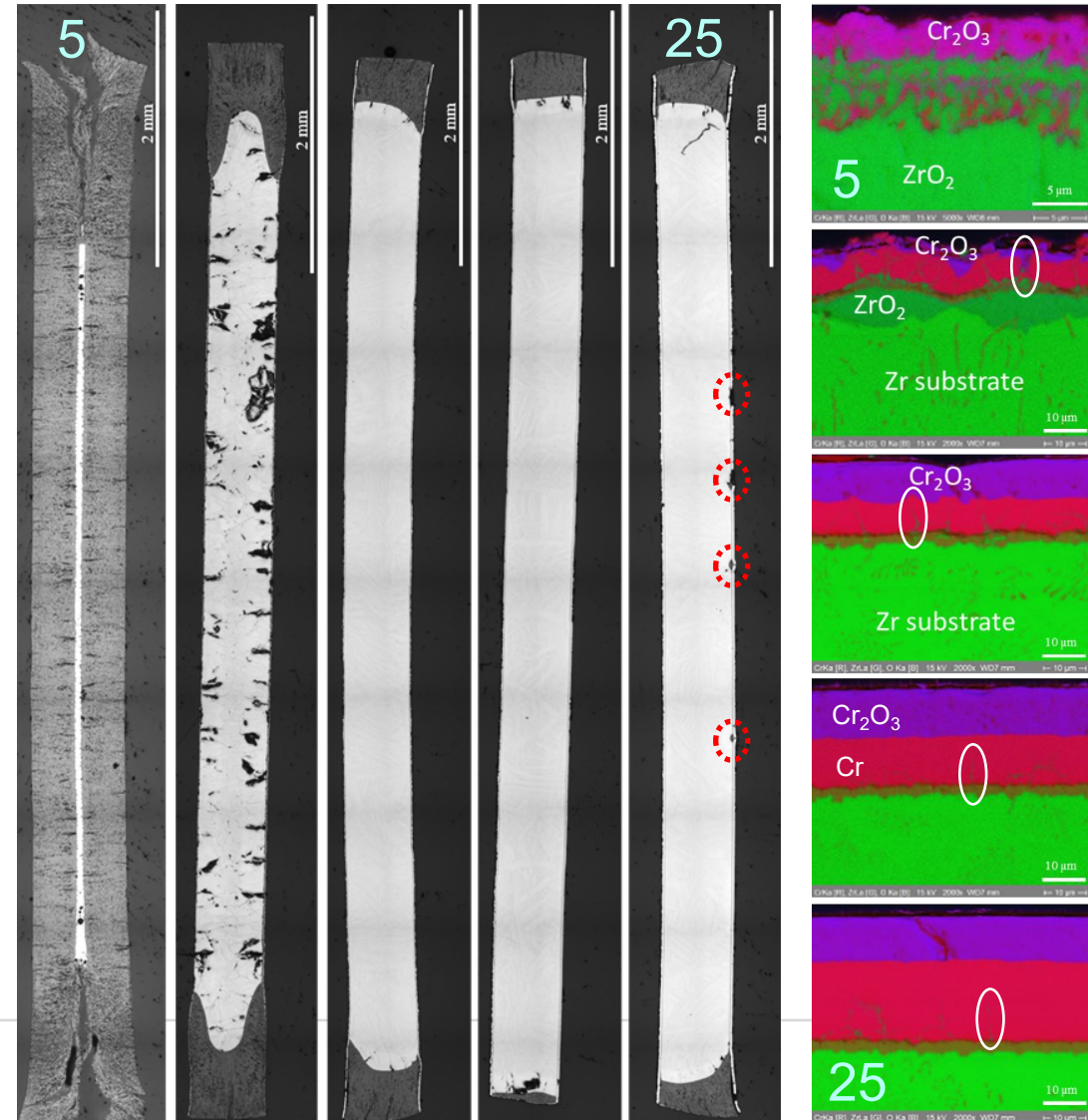
- Enhanced oxidation at poorly coated edges (edge effect)
- Four-layer structure for all samples:  
 $\text{Cr}_2\text{O}_3/\text{Cr}/\text{ZrCr}_2/\text{Zry}$
- 2-5  $\mu\text{m}$   $\text{Cr}_2\text{O}_3$  layer
- $\sim 1 \mu\text{m}$   $\text{ZrCr}_2$  interface layer
- ➔ Protective effect for all samples
- 5  $\mu\text{m}$  Cr: rough interface,  $\text{ZrO}_2$  diffusion paths along Cr GBs



# Post-test examination of 1200°C samples



- Strong edge effects
- 5 μm Cr: Almost complete oxidation of sample
- 10 μm Cr: Degraded coating and significant  $\alpha$ -Zr(O) formation
- 15-25 μm Cr: 4-layer structure with  $ZrO_2$  paths along Cr GBs
- 25 μm Cr: local defects in coating
- ➔ Best protection for 15-20 μm Cr thickness



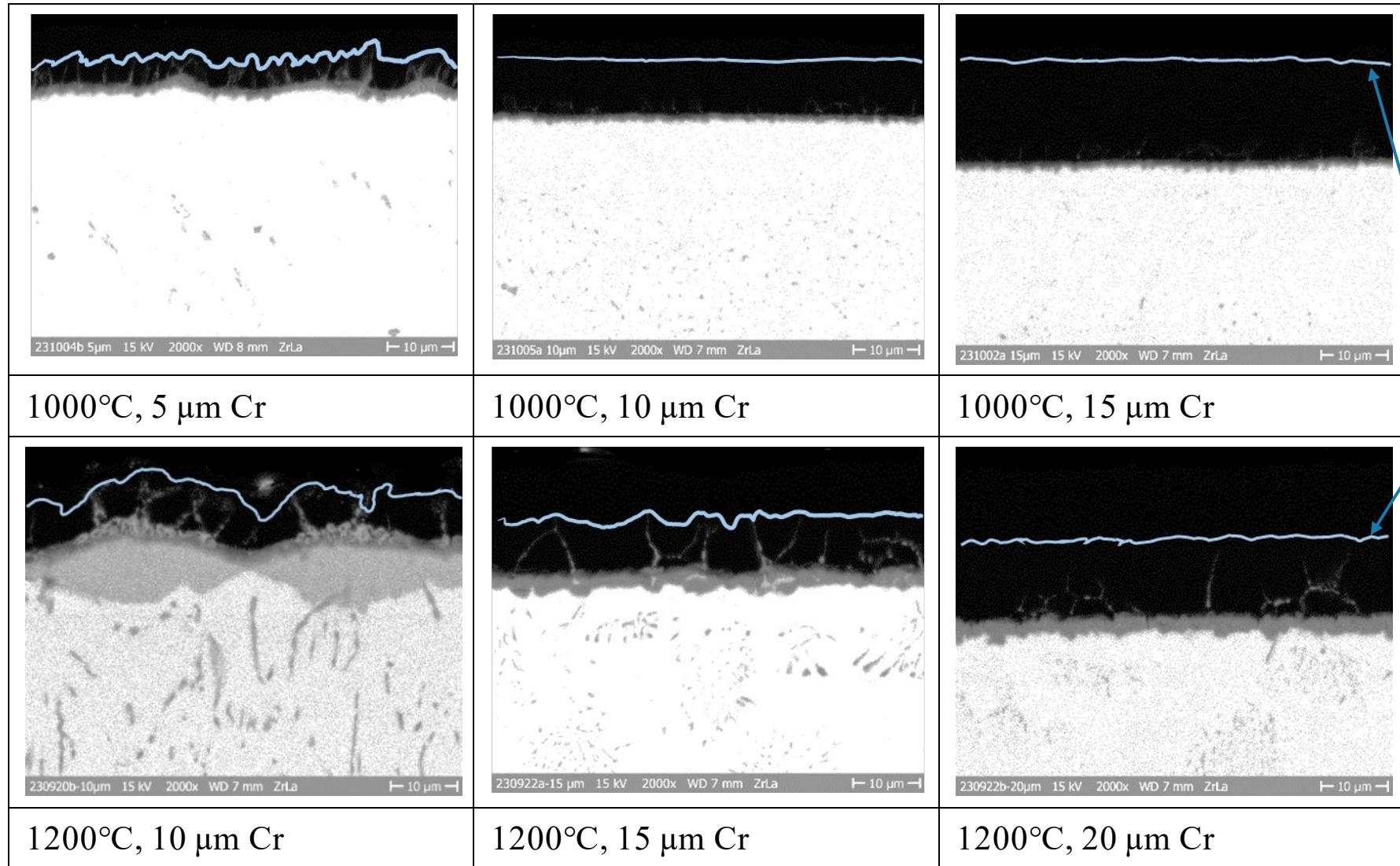
# Special feature only for 25- $\mu\text{m}$ sample at 1200°C

Failure of Cr coating  
during oxidation



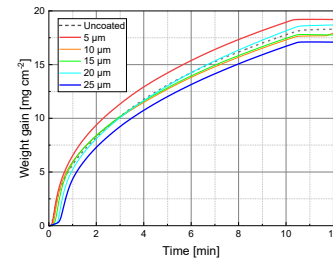
➔ Indication for too thick Cr coating resulting in thermo-mechanical mismatch?

# ZrO<sub>2</sub> diffusion paths along Cr grain boundaries

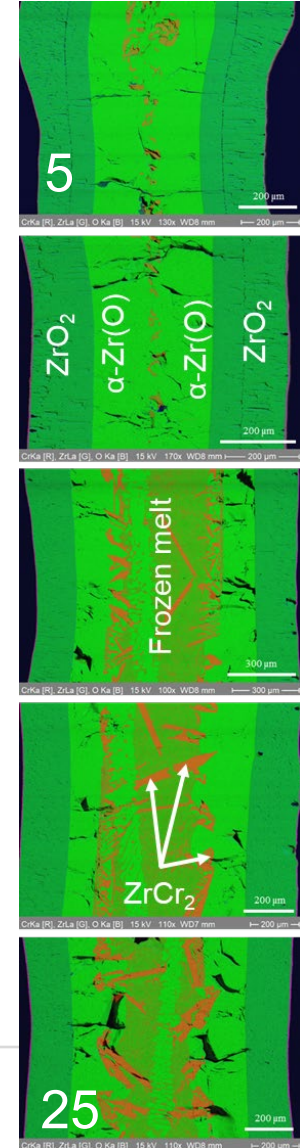
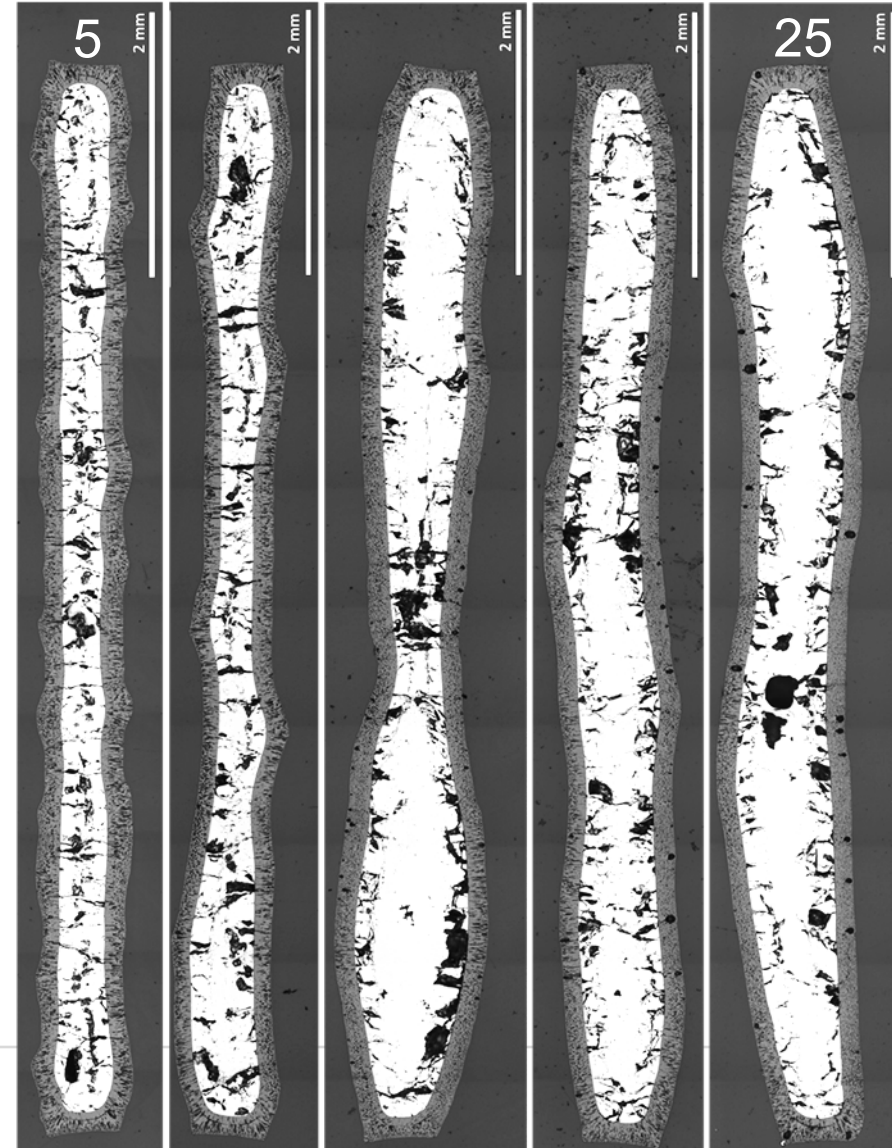


Cr/Cr<sub>2</sub>O<sub>3</sub>  
interface

# Post-test examination of 1400°C samples



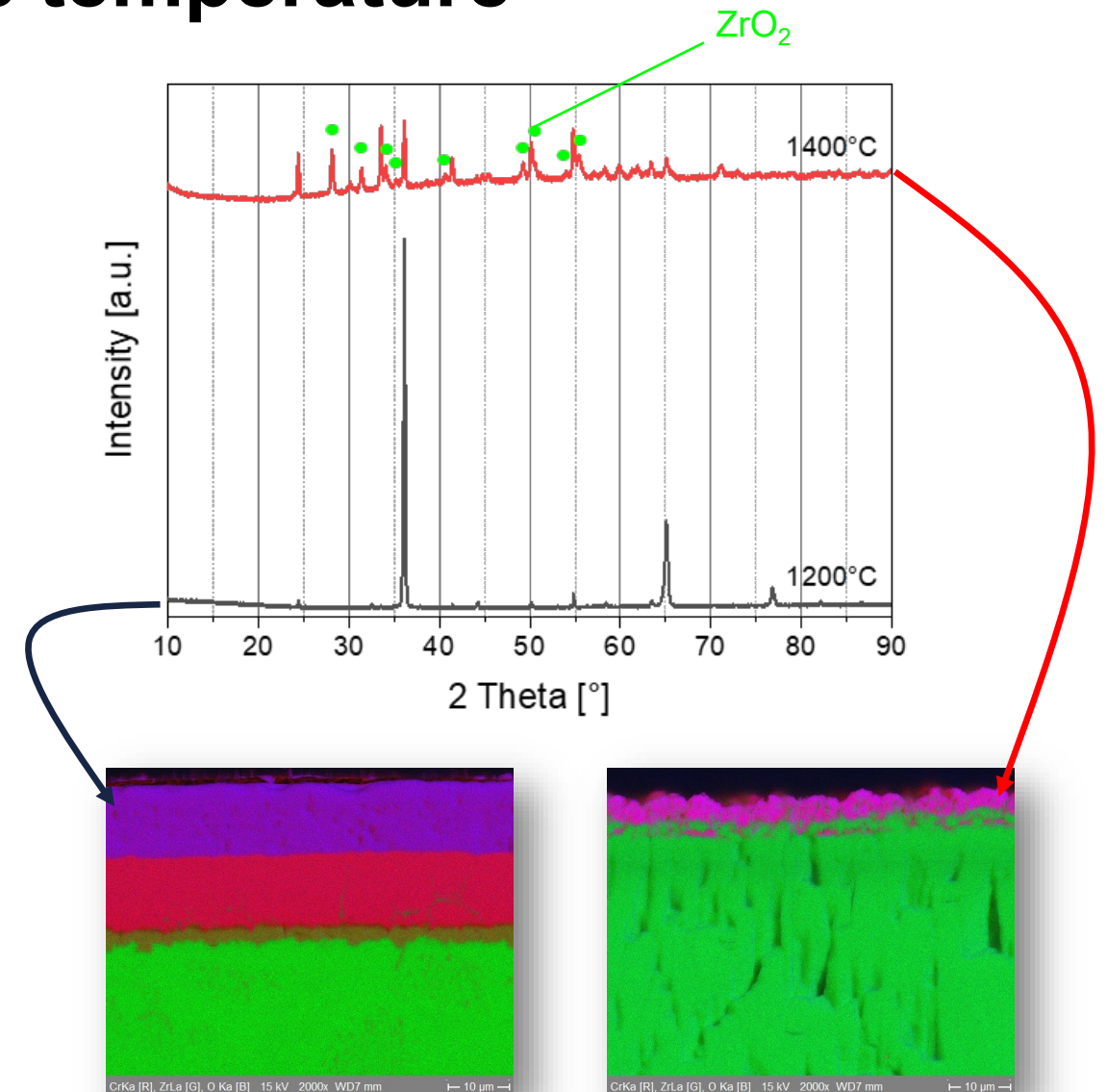
- Significant oxidation of all samples, almost independent on Cr thickness
- Increasing eutectic melt formation with thicker Cr coating
- $ZrCr_2$  precipitates in frozen melt
- $Cr_2O_3$  layer on surface
- ➔ No protective effect of Cr coating above eutectic temperature (1330°C)





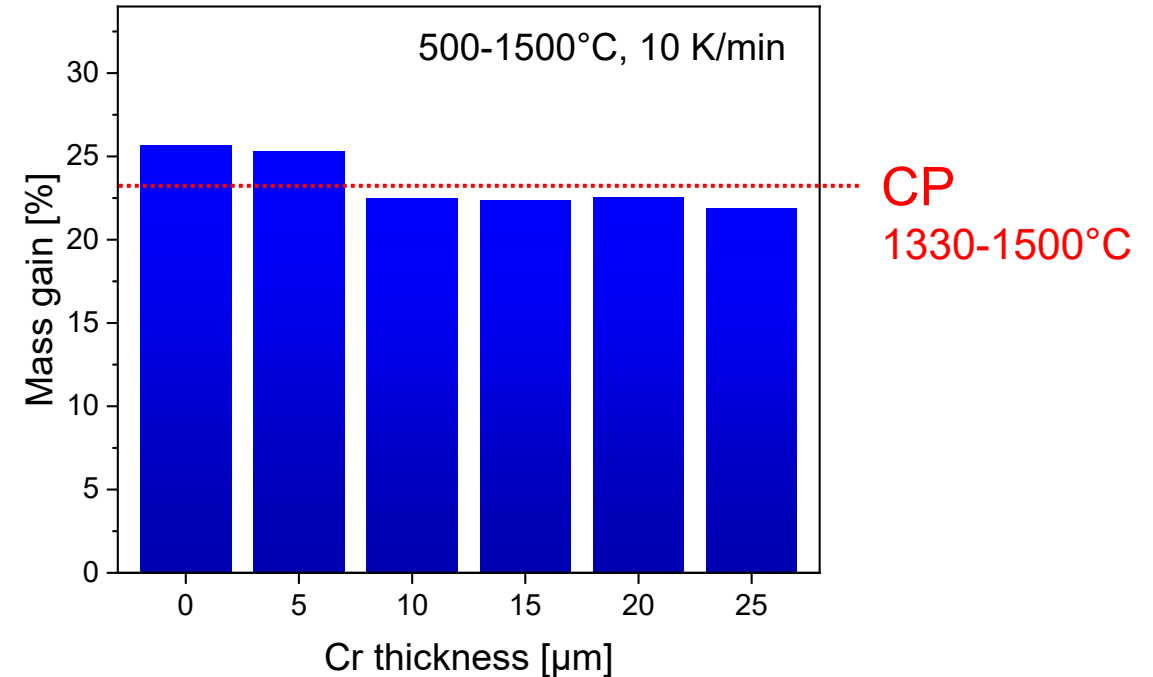
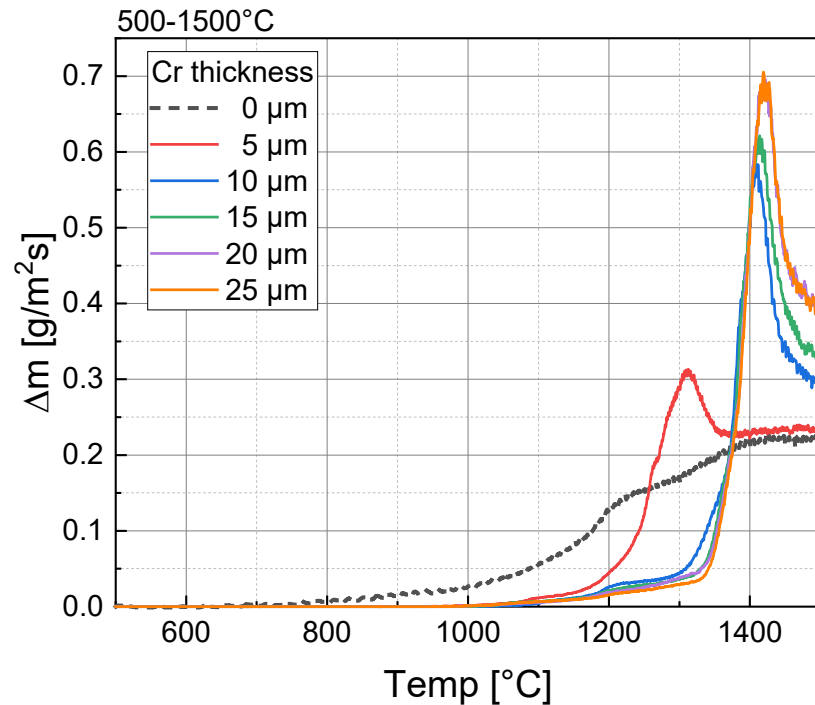
# XRD below and above eutectic temperature

- 1200°C: Strong (110) texture of the epitaxially grown  $\text{Cr}_2\text{O}_3$
- 1400°C: Evenly distributed  $\text{Cr}_2\text{O}_3$  grains
- ➔ Initially formed  $\text{Cr}_2\text{O}_3$  reduced by Zr-Cr eutectic melt and reformed on top of the  $\text{ZrO}_2$  layer



# Transient tests

# Oxidation rates vs. temperature

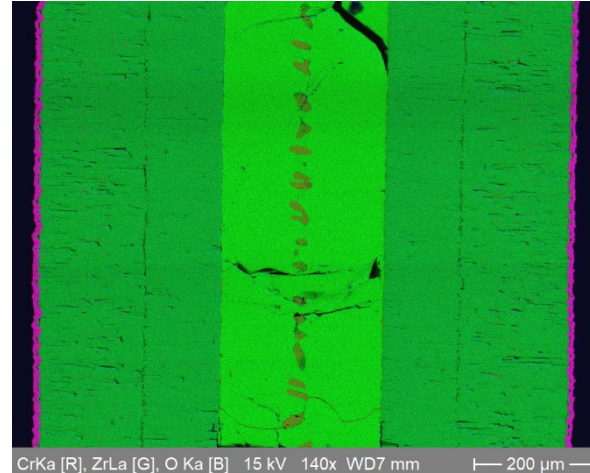
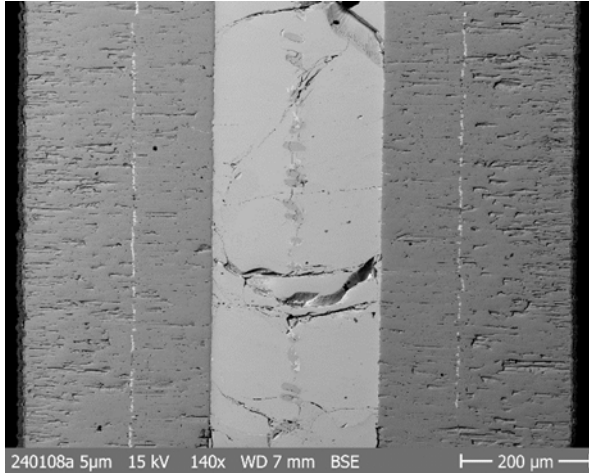


- Protective effect of all coatings up to 1200°C
- Early failure of 5-μm sample above 1200°C due to oxidation and mutual diffusion
- 10-25-μm samples: Rapid increase of oxidation rates above eutectic temperature of 1330°C
- Comparable integral oxidation for all samples

# Post-test examination samples after transient tests

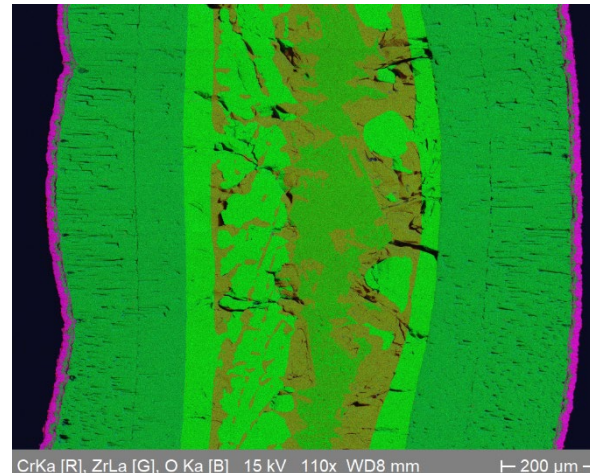
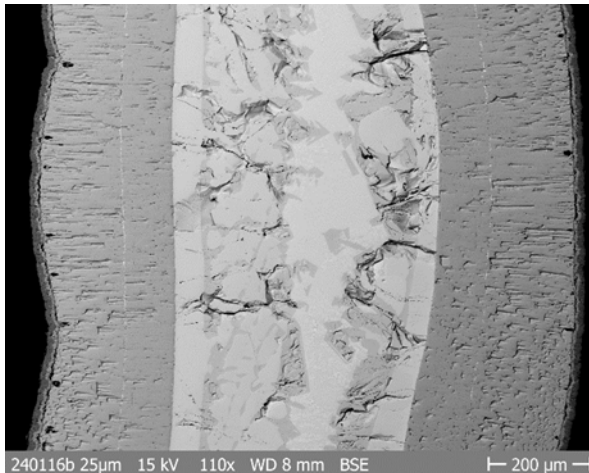
Examples: 5  $\mu\text{m}$  and 25  $\mu\text{m}$  Cr

5  $\mu\text{m}$



- Inverse “crocodile skin” of samples with  $\geq 10 \mu\text{m}$  Cr
- Thin superficial (re-formed)  $\text{Cr}_2\text{O}_3$  layer
- Thick  $\text{ZrO}_2$  layer with tin line

25  $\mu\text{m}$



- Increasing eutectic melt formation with thicker Cr coating in the center of the sample

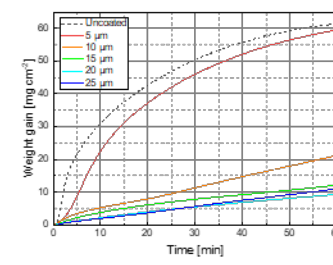
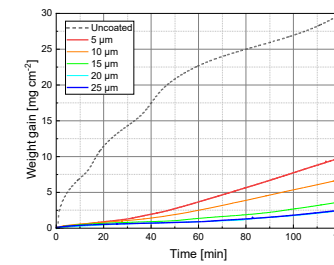
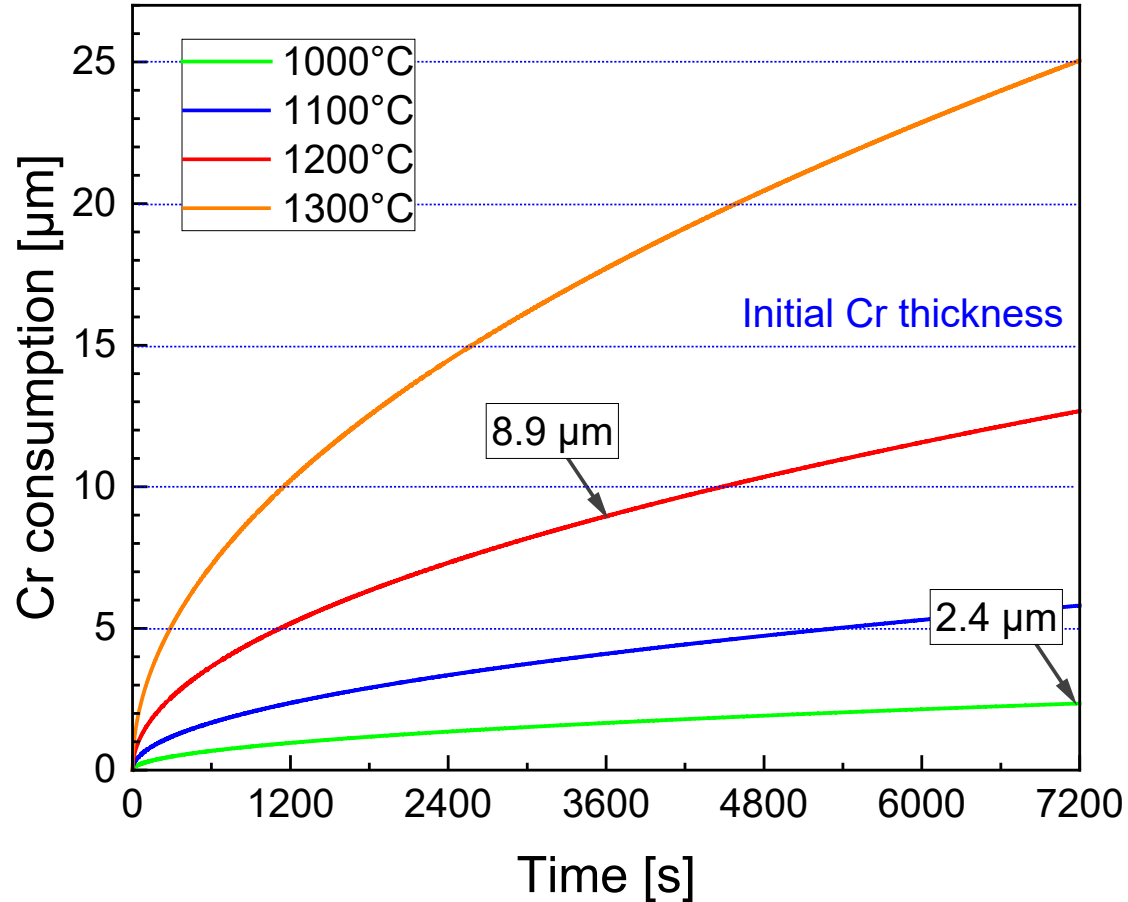
Optical micrographs

EDS mappings

# Estimation of Cr consumption

Based on Brachet, Proceedings TOPFUEL2024, Grenoble, France  
(considering Cr oxidation and diffusion of Cr into Zry)

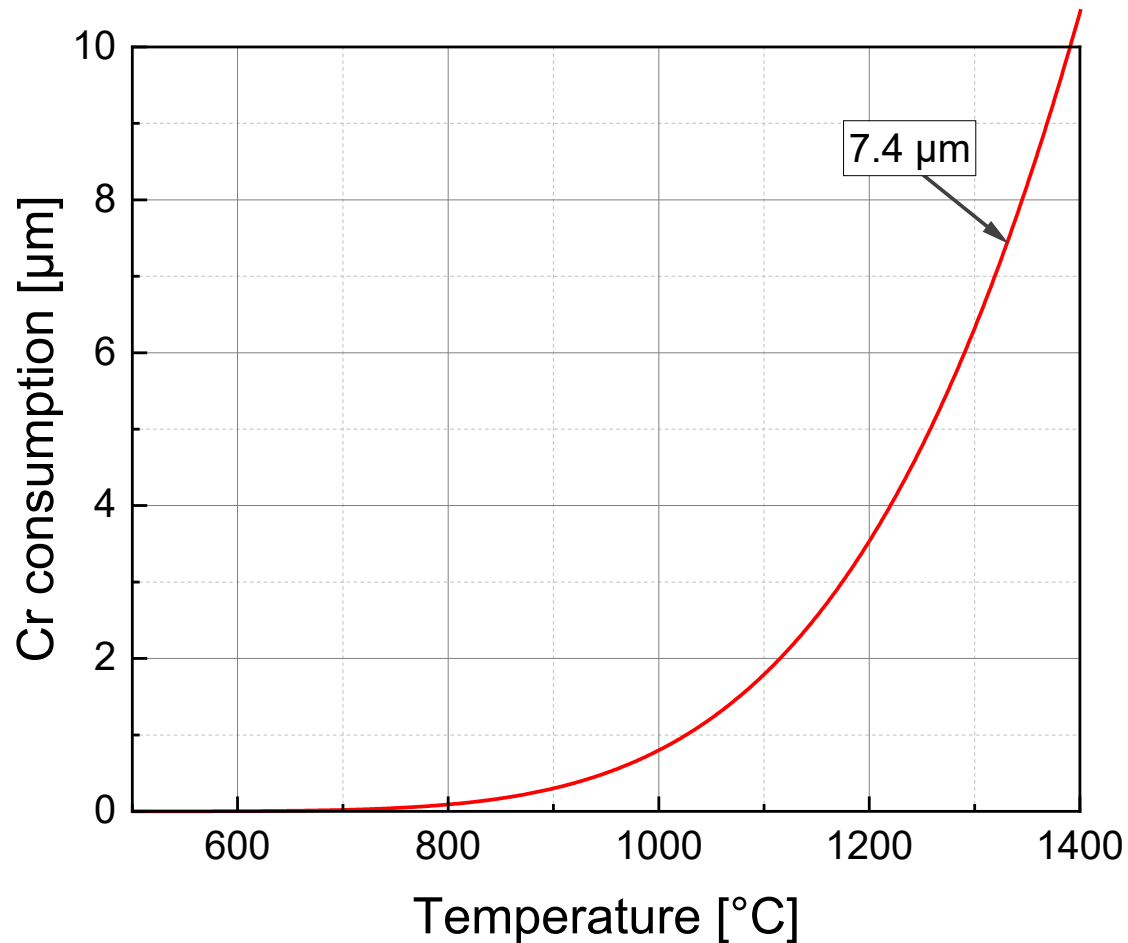
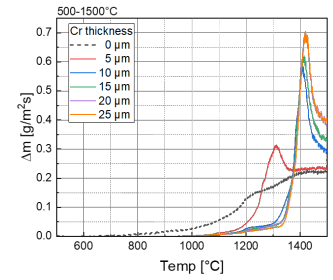
# Cr consumption during isothermal tests



- 1000°C: only partial consumption of Cr coating for all samples for 2 hours
- 1200°C: full consumption of 5-µm Cr, partial consumption of thicker coatings
- Good correspondence with experimental results

Cr consumption due to oxidation and diffusion

# Cr consumption during transient tests



- 7.4  $\mu\text{m}$  Cr consumed when eutectic temperature is reached
- Complete consumption of Cr coating at this point for 5- $\mu\text{m}$  coating
- Partial consumption of thicker coatings
- Good correspondence with experimental results

Cr consumption due to oxidation and diffusion

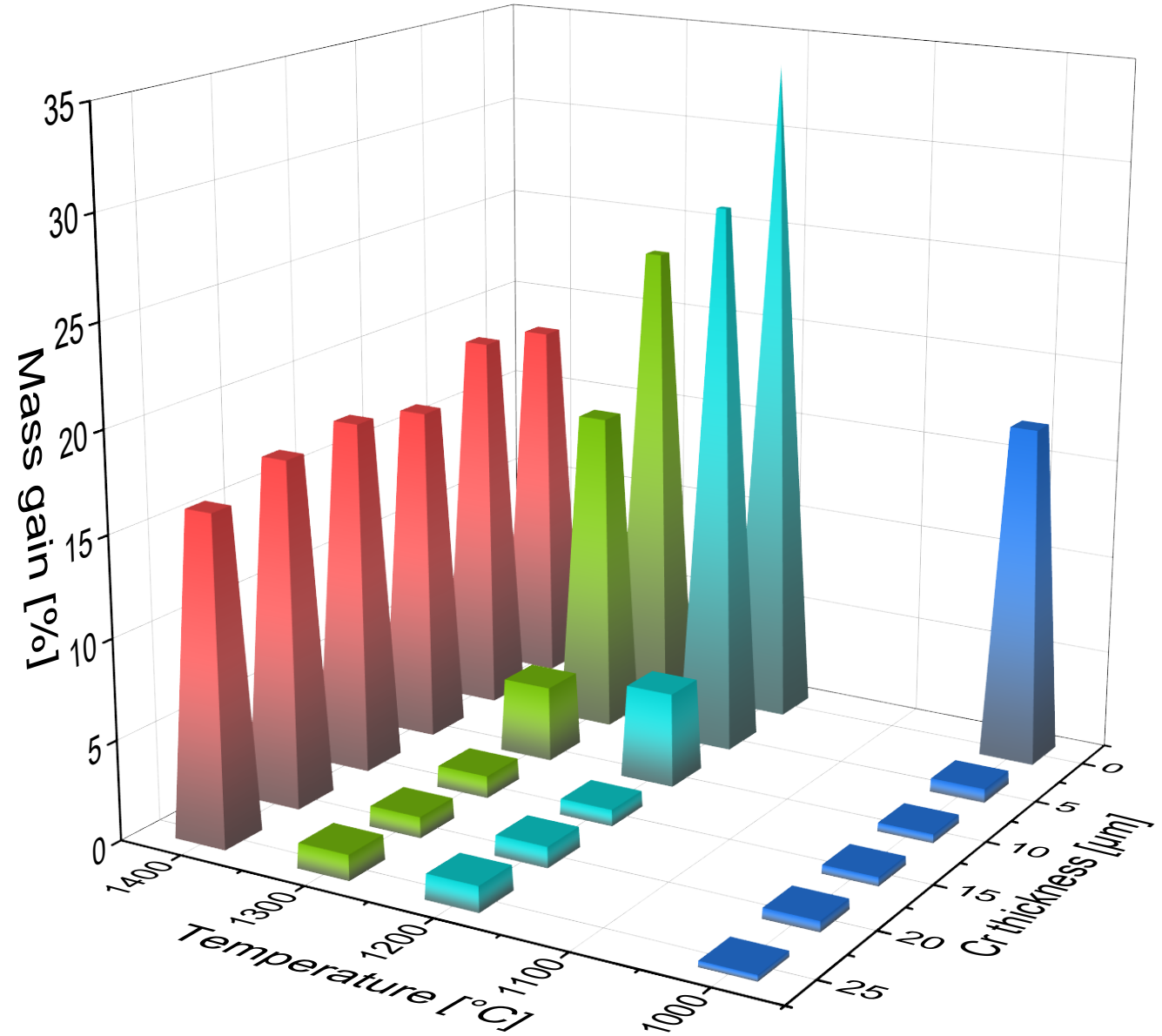
# Conclusion

- Increasing protective effect with increasing Cr thickness up to 1300°C
  - Oxidation and degradation are determined by diffusion processes
- Optimal (PVD) Cr thickness is between 15 and 20  $\mu\text{m}$ 
  - Thinner coating: early consumption and loss of protective effect
  - Too thick coating: Thermomechanical stresses may cause cracks in Cr coating
- Rapid failure of Cr coating at 1330°C with complete loss of protective effect caused by Cr-Zr eutectic interaction
- The more metallic Cr is present when the eutectic temperature is reached, the more eutectic melt is formed
- Oxidation kinetics above 1330°C determined by Zry oxidation
- ➔  $\text{Cr}_2\text{O}_3$  kinetics  $\rightarrow$  transition  $\rightarrow$   $\text{ZrO}_2$  kinetics
- ➔ Slow transition for  $T < 1330^\circ\text{C}$ , fast transition for  $T > 1330^\circ\text{C}$



# Graphical summary

Calculated mass gain based on layer thicknesses vs. temperature and Cr thickness



# Acknowledgment

- Injae Lee's internship at KIT was supported by the Korean KONICOF program
- HGF program NUSAFE for funding
- Jean-Christophe Brachet for fruitful discussions during post-test analyses
  
- Thank YOU for your patience



**Jean-Christophe Brachet**

CEA

## **Effect of initial Cr-coating thickness on the high-temperature steam oxidation behavior of Cr-coated Zr-based alloys: Comparison between TGA experiments conducted at several institutes using “Equivalent Chromium Reacted” (ECrR) parameter**

Karlsruhe Institute of Technology (KIT) has recently carried out several Thermo-Gravimetric Analysis (TGA) oxidation tests at High-Temperature (HT) in steam environment on Zircaloy-4 sheets coated by Cr using Physical Vapor Deposition (PVD), with initial Cr coating thicknesses ranging from 5 to 25  $\mu\text{m}$ . Along with observations made at CEA and in other research institutes, these recent TGA data from KIT confirm that increasing the initial Cr coating thickness reduces the oxidation kinetics at HT of Cr-coated Zr-based alloys. To take this effect into account, CEA has recently derived a new “Equivalent Cladding Reacted” parameter, called: “Equivalent Chromium Reacted” (ECrR) [1] [2], expressed as a function of HT oxidation conditions (temperature and time) and the initial Cr coating thickness:

$$\text{ECrR (\%)} = 6.73 \times 105 \exp(-15784/T) \times (t)^{1/2} / X_0$$

*(T in Kelvin, t in seconds, X<sub>0</sub> being the initial Cr-coating thickness in  $\mu\text{m}$ )*

This simple parameter appears efficient to predict the overall “consumption kinetics” of Cr coating upon HT oxidation. Moreover, this new metric has been successfully used to account for the initial Cr coating thickness effect on the Post-Quenching (PQ) residual cladding strength and ductility, following one-sided HT steam oxidation. Regardless of the initial Cr thickness, ranging from  $\sim 5 \mu\text{m}$  to  $\sim 25 \mu\text{m}$ , it was demonstrated that the PQ Ductile-to-Brittle Transition (DBT) of the failure mode in the Cr-coated cladding occurs at an apparent “critical” value of the ECrR parameter of nearly 70% [1]. Indeed, for Cr-coated claddings steam oxidized at 1100-1300°C and when the Cr-coating loses its protectiveness, it has been shown that this ECrR value corresponds to an averaged oxygen content that has diffused into the prior- $\beta\text{Zr}$  reaching a value higher than  $\sim 0.4\text{wt.}\%$  [2] which is known to be a “critical” value inducing DBT of the water quenched prior- $\beta\text{Zr}$  value at room temperature [3].

Furthermore, as will be shown in this presentation and illustrated in Figs 1 & 2, the use of this new “ECrR” allows rationalizing and capturing the effect of the initial Cr coating on the Weight Gain (WG) evolution during HT oxidation for various initial Cr coating thicknesses, oxidation temperatures, and durations, and under both isothermal and anisothermal conditions. Fig. 2 also highlights an acceleration of the WG increase beyond an ECrR of about 70-100%, consistent with the expected loss of HT oxidation protectiveness of the Cr coating beyond this “critical” ECrR range.

**References:**

- [1] Brachet, J.-C., Guilbert, T., Hamon, D., Nony, G., & Gokelaere, P. (2024). "A new « ECR » parameter to support high-temperature (one-sided) steam oxidation behavior of Cr-coated Zr-based E-ATF claddings, in relation with their post-quenching (PQ) mechanical strength and ductility (for LOCA and slightly beyond conditions)", Proceedings of the Topfuel / Reactor Fuel Performance International Symposium, 29 September – 3 October 2024, Grenoble, France.
- [2] Brachet, J.-C., Guilbert, T., Urvoy, S., Rouesne, E., Peyret, M., Vandenberghe, T., Prou, C., Le Hong, T., Hamon, D., "Some practical methodologies to assess the overall high temperature (one-sided) steam oxidation protectiveness of chromium-based coatings on a zirconium-based substrate, as Enhanced - Accident Tolerant (Nuclear) Fuels (E-ATF) claddings", Journal of Nuclear Materials (2025), doi: <https://doi.org/10.1016/j.jnucmat.2025.155620>
- [3] Brachet, J.-C., Maillot, V., Portier, L., Gilbon, D., Lesbros, A., Waeckel, N., Mardon, J.-P., "Hydrogen Content, Pre Oxidation and Cooling Scenario Influences on Post-Quench Mechanical Properties of Zy-4 and M5TM Alloys in LOCA Conditions - Relationship with the Post-Quench Microstructure", ASTM 15<sup>th</sup> International Symposium on Zirconium in the Nuclear Industry, June 24-28, 2007, Sunriver, Oregon, USA, Journal of ASTM International, Vol. 5, No. 4, Paper ID JAI101116, (2008)

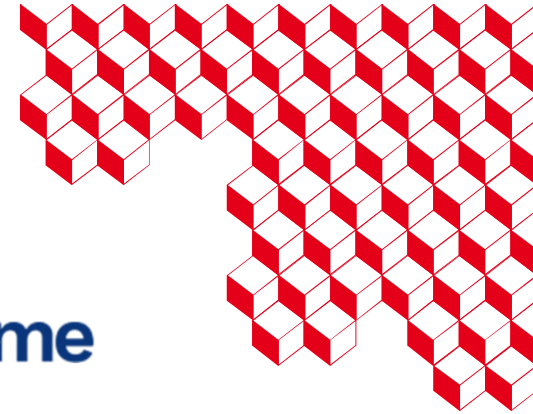


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# Effect of initial Cr-coating thickness on the HT steam oxidation behavior of Cr-coated Zr-based alloys: Comparison between TGA experiments conducted at several institutes using “Equivalent Chromium Reacted” (ECrR) parameter

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## Main references:

[1] J.-C. Brachet, et al., “High Temperature Steam Oxidation of Chromium-Coated Zirconium-Based Alloys: Kinetics and Process”, *Corrosion Science* 167 (2020) 108537, doi: <https://doi.org/10.1016/j.corsci.2020.108537>

[2] J.-C. Brachet, et al., “Evaluation of Equivalent Cladding Reacted parameters of Cr-coated claddings oxidized in steam at 1200°C in relation with oxygen diffusion/partitioning and post-quench ductility”, *JNM* 533 (2020) 152106, <https://doi.org/10.1016/j.jnucmat.2020.152106>

[3] J.-C. Brachet et al., “A new « ECR » parameter to support high-temperature (one-sided) steam oxidation behavior of Cr-coated Zr-based E-ATF claddings, in relation with their post-quenching mechanical strength and ductility...”, *Proceedings of Topfuel-2024, Grenoble, France, (Sept. 29th - Oct. 03rd 2024)*;

[4] J.-C. Brachet, et al., “Some practical methodologies to assess the overall high temperature (one-sided) steam oxidation protectiveness of Cr-based coatings on a zirconium-based substrate...”, *Journal of Nuclear Materials* (2025), doi: <https://doi.org/10.1016/j.jnucmat.2025.155620>

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30<sup>th</sup> Int. QUENCH Workshop, KIT (Karlsruhe, Germany), 16-18<sup>th</sup> Dec. 2025

Recall - Consumption kinetics of Cr coatings on Zr-based substrate upon HT steam oxidation (1000-1300°C, LOCA and slightly beyond conditions) by two main mechanisms:

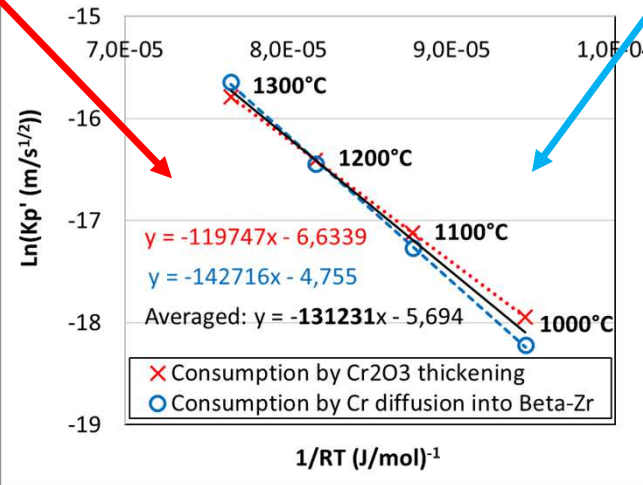
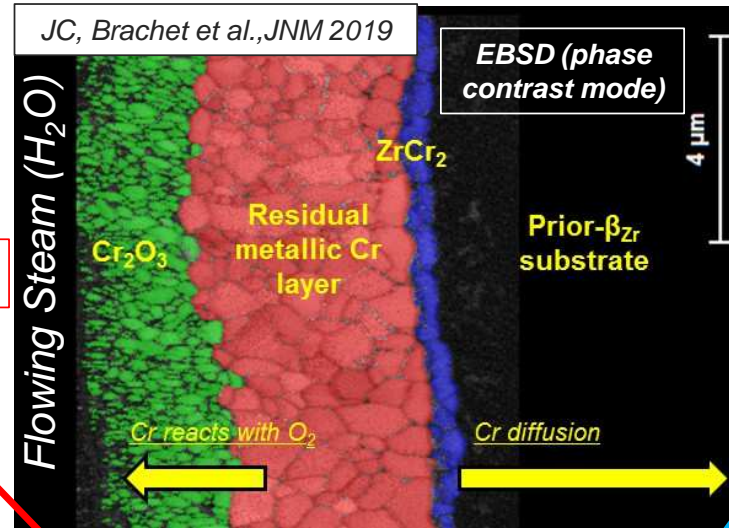
(1) Outer Cr<sub>2</sub>O<sub>3</sub> scale thickening

$$\Delta Cr(\text{consumed by } Cr_2O_3) = Kp_1' \sqrt{\text{oxidation time}}$$

(3) Cr volatilization and Cr consumption due to the interlayer ZrCr<sub>2</sub> thickening are neglected (i.e., less than ~2µm Cr consumed by these mechanisms...)

(2) Cr diffusion into the β<sub>Zr</sub> substrate

$$\Delta Cr(\text{Cr diffusion into } \beta_{Zr}) = Kp_2' \sqrt{\text{oxidation time}}$$



Due to similar parabolic rate constant (Kp') values, one can identify an “averaged” Kp' describing the overall contributions of both Cr-coating consumption mechanisms

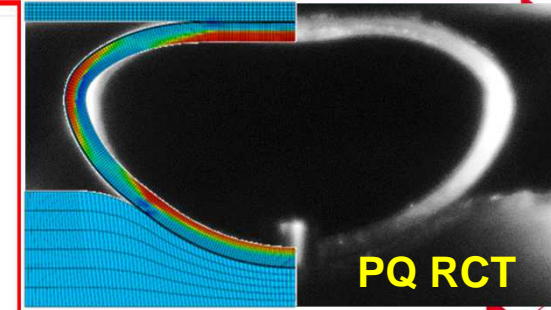
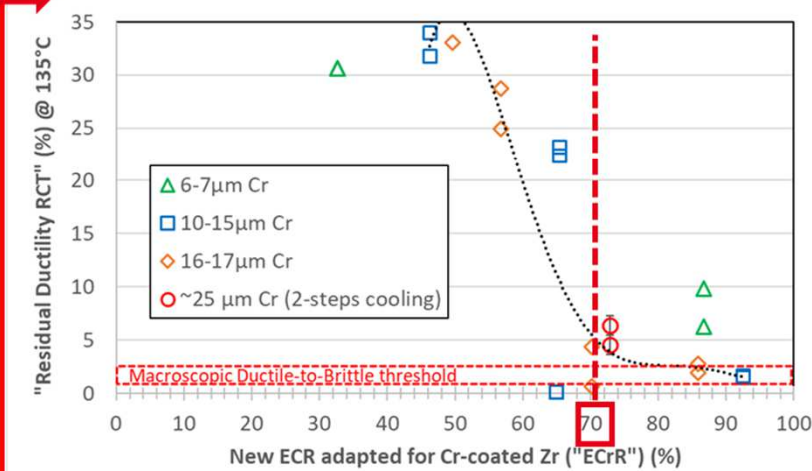
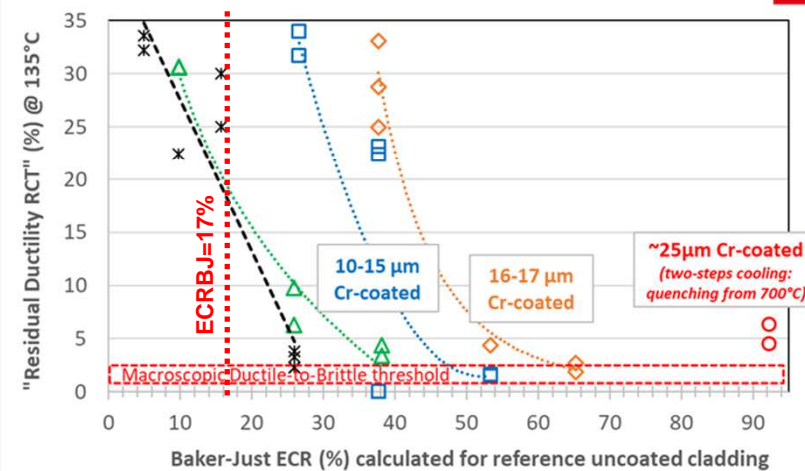
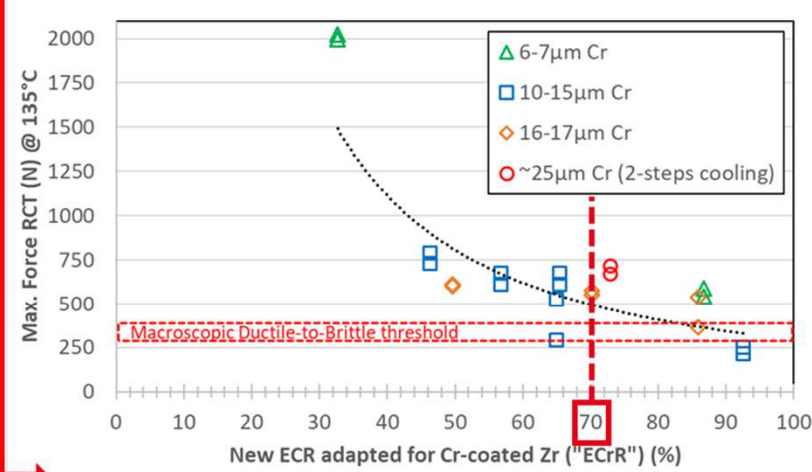
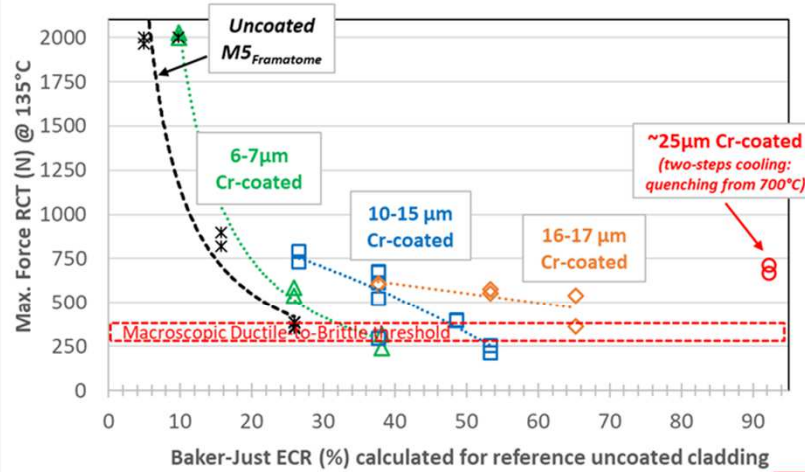
$$\Delta Cr_{(Cr_2O_3 + Cr \text{ diffusion into } \beta\text{-Zr})} = 2 \times Kp'_{\text{Averaged}} \sqrt{\text{oxidation time}} = 6,73 \cdot 10^3 \cdot \exp(-15784/T) \cdot \sqrt{\text{oxidation time}}$$

With: ΔCr in µm, T in Kelvin and t in seconds

JC, Brachet et al., Topfuel, 2024

New ECR parameter, i.e., « Equivalent Chromium Reacted » proposed, taking into account the initial Cr-coating thickness ( $X_0$ ):

$$ECrR (\%) = 6,73 \cdot 10^5 \cdot \exp(-15784/T) \cdot (t)^{1/2} / X_0 \quad (X_0 \text{ in } \mu\text{m})$$



**Partial Conclusion (1):**

- New "ECrR" parameter helps to "rationalise" the PQ clad mechanical properties of Cr-coated materials derived from RCT, by taking into account the initial Cr-coating thickness influence

**Partial Conclusion (2):**

- After 1-sided steam oxidation & water quenching, determination of an apparent "critical ECRR" ~ 70% which corresponds to Ductile-to-Brittle-Transition derived from RCT @ 20 & 135°C

JC, Brachet et al., Topfuel, 2024

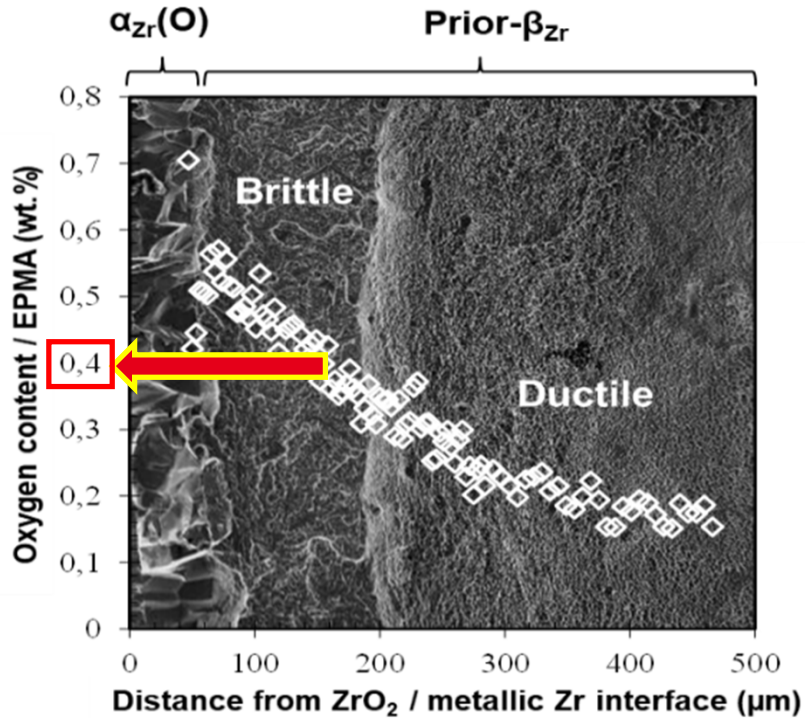


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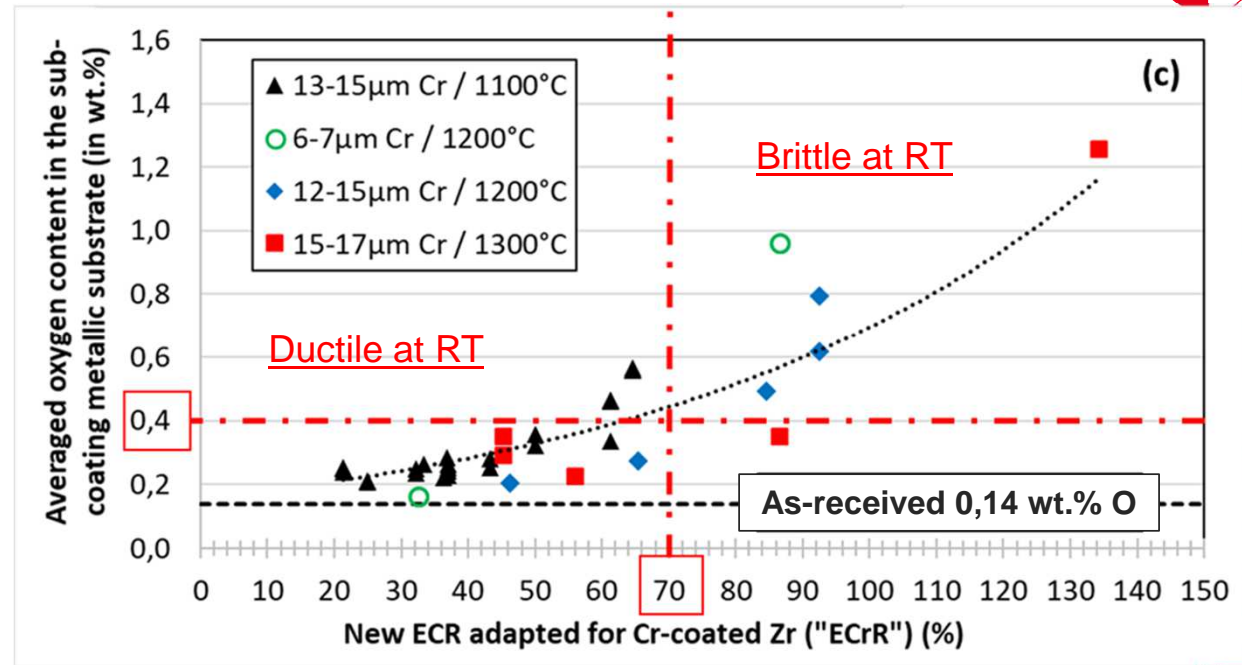
30<sup>th</sup> Int. QUENCH Workshop, KIT (Karlsruhe, Germany), 16-18th Dec. 2025

Relationship between the apparent critical « ECrR » ~ 70% inducing Ductile-to-Brittle transition of the failure mode of HT (one-sided) oxidized Cr-coated claddings following water quenching down to RT vs. the prior- $\beta_{Zr}$  oxygen content  
*(neglecting the additional influence of Cr diffusion and/or of potential H uptake...)*

Cross-section fractograph of an uncoated Zr-based cladding after HT oxidation and PQ Impact testing at RT:



JC. Brachet, V. Maillot et al.,  
 J. of ASTM International (2008)



JC, Brachet et al., JNM, 2025



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30<sup>th</sup> Int. QUENCH Workshop, KIT (Karlsruhe, Germany), 16-18th Dec. 2025



### Partial conclusions:

New “ECrR” parameter helps to “rationnalise” the PQ clad mechanical properties of Cr-coated materials derived from RCT, by **taking into account** :

- the initial **Cr-coating thickness** influence : within the **5-30 $\mu$ m** thicknesses range
- **oxidation duration** : from a few minutes to several hours
- **oxidation temperature** : within the **1100-1300°C** temperature range

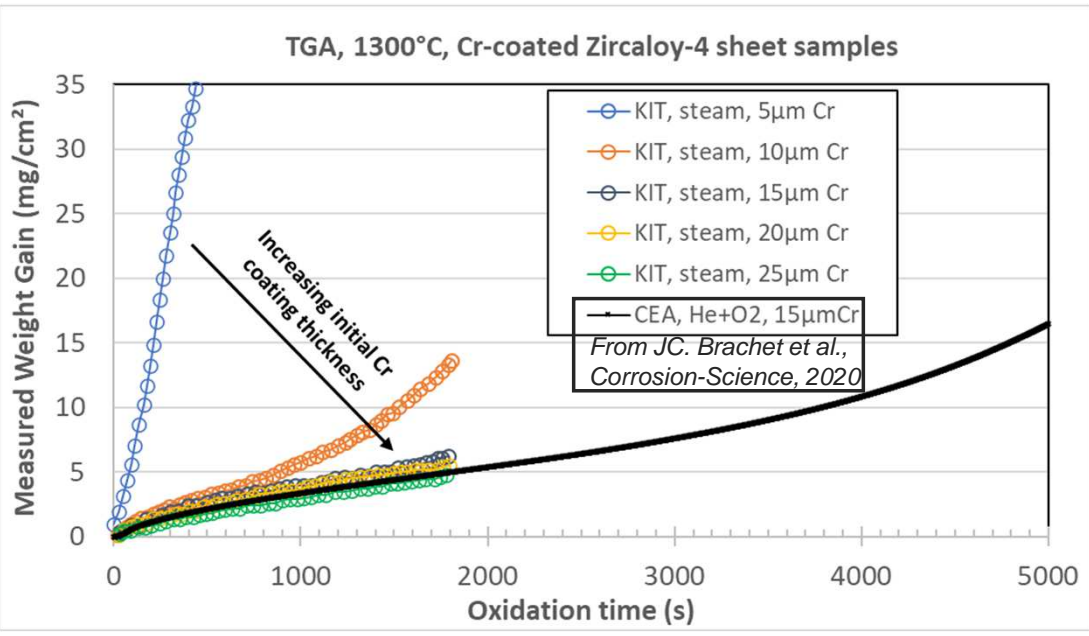
⇒ Apparent **“critical ECrR”** ~ 70% which corresponds to:

- Achievement of **~0,4 wt. % of oxygen** having diffused within the residual **prior- $\beta_{Zr}$  layer substrate**
- **PQ Ductile-to-Brittle** transition of the macroscopic failure mode (derived from PQ RCT and/or from PQ impact testing at RT...)

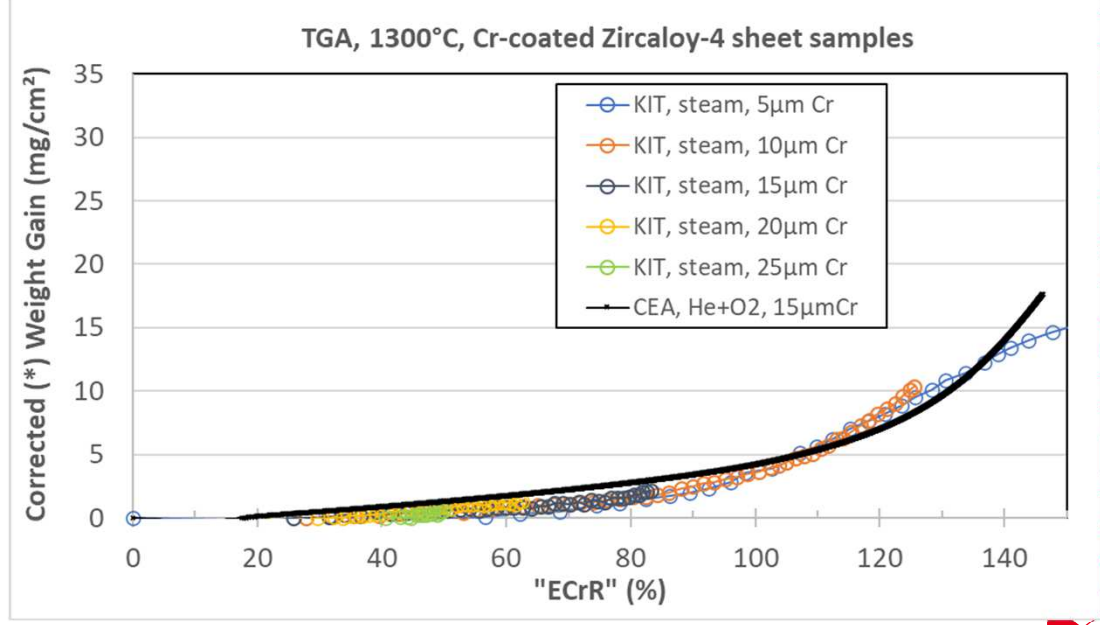
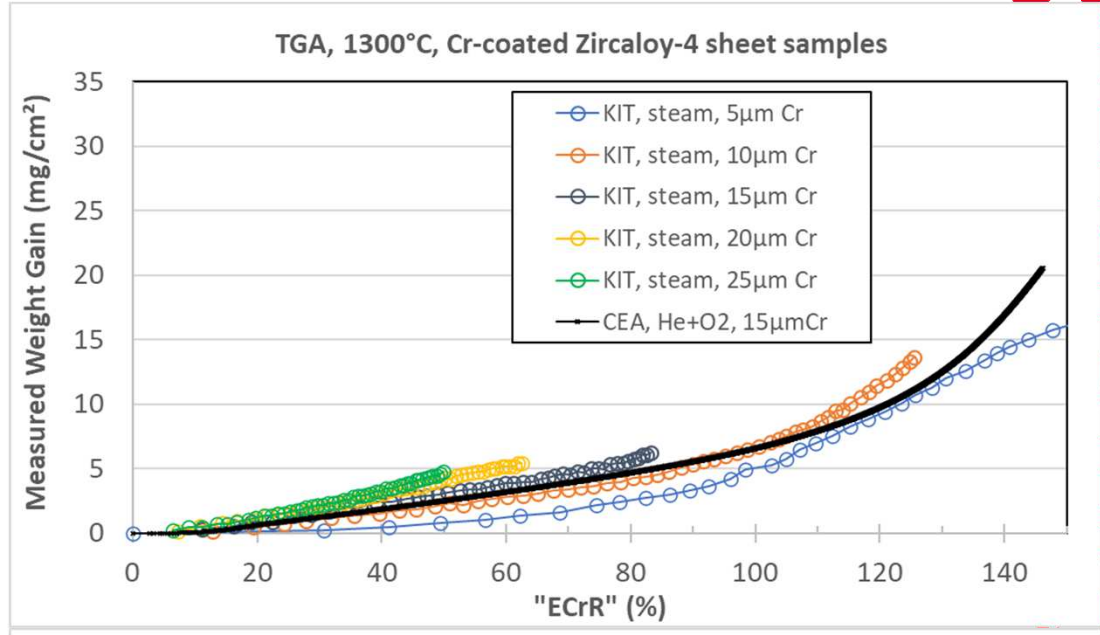
### Aim of the present study/analysis:

Extend and apply these new “ECrR” metrics to Cr-coated materials developed and studied at different institutes and for different initial thicknesses, in relation with their continuous Weigh-Gain (WG) evolution, as measured by Thermo-Gravimetric Analysis (TGA) upon one-sided steam oxidation at HT, for both isothermal and anisothermal (transient) conditions

Ex. 1 (1/2): KIT TGA data obtained on Cr-coated Zirc-4 with Cr thicknesses ranging from 5 to 25µm -  $T_{\text{oxidation}} = 1300^{\circ}\text{C}$   
 (see previous Martin S. presentation, submitted to JNM...)

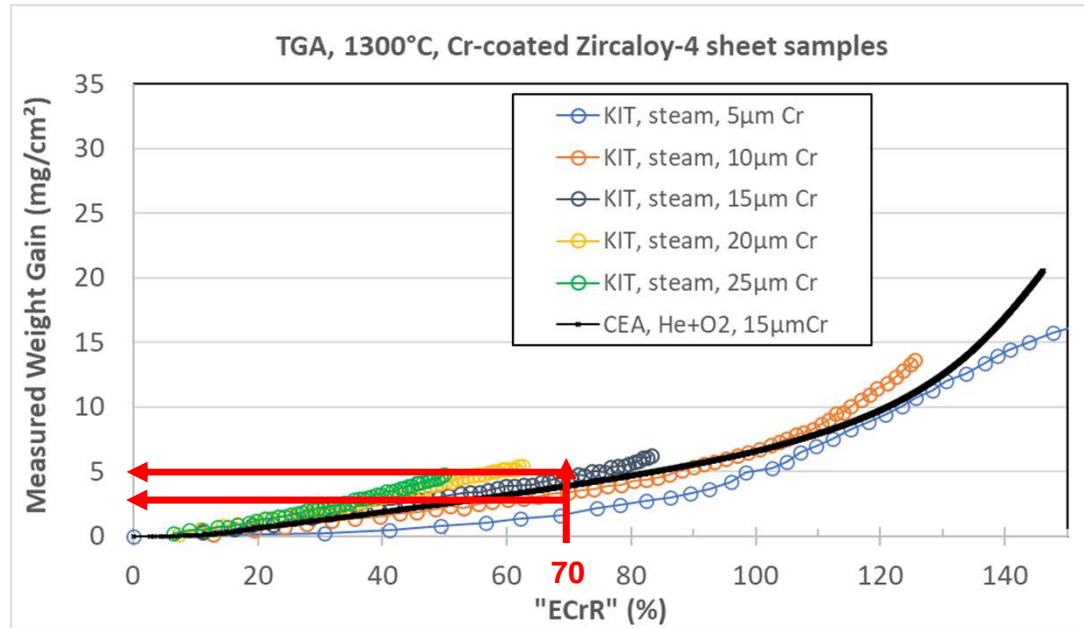


(\*) Attempts have been done to correct the « extra-WG » measured due to uncoated or poorly coated samples areas with a quite conservative assumption that 10% of the total surface is uncoated...



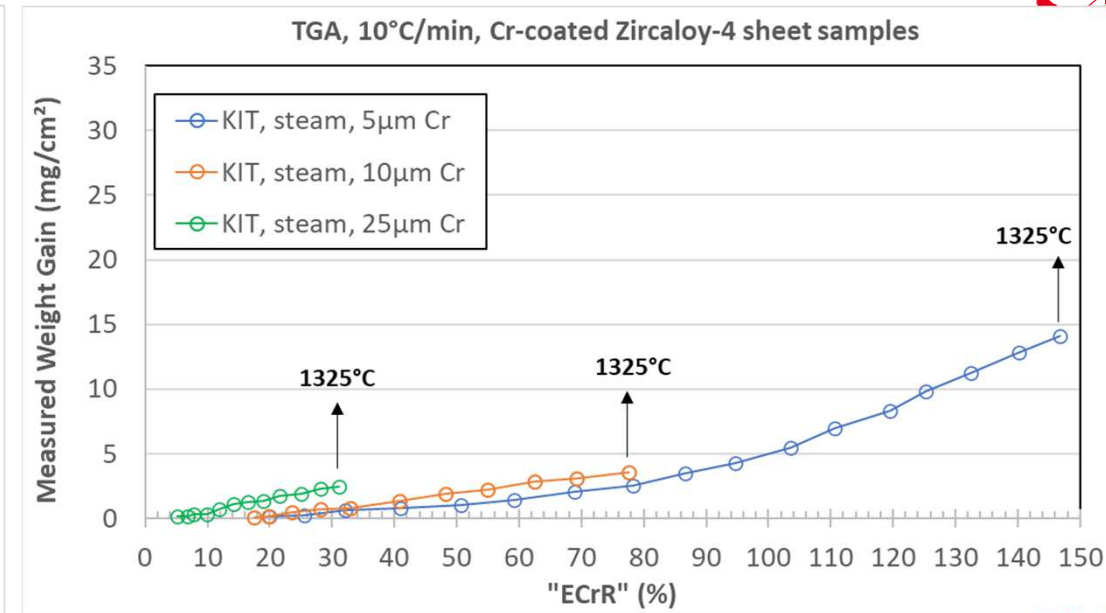
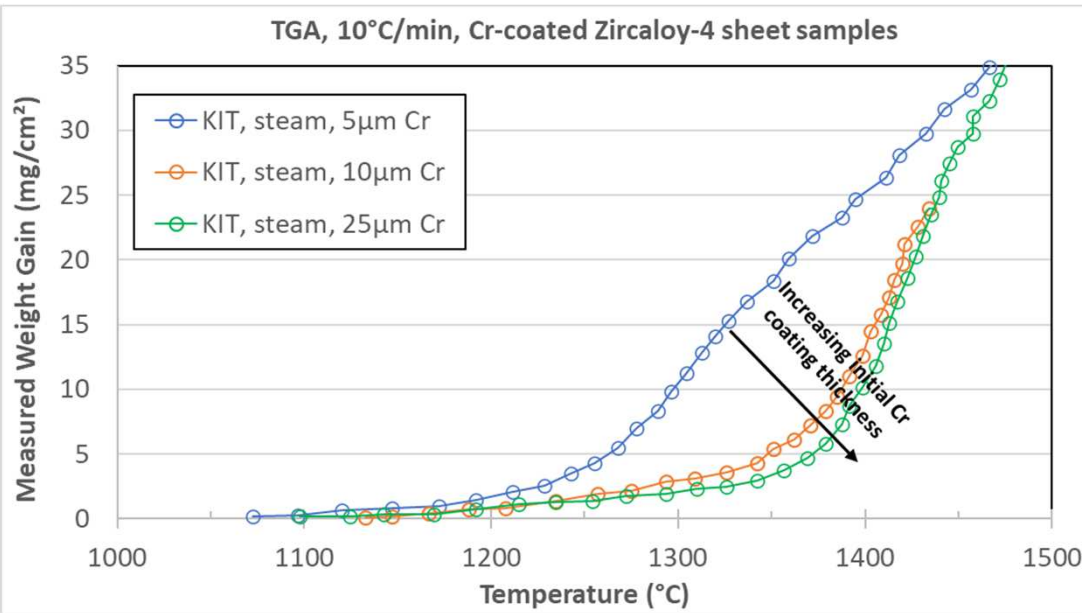
[jean-christophe.brachet@cea.fr](mailto:jean-christophe.brachet@cea.fr)

Ex. 1 (2/2): KIT TGA data Cr = 5 - 25 $\mu$ m; T<sub>oxidation</sub> = 1300°C



**Apparent « critical ECrR = 70% »**  
(corresponding to HT oxidation kinetics acceleration,  
i.e., loss of Cr coating protectiveness threshold )  
⇔ **Apparent « critical WG » ~3-5 mg/cm<sup>2</sup>**

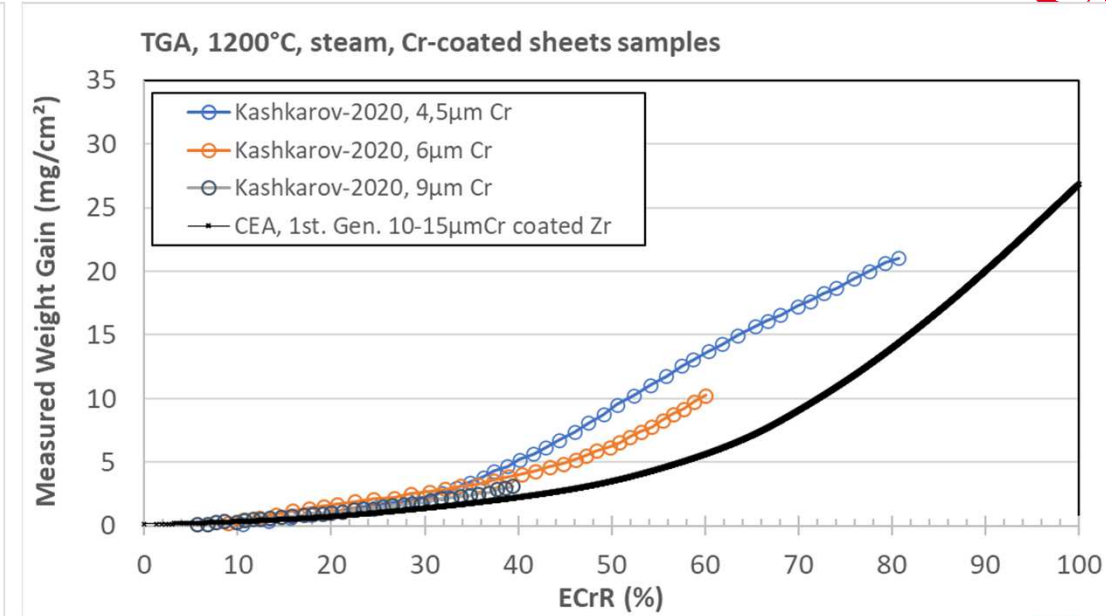
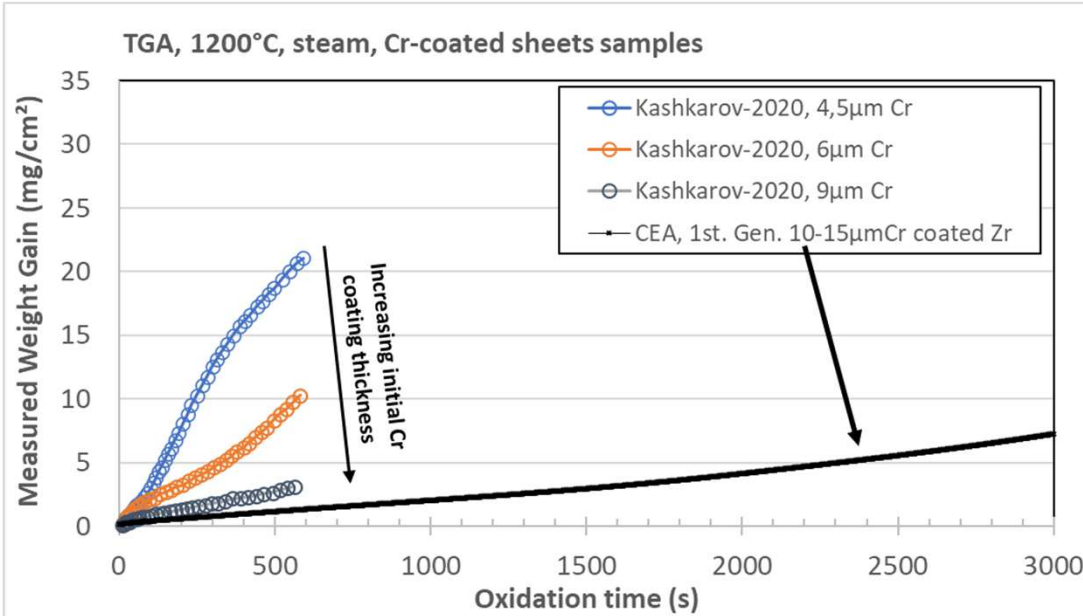
Ex. 2: KIT TGA data Cr = 5 - 25 $\mu$ m, Transient (anisothermal) conditions, 10°C/min up to 1500°C;



No correction of the uncoated or poorly coated surfaces influence on the measured WG

Rem.: data obtained above 1325°C not considered here, because of the « Zr-Cr eutectic » reaction inducing fast loss of the coating's protectiveness...

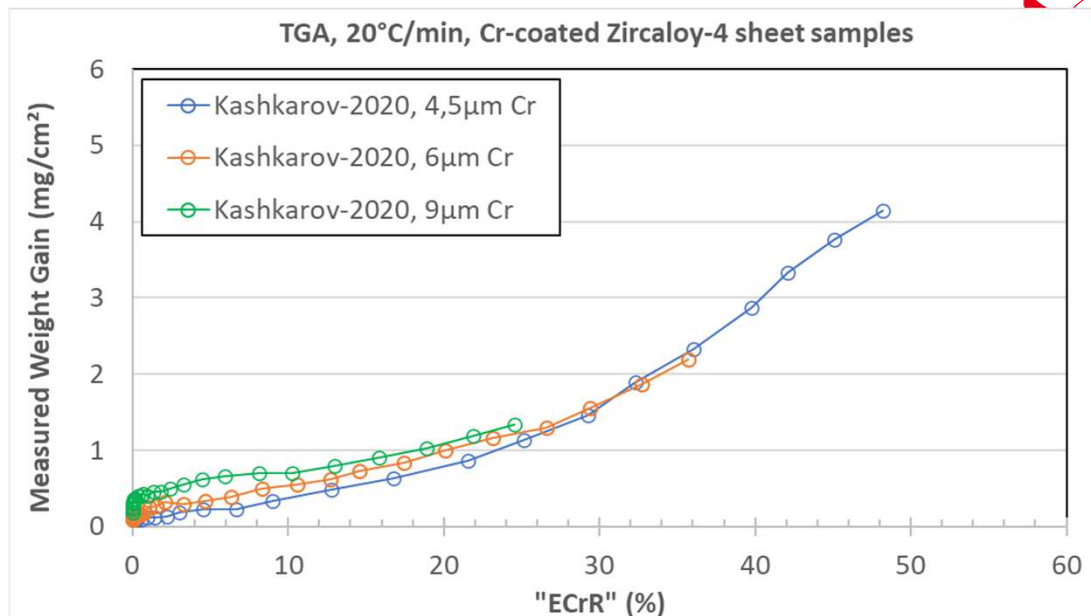
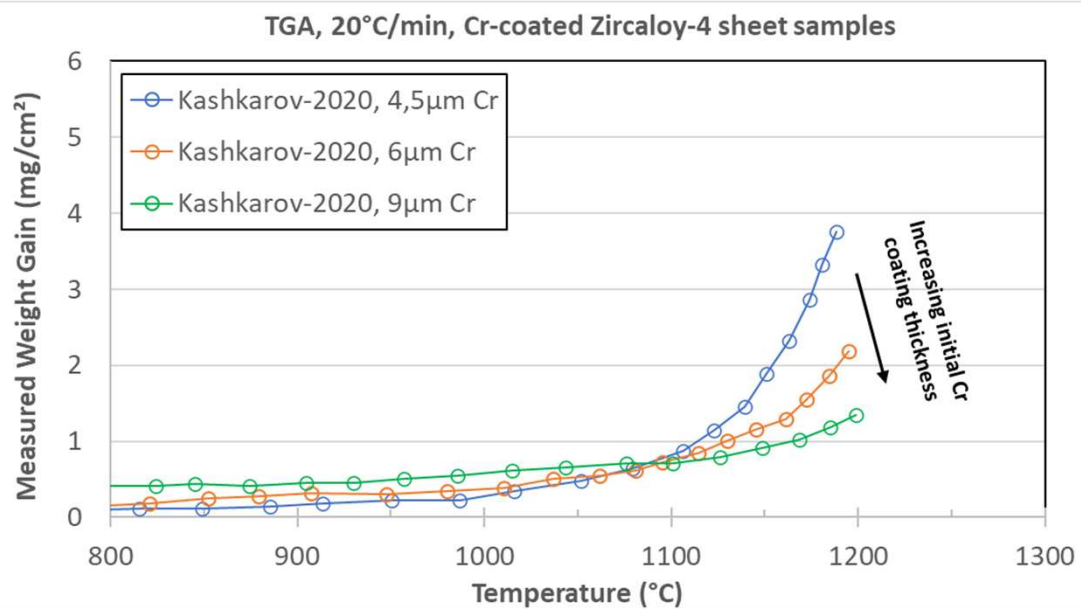
Ex. 3 (1/2): Previous KIT TGA data obtained on 1<sup>st</sup> generation Cr-coated E110, isothermal conditions, 1200°C  
Kashkarov et al., Corrosion Science, 2020



No correction of the uncoated or poorly coated surfaces influence on the measured WG

Apparent loss of Cr protectiveness (*i.e.*, *oxidation kinetics acceleration*) seems to occur earlier, for an **ECrR~40%**. Could be due to not fully optimized Cr-coating of these first generation coated E110 materials, having quite low Cr thicknesses...

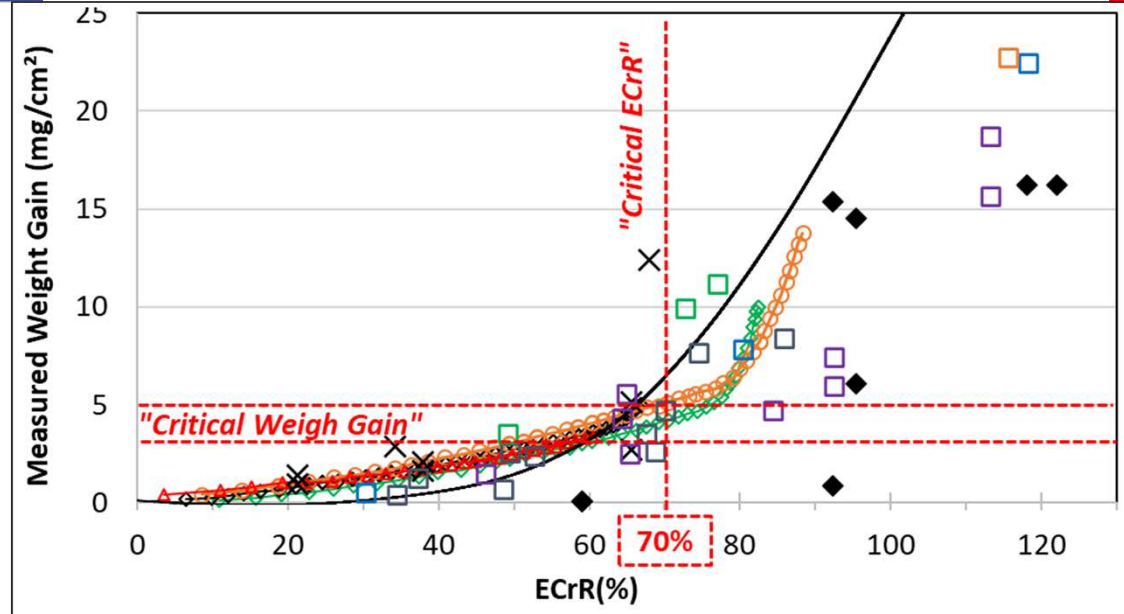
Ex. 3 (2/2): Previous KIT TGA data obtained on 1<sup>st</sup> generation Cr-coated E110, transient (20°C/min) conditions => 1200°C  
 Kashkarov et al., Corrosion Science, 2020



No correction of the uncoated or poorly coated surfaces influence on the measured WG

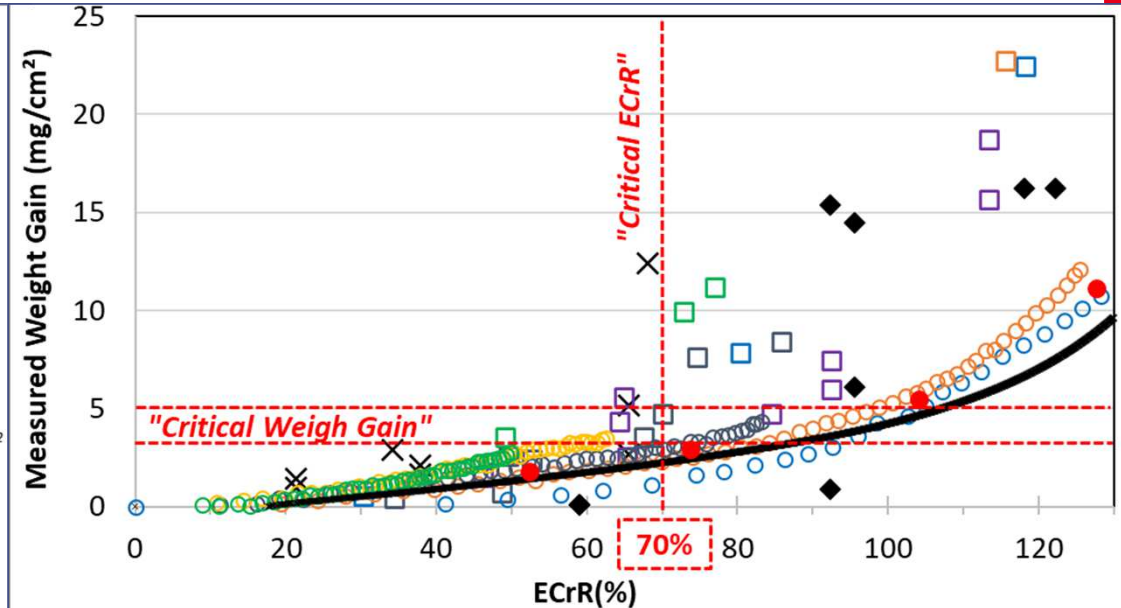
Confirmation of the capacity of the ECrR metrics to account for the effect of the initial Cr thickness not only in isothermal conditions but also for transient conditions which are more LOCA-prototypical...

- × 1100°C, 15µm Cr
  - 1200°C, 7µm Cr
  - 1200°C, 10µm Cr
  - 1200°C, 10-15µm Cr
  - 1200°C, 15-17µm Cr
  - 1200°C, 22-28µm Cr
  - ◆ 1300°C, 15µm Cr
- 7-15cm long Cr-coated M5 plugged clad segments, CEA 1-sided steam oxidation + water quenching data, for several initial Cr thicknesses, oxidation temperatures and durations
- ◇ 1200°C, Kang-2025, AIP-12µm Cr
  - ◇ 1200°C, Kang-2025, MS-13,5µm Cr
  - ◇ 1200°C, Kang-2025, AIP-16µm Cr
- short Cr-coated plugged clad segments, SNU 1-sided TGA steam oxidation data, for three initial Cr thicknesses and for two coating processes
- △ 1200°C, Deng-2025, 13µmCr
- TGA (steam) on sheet sample's geometry
- 1200°C, CEA-2017, 15µm Cr



PQ weighing – CEA data – Cr ~ 5 - 25µm / different oxidation durations and temperatures (1100-1300°C)  
 + one TGA – CEA data for Cr = 15µm carried out at 1200°C (steam environment)...  
 + TGA - 1200°C from Kang et al. – Cr = 12-16µm, JNM-2025  
 + TGA - 1200°C from Deng et al. – Cr = 13µm, JMR&T-2024

- × 1100°C, 15µm Cr
  - 1200°C, 7µm Cr
  - 1200°C, 10µm Cr
  - 1200°C, 10-15µm Cr
  - 1200°C, 15-17µm Cr
  - 1200°C, 22-28µm Cr
  - ◆ 1300°C, 15µm Cr
- 7-15cm long Cr-coated M5 plugged clad segments, CEA 1-sided steam oxidation + water quenching data, for several initial Cr thicknesses, oxidation temperatures and durations
- 1300°C, Steinbrueck-2025, 5µm Cr (\*)
  - 1300°C, Steinbrueck-2025, 10µm Cr (\*)
  - 1300°C, Steinbrueck-2025, 15µm Cr (\*)
  - 1300°C, Steinbrueck-2025, 20µm Cr (\*)
  - 1300°C, Steinbrueck-2025, 25µm Cr (\*)
  - × 1300°C, Brachet-2020, 15µm Cr, He+O<sub>2</sub> (\*)
  - 1300°C, Li-2024, Post-oxidation weighing, 17µmCr
- TGA (steam, except CEA data with He+O<sub>2</sub> environment) - sheet sample's geometry
- (\*) 5% uncoated surface correction



**PQ weighing – CEA data – Cr ~ 5 - 25µm / different oxidation durations and temperatures (1100-1300°C)**  
**+ one TGA – CEA data for Cr = 15µm carried out at 1300°C (He+O<sub>2</sub>)...**  
**+ TGA - 1300°C from Steinbrueck et al. – Cr = 5 – 25µm, this workshop, to be published in JNM**  
**+ PQ weighing data - 1300°C – Cr = 17µm from Li et al. JMR&T-2024**



## Some conclusions , on-going and further work

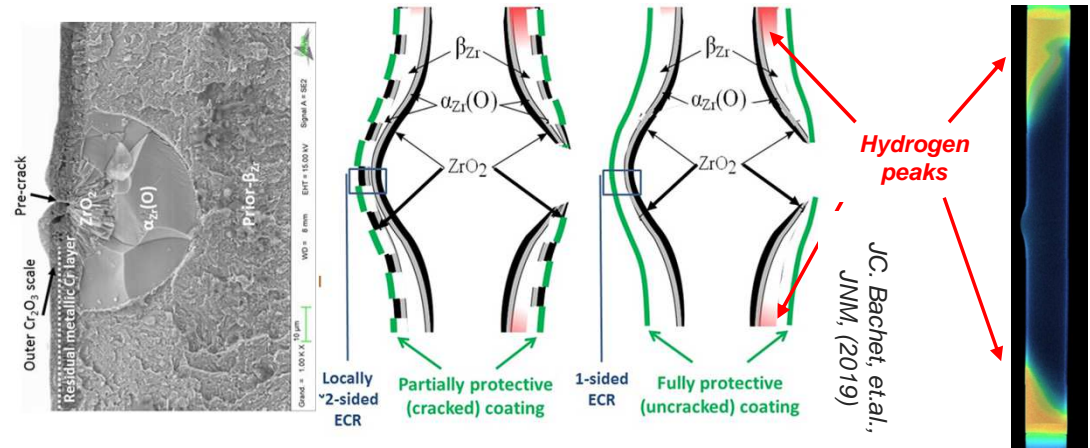
Beyond its practical use in relationship with PQ clad mechanical properties of Cr-coated materials having experienced one-sided HT steam oxidation (1100-1300°C) and quenching, new “ECrR” metrics appear to be useful to rationalise the continuous WG evolutions derived from TGA experiments, taking into account the initial Cr-coating thickness influence + oxidation temperature and duration.

Thus, the ECrR parameter should be a practical metrics to compare Cr-coating’s relative performances upon HT oxidation even with different initial Cr thicknesses and/or different oxidation temperatures.

Additionally, this approach can be used in transient (*more LOCA-prototypical*) conditions...

### On-going and further work:

- account for the effect of pre-damaged / pre-cracked coatings
- ⇒ **“Connect-NM / Crocodox”** project
- account for two-sided oxidation conditions and the associated 2<sup>dary</sup> hydriding resulting from clad ballooning and burst



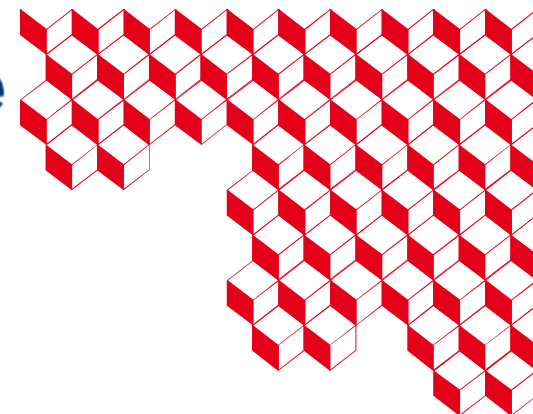
F. Ott et al. (CEALLB),  
neutron tomography  
carried out at LL  
(Grenoble, France)



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# Thank you for your attention

*This work has been funded by the French Nuclear Institute (I3P). Many thanks to the numerous colleagues and students at CEA who have contributed to the development and evaluation of E-ATF Cr-coated Zr-based claddings over past twelve years, and to our industrial partners for partial funding and fruitful discussions (and Framatome for providing the M5<sub>Framatome</sub> substrate)*

*M5<sub>Framatome</sub> is a trademark or a registered trademark of Framatome or its affiliates in the USA or other countries*



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**Back slides...**



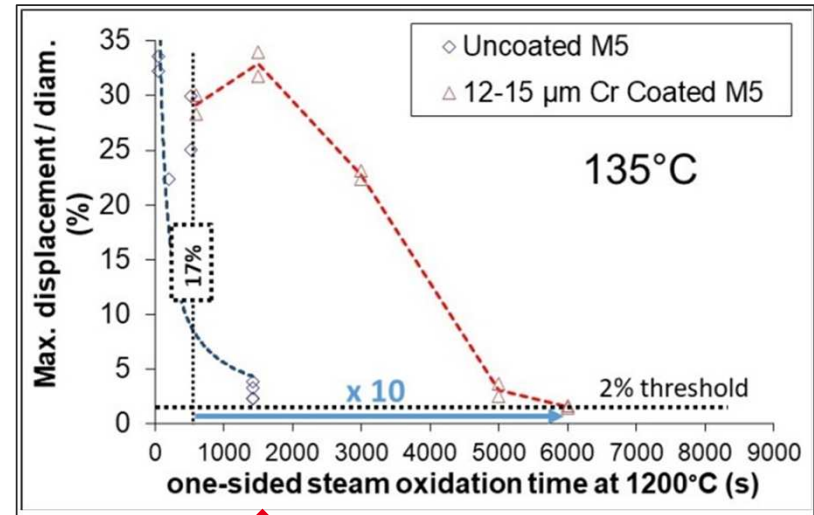
[jean-christophe.brachet@cea.fr](mailto:jean-christophe.brachet@cea.fr)



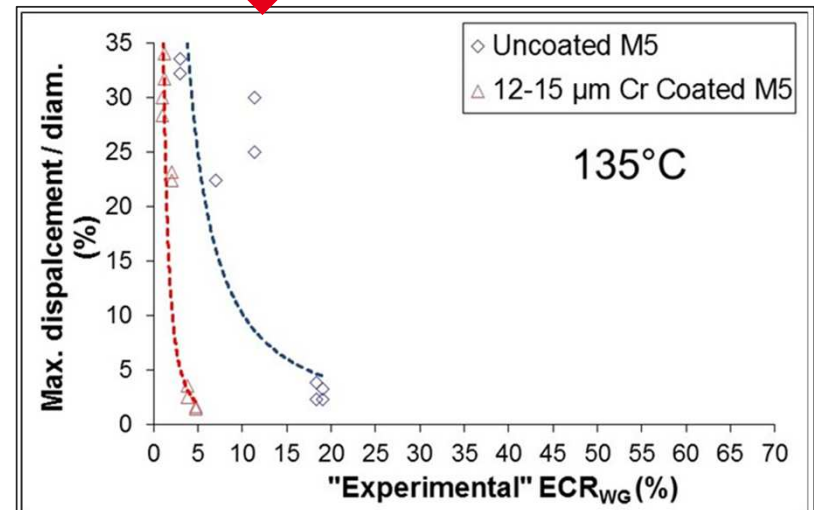
## New « ECrR » / Introduction (1/2)

⇒ Following HT steam oxidation (for LOCA and beyond conditions), both experimental (based on measured Weight Gain) and calculated “ $ECR_{BJ/CP}$ ” (used since the 70ties for the uncoated Zr-based claddings) are not adapted “metrics” to rely on the PQ mechanical properties of Cr-coated claddings;

⇒ Fundamentally due to the different underlying HT oxidation mechanisms (between uncoated & coated materials) and the different induced oxygen diffusion profiles and partitioning into the Zr-base ( $\beta_{Zr}$ ) substrate

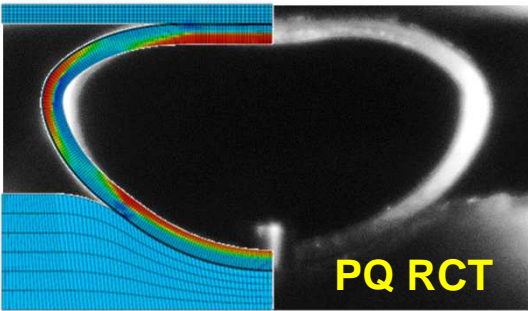


Seems to be contradictory?



Materials	Oxidation time at 1200 °C (s)	WG (mg/cm <sup>2</sup> )	$ECR_{WG}$ (%)	Fraction of ECR corresponding to oxygen which has diffused into the metallic substrate
Uncoated M5 <sub>Framatome</sub>	60 - 1420s	4 - 24	3 - 20	20-30 %
12-15µm Cr-coated M5 <sub>Framatome</sub>	9000	15 - 16	12 - 13	85 %

Brachet et al., JNM 2020

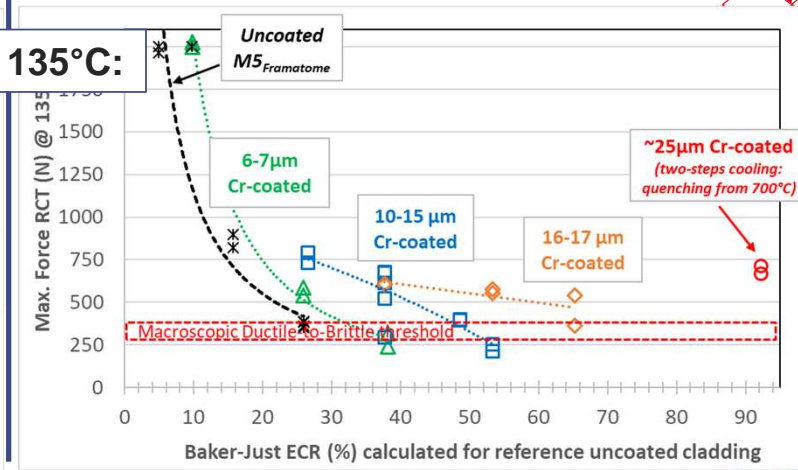
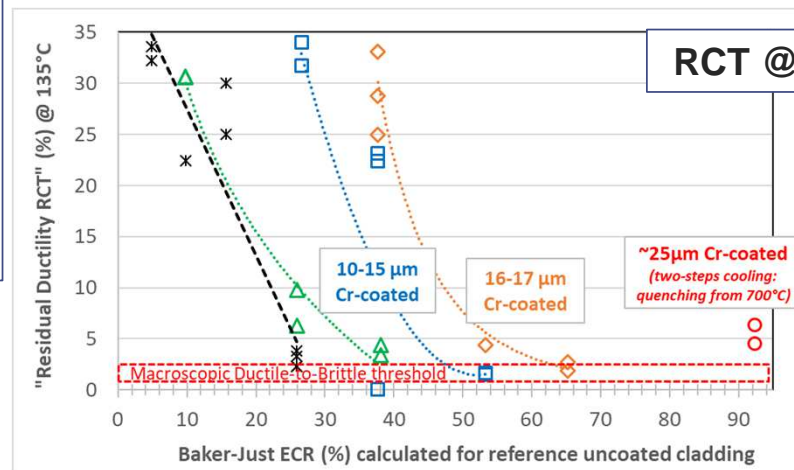
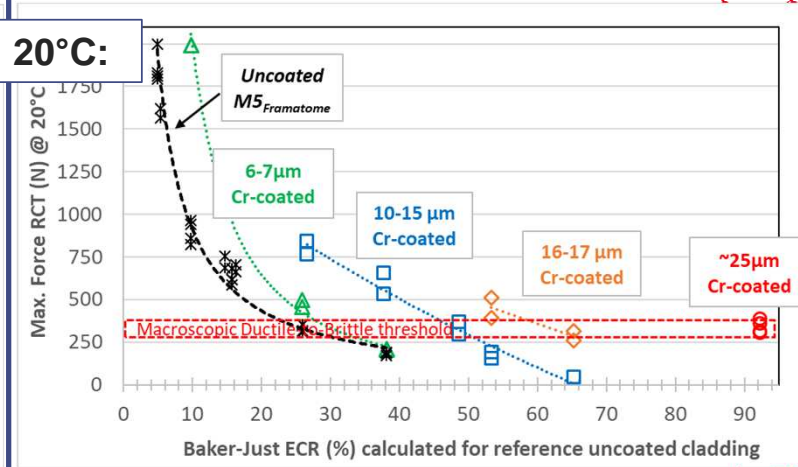
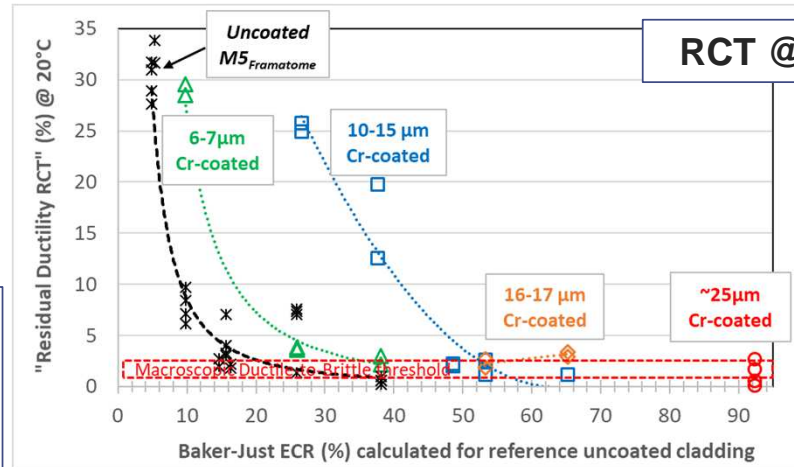


## New « ECrR » / Introduction (2/2)

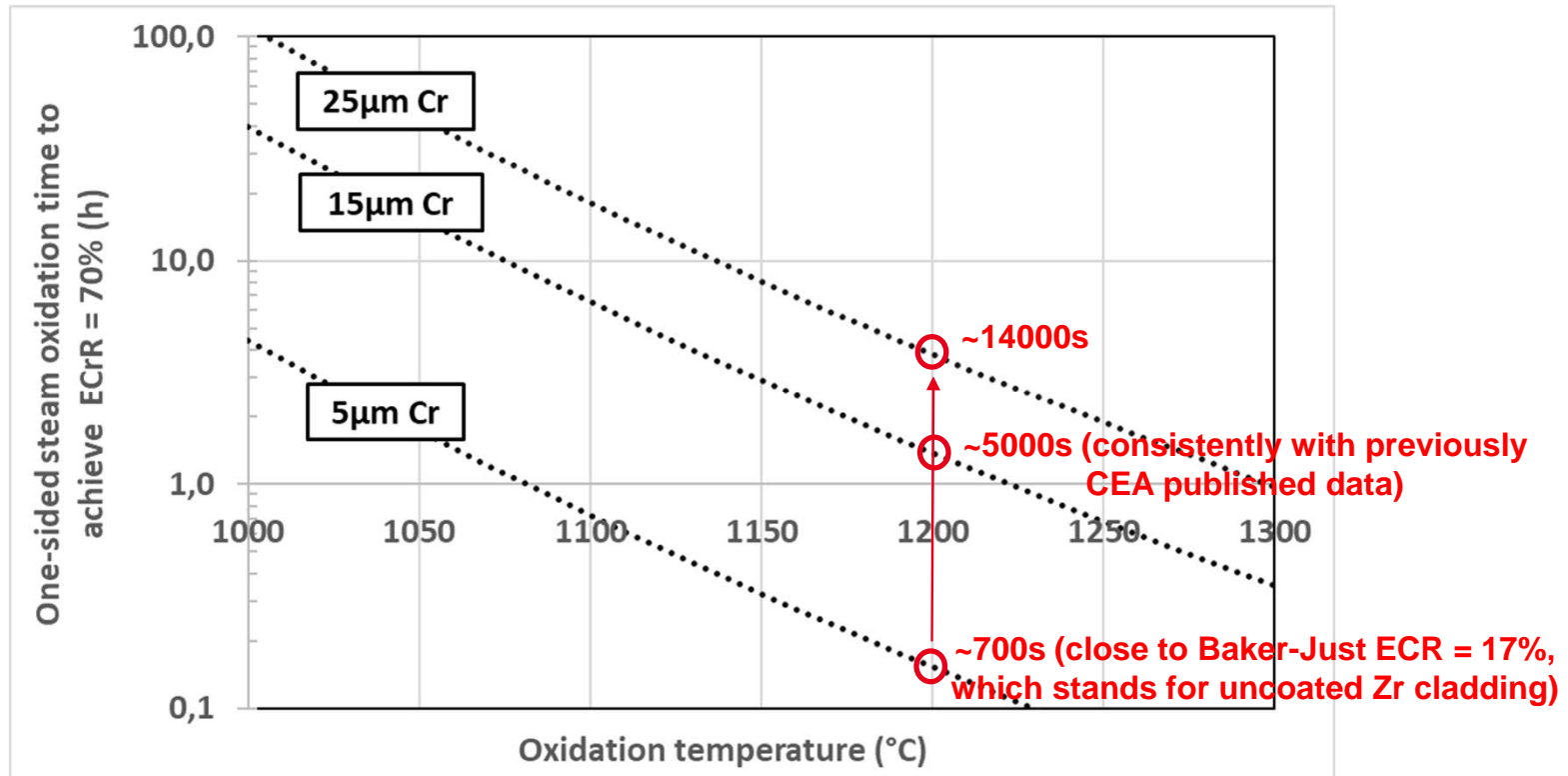
Offset strain (~ « Residual ductility »)

Max. Force (~ « Residual strength »)

=> Additional limitation by using conventional approaches (i.e., calculated Baker-Just or Cathcart-Pawel ECR correlations that have been derived for the uncoated reference claddings and/or experimental / WG ECR) is that such parameters are **not able to account for the influence of the initial Cr-coating thickness**

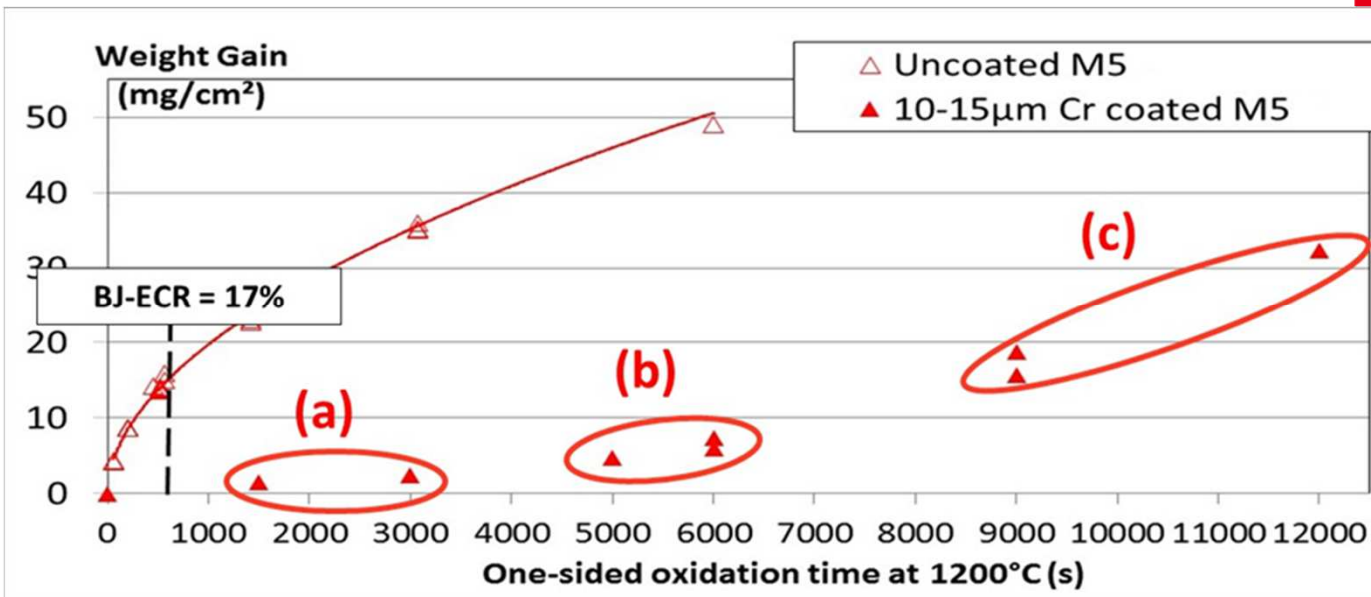
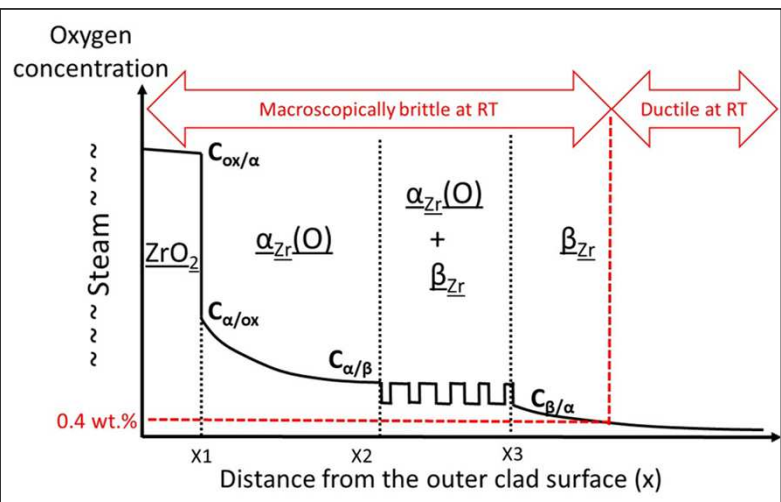


Using the “critical” ECrR=70% threshold value, one can calculate typical “grace time” of Cr-coated Zr based claddings before reaching PQ Ductile-to-Brittle transition vs. initial Cr thickness (for one-sided steam oxidation and ~0.6 mm thick claddings):

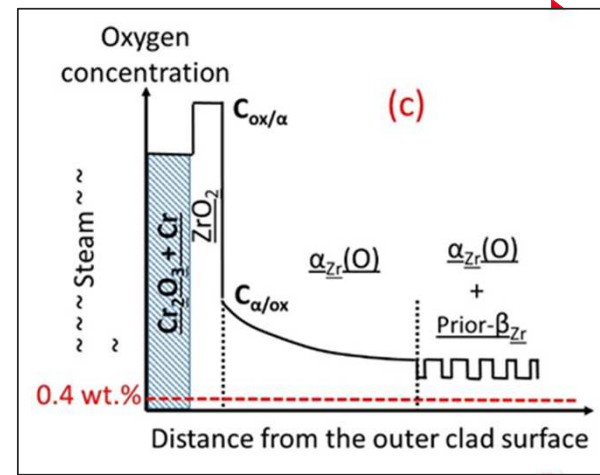
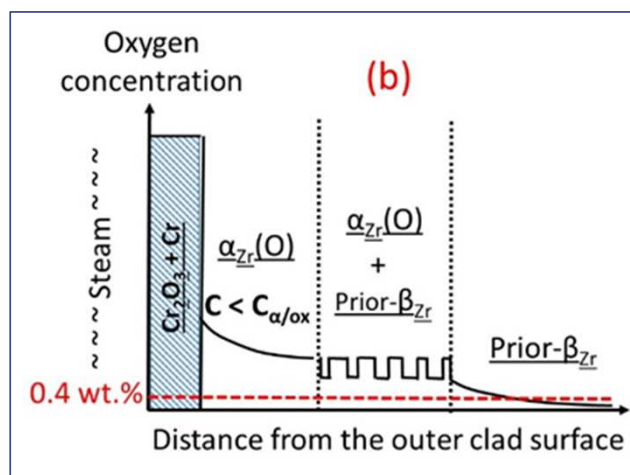
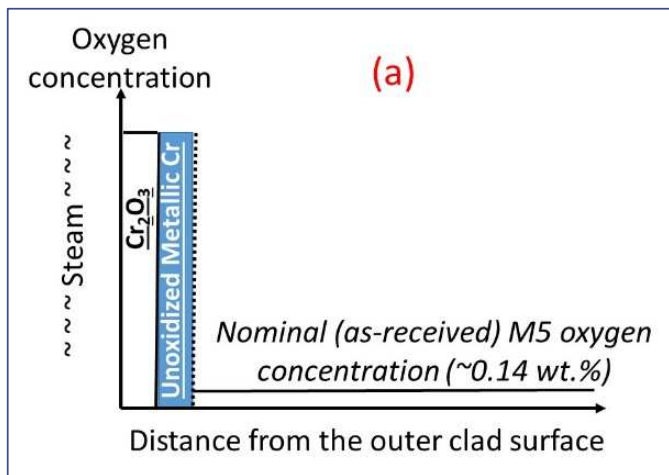


⇒ Among other results, such predictions confirm that **Cr-thickness lower than 10µm brings limited “grace time”...**

Uncoated:



Cr-coated:



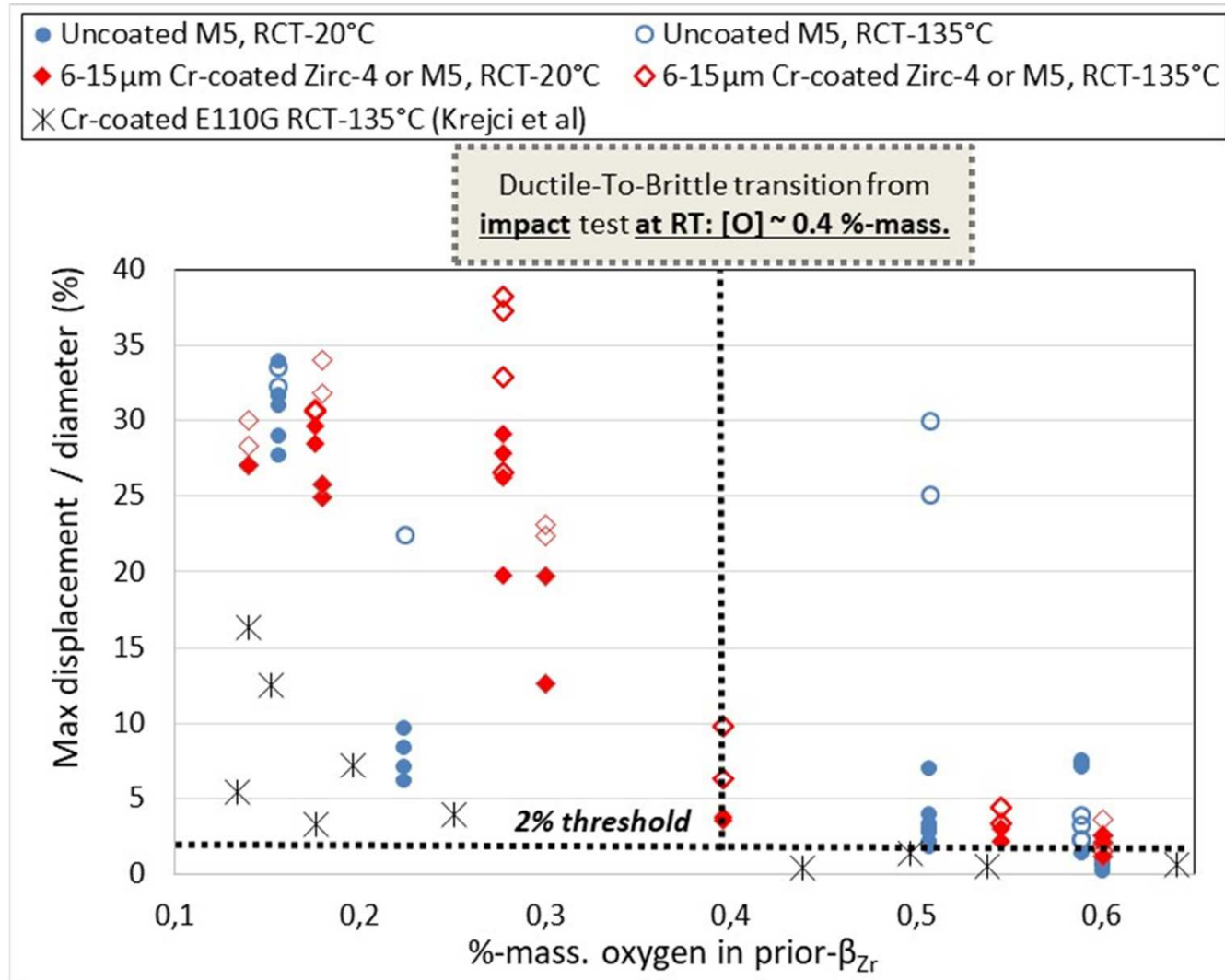
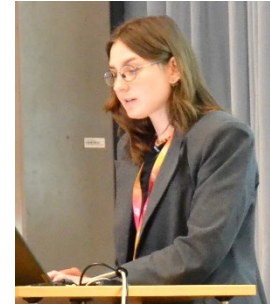


Figure 1 - Post-Quenching “residual ductility” derived from RCTs performed at 20 and 135 °C on uncoated and 6 to 15 μm thick Cr-coated zircaloy-4 or M5<sub>Framatome</sub>, and from Krejci et al. on Cr-coated E110G substrate **Erreur ! Source du renvoi introuvable.**, as a function of the mean oxygen content of the residual prior-β<sub>Zr</sub> layer





**Diana Bachurina**

KIT

## **Steam Oxidation of Cr-Coated Zircaloy-4 Rods Across a Wide Range of Heating Rates**

Although Cr-coated zirconium tubes have been extensively investigated in recent years, many open questions remain, particularly regarding their behavior above 1330 °C – the eutectic temperature in the Cr-Zr system. Once this reaction occurs, the protective properties of the coating are lost, and oxidation proceeds more severely than in uncoated Zr alloys. In this study, we examined the effect of heating rate on high-temperature steam oxidation and degradation of Cr-coated Zry-4 rods above the eutectic temperature.

Zircaloy fuel cladding coated with a 15 µm Cr layer using the PVD method (Oerlikon) was tested (12.5 cm length, ø10.75 mm outer, ø9.3 mm inner). Experiments were conducted in the QUENCH-Single Rod facility under steam conditions. Heating rates of 5, 10, 30, 50, 100, and 300 K/min were applied. Steam was introduced at 800 °C, and the temperature increased up to 1500 °C. After testing, samples were examined using optical and electron microscopy. A source of uncertainty arose during internal temperature measurements: samples at lower heating rates experienced overheating, while those at higher rates were slightly underheated. This should be considered when interpreting the results.

Macro- and microscopic analysis revealed that at 5 K/min, no “crocodile skin” structure formed; instead, a brittle oxide scale appeared. At 10 K/min and above, “crocodile skin” ridges developed, while eutectic microstructure was first observed at 30 K/min. The area covered by eutectic structure showed no clear dependence on heating rate.

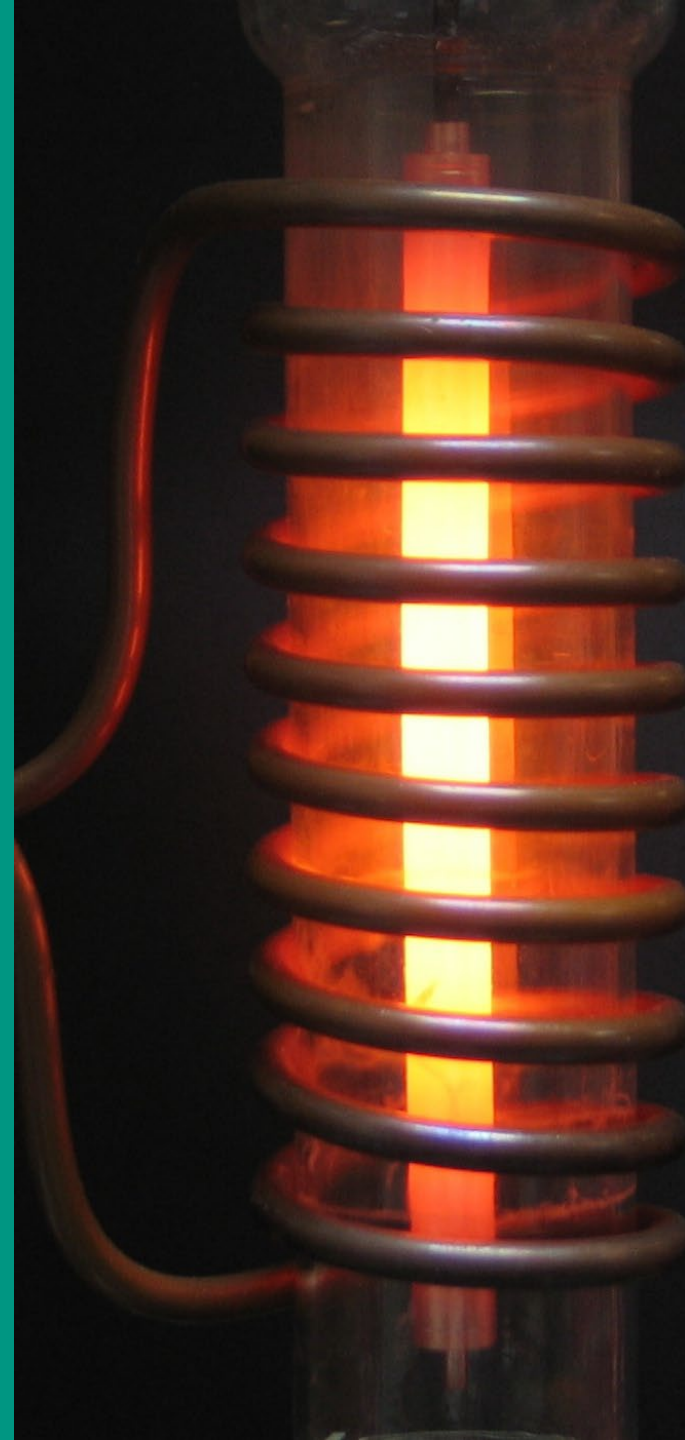
Oxide scale thicknesses ( $ZrO_2$  and  $Cr_2O_3$ ) decreased with increasing heating rate.  $ZrO_2$  thickness matched theoretical predictions for uncoated Zr alloys at higher heating rates, but measured thicknesses at  $\leq 30$  K/min were higher, likely due to temperature overshoot during testing.

Hydrogen release was also monitored. The  $H_2$  release rate increased with heating rate, reaching  $\approx 6$  L/h at 5 K/min and about ten times higher at 100 K/min. Maximum release rates not only increased with heating rate but also shifted to higher temperatures. Total  $H_2$  release decreased with heating rate and was already lower than that of uncoated samples at 100 K/min.

# Steam Oxidation of Cr-Coated Zircaloy-4 Rods Across a Wide Range of Heating Rates

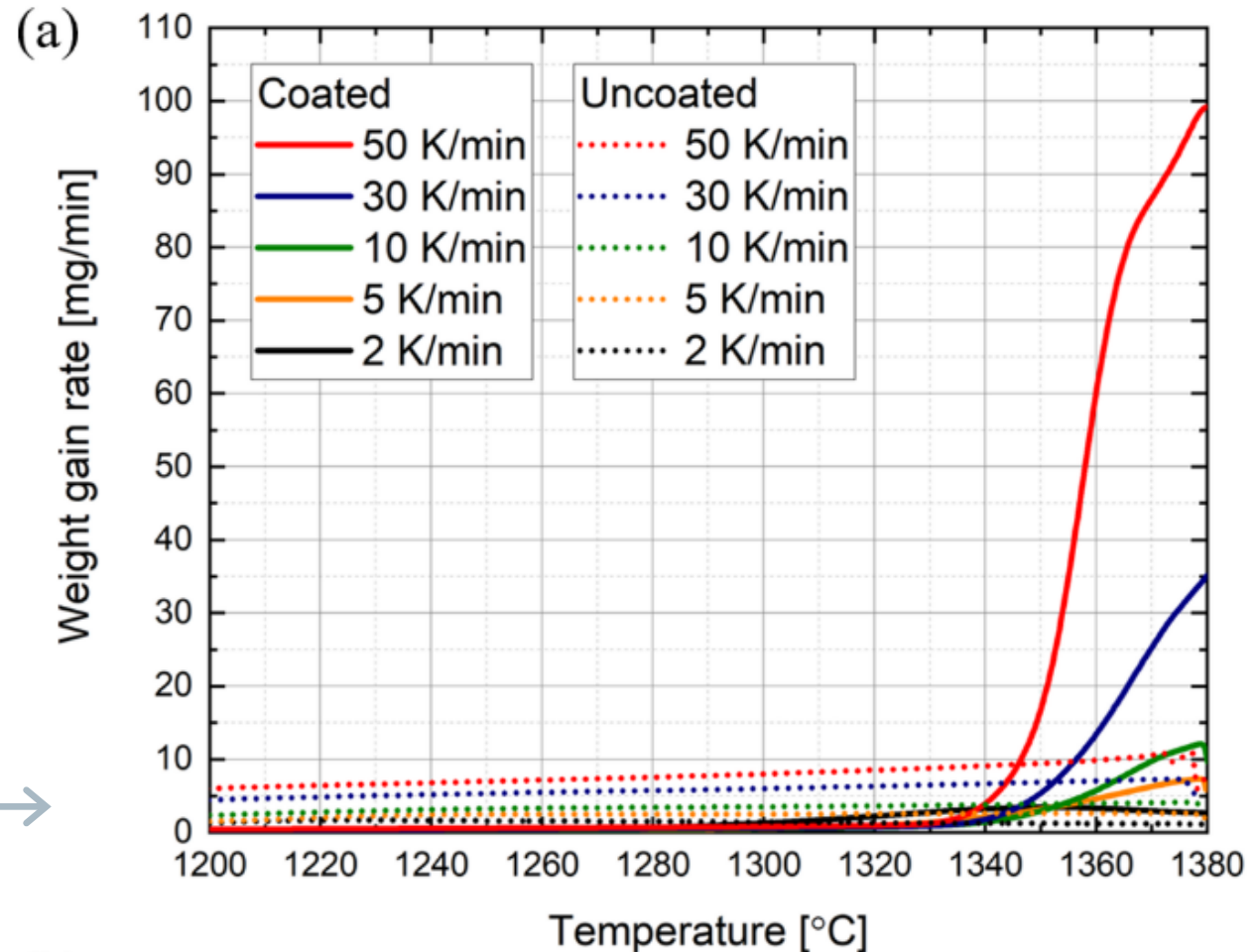
Diana Bachurina, Ulrike Stegmaier, Jaeyoon Bae,  
Martin Steinbrück

QUENCH Workshop, 16-18 December 2025



# Background

- Aim: examine the effect of heating rates on high-temperature steam oxidation and degradation of Cr-coated Zry-4 rods above eutectic temperature
- Previous data on oxidation in  $O_2$  limited to **50 K/min**

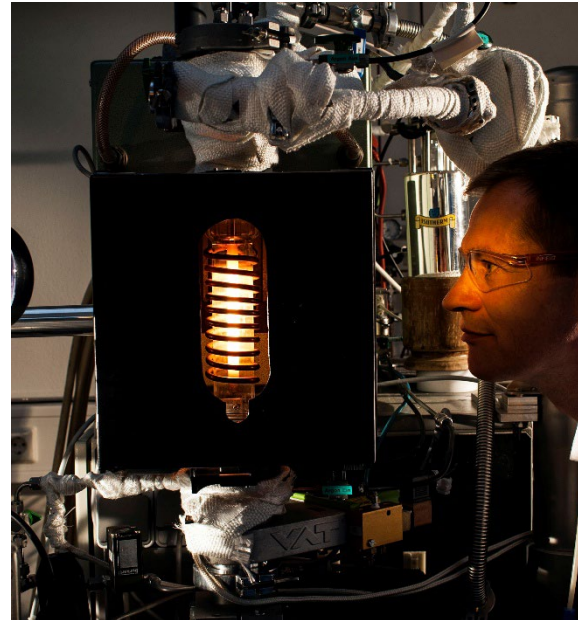


Kim d. et al, DOI:10.1016/J.JNUCMAT.2023.154538

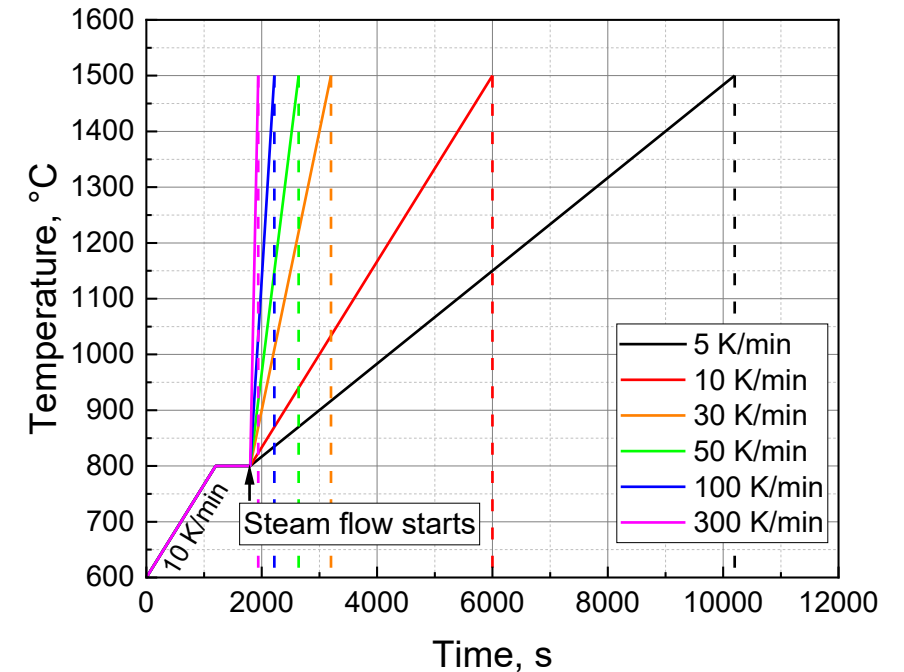
# Materials and methods



Zry-4  
Cr-coating (Oerlikon), PVD,  
15  $\mu\text{m}$  thick  
12 cm long,  $\varnothing$ 10.75 mm outer,  
 $\varnothing$ 9.3 mm inner  
+ uncoated plugs



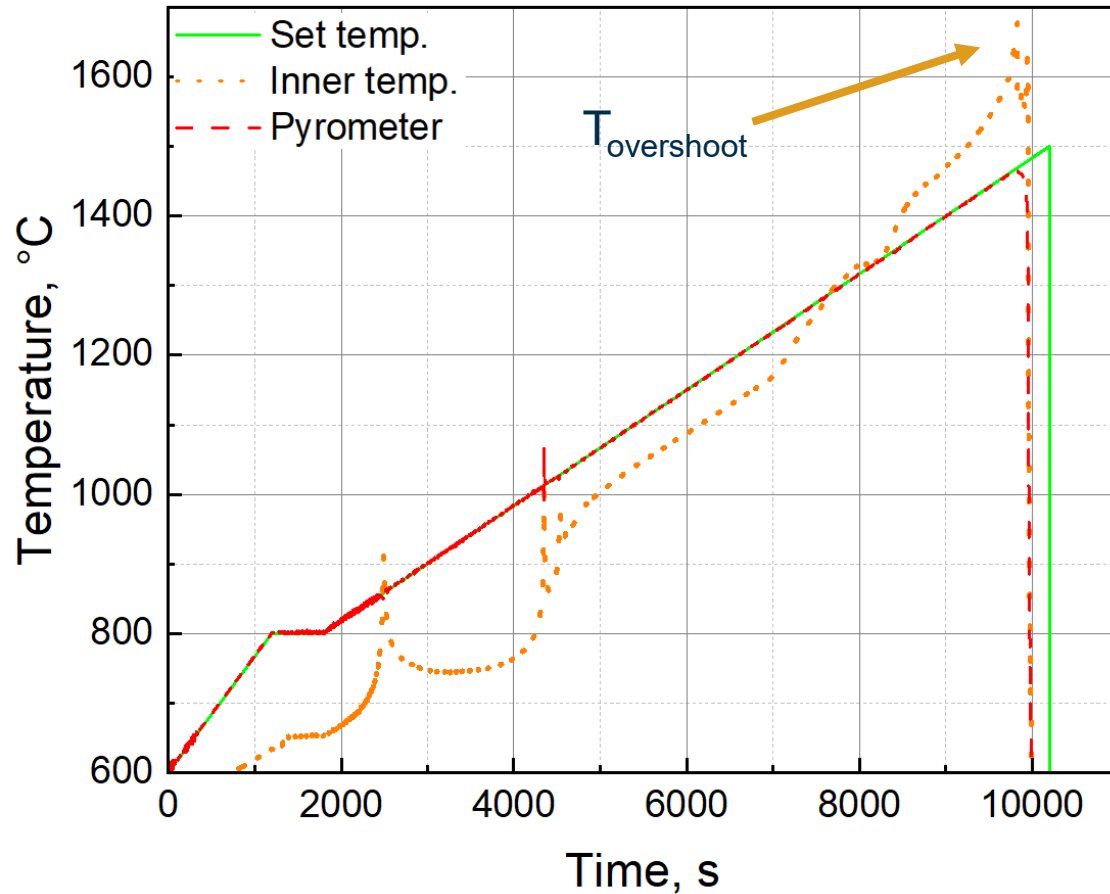
QUENCH-SR  
Atmosphere – steam starting 800°C  
Argon flow <800°C and >1500°C 40l/h  
Coupled with mass spectrometry



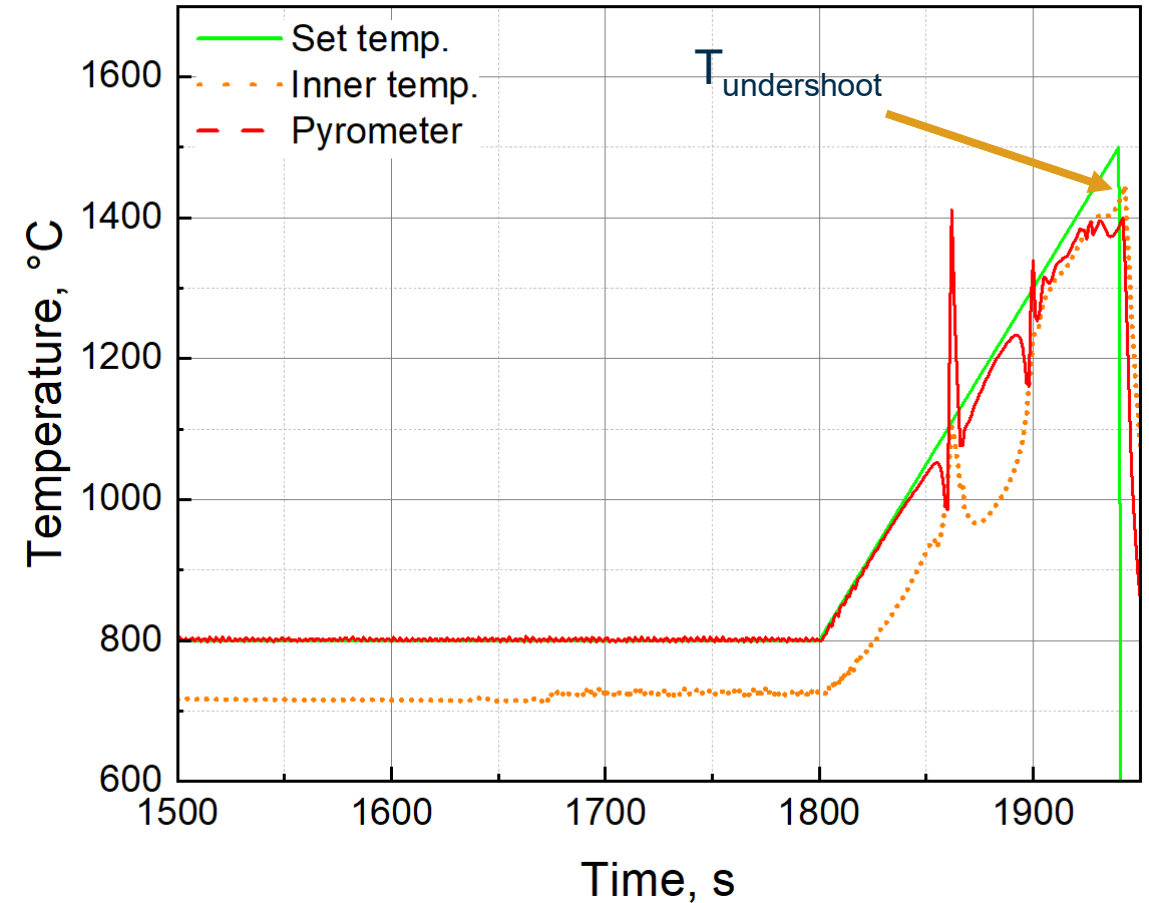
Post-test examination  
OM, SEM

# Source of Uncertainty

241028a 5 K/min Cr-coated Zry-4



241031b 300 K/min Cr-coated Zry-4





# Results

# Macroscopic examination

As-received 5K/min 10K/min 30K/min 50K/min 100K/min 300K/min



Cr-Coated Zry-4 (PVD)

As-received 5K/min 30K/min 100K/min



Uncoated Zry-4

# Macroscopic examination

As-received 5K/min 10K/min 30K/min 50K/min 100K/min 300K/min



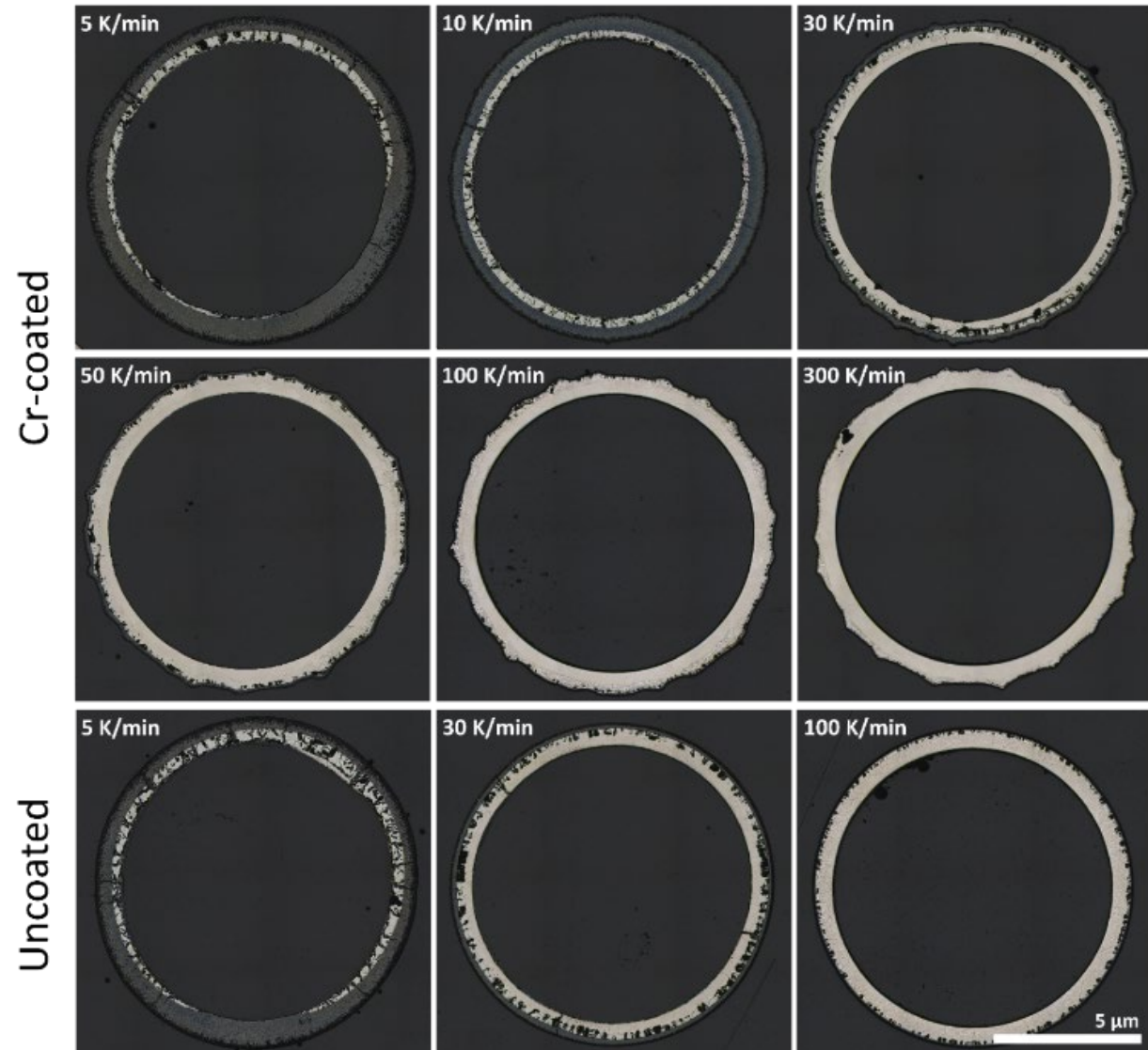
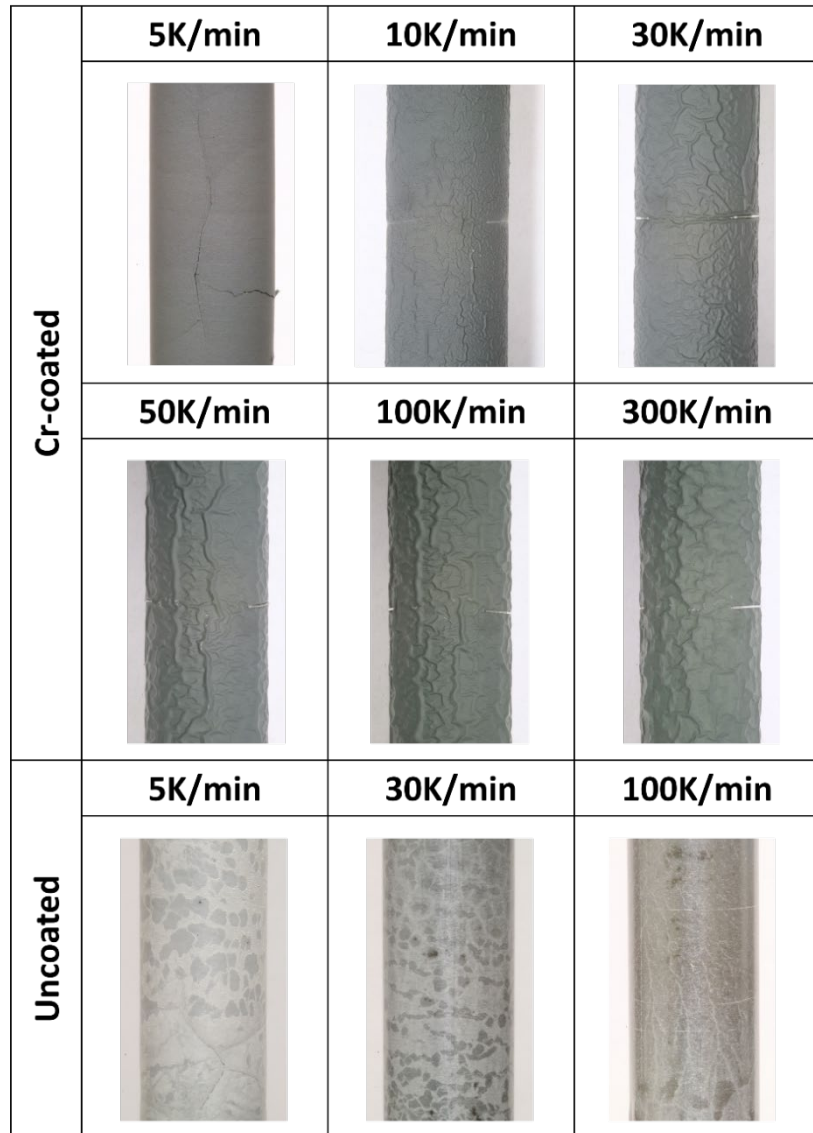
Cr-Coated Zry-4 (PVD)

Cr-coated	5K/min	10K/min	30K/min
	50K/min	100K/min	300K/min
Uncoated	5K/min	30K/min	100K/min

Magnified



# Microscopic examination





# Microscopic examinations

# Microscopic examination

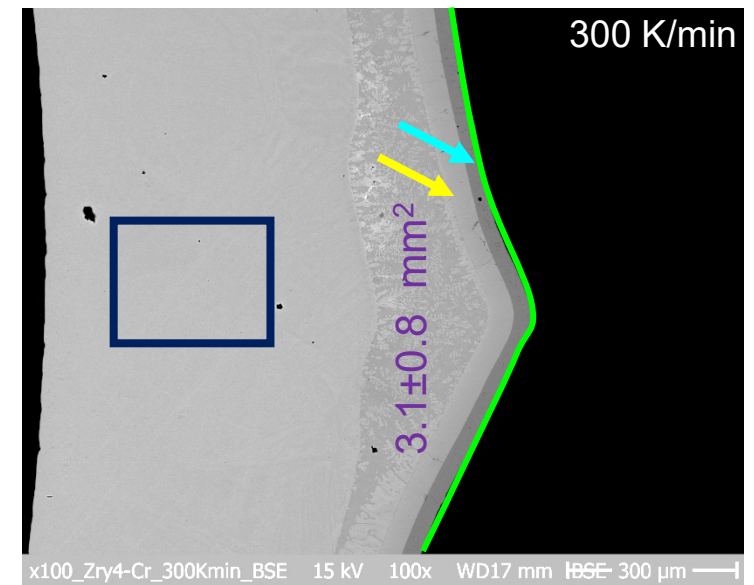
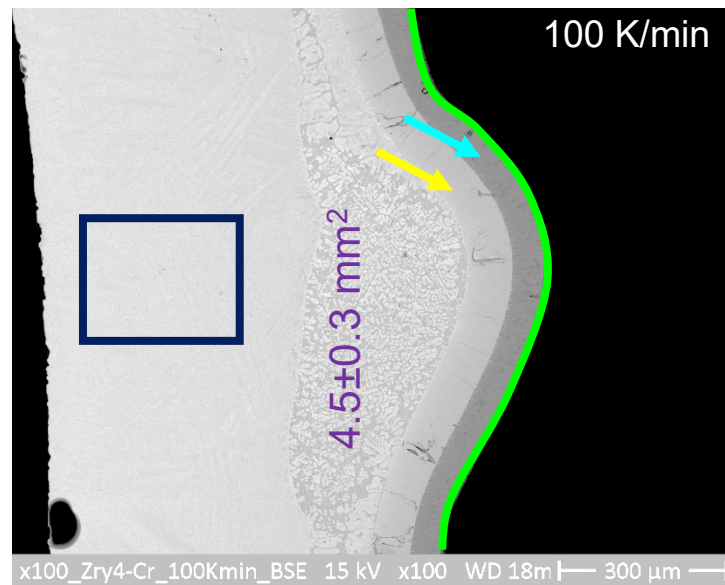
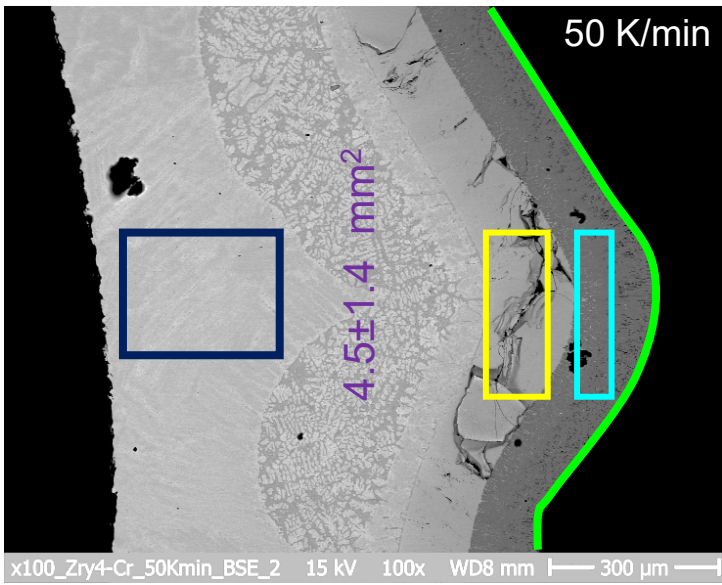
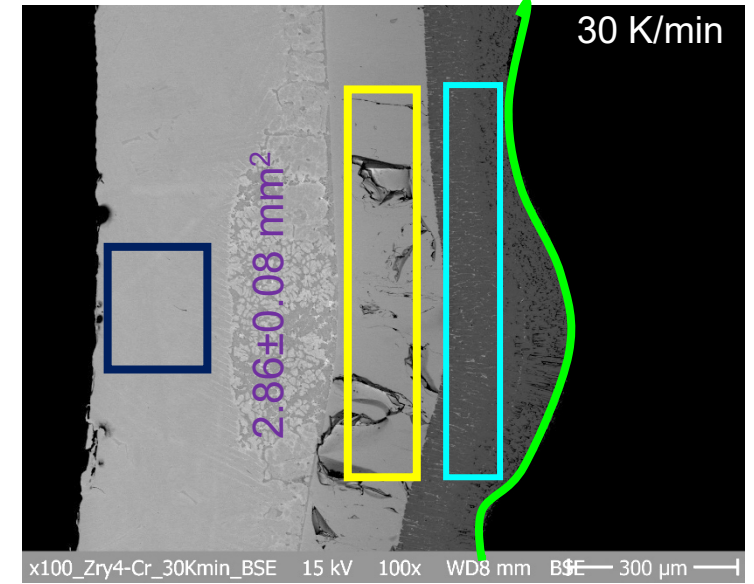
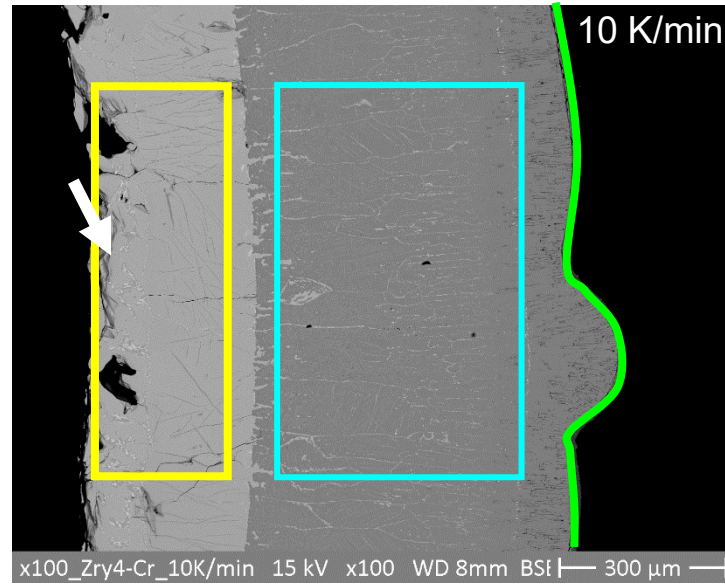
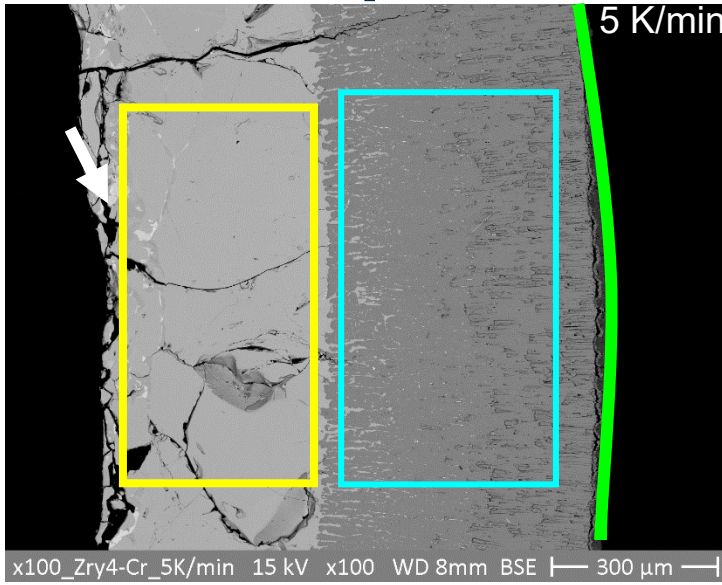
Cr<sub>2</sub>O<sub>3</sub>

ZrO<sub>2</sub>

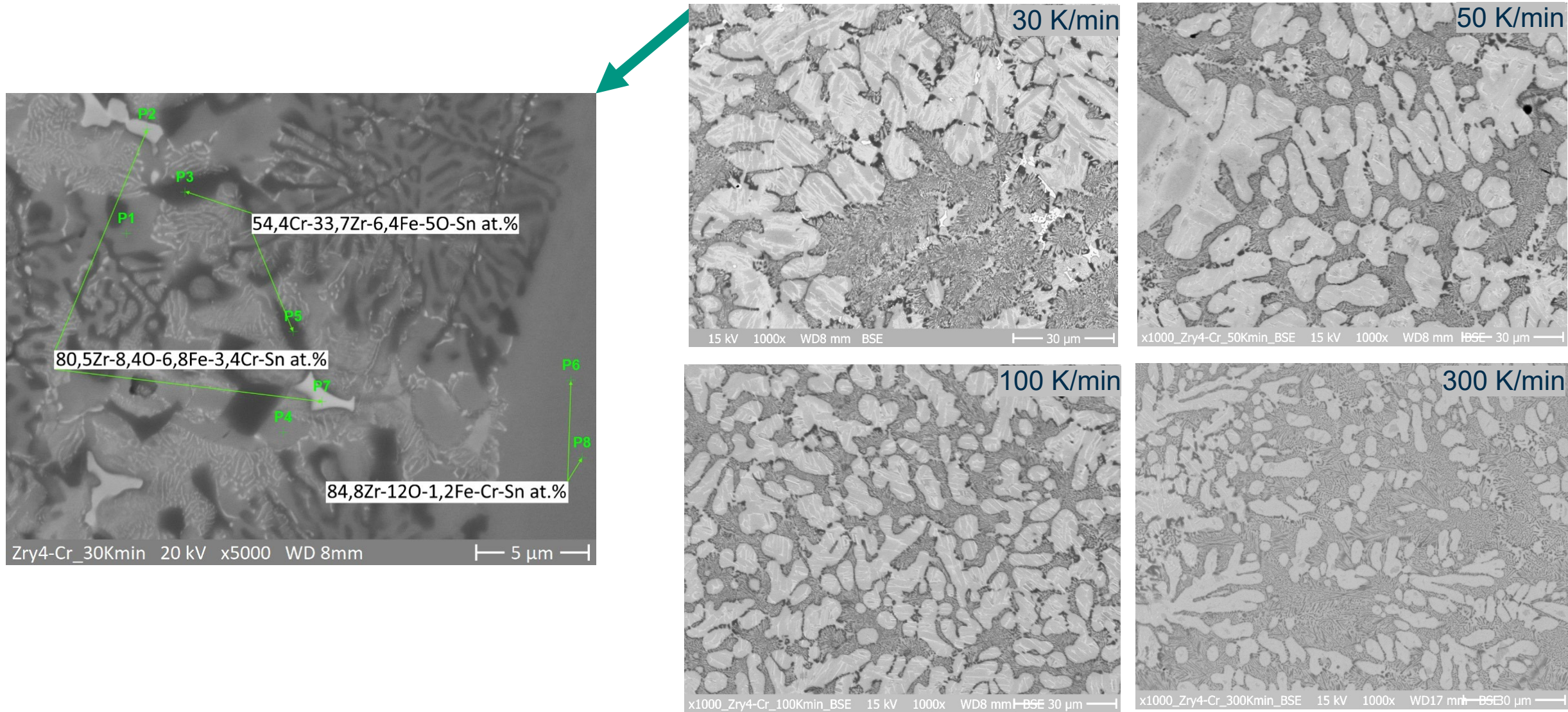
αZr(O)

prior β

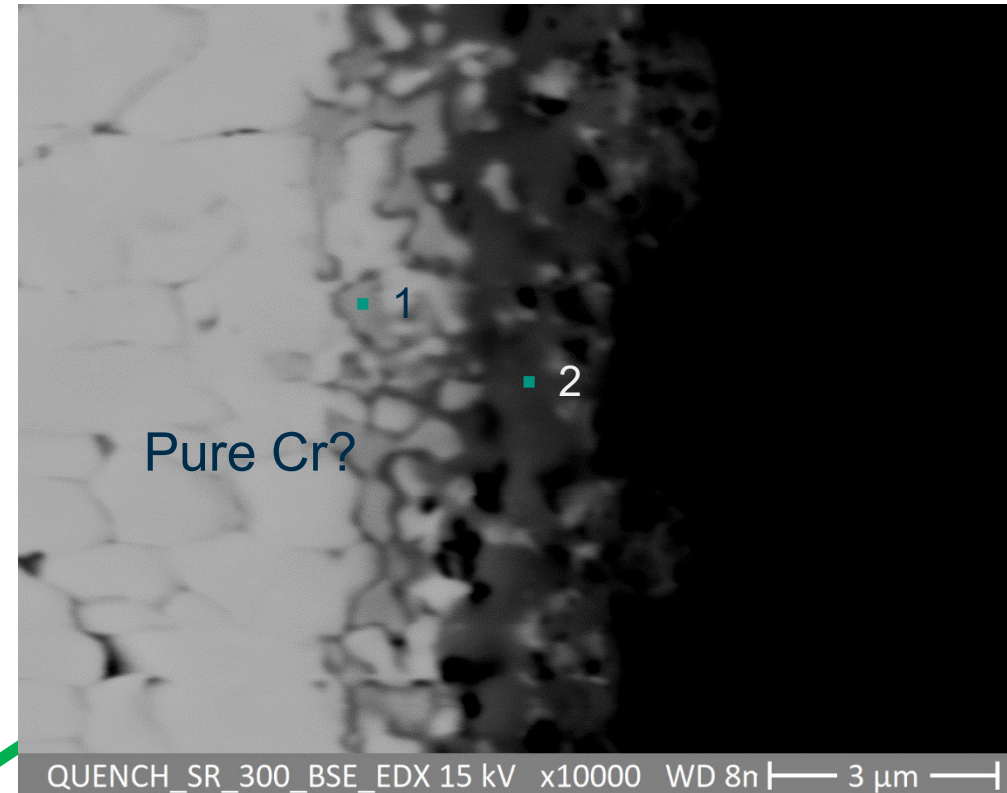
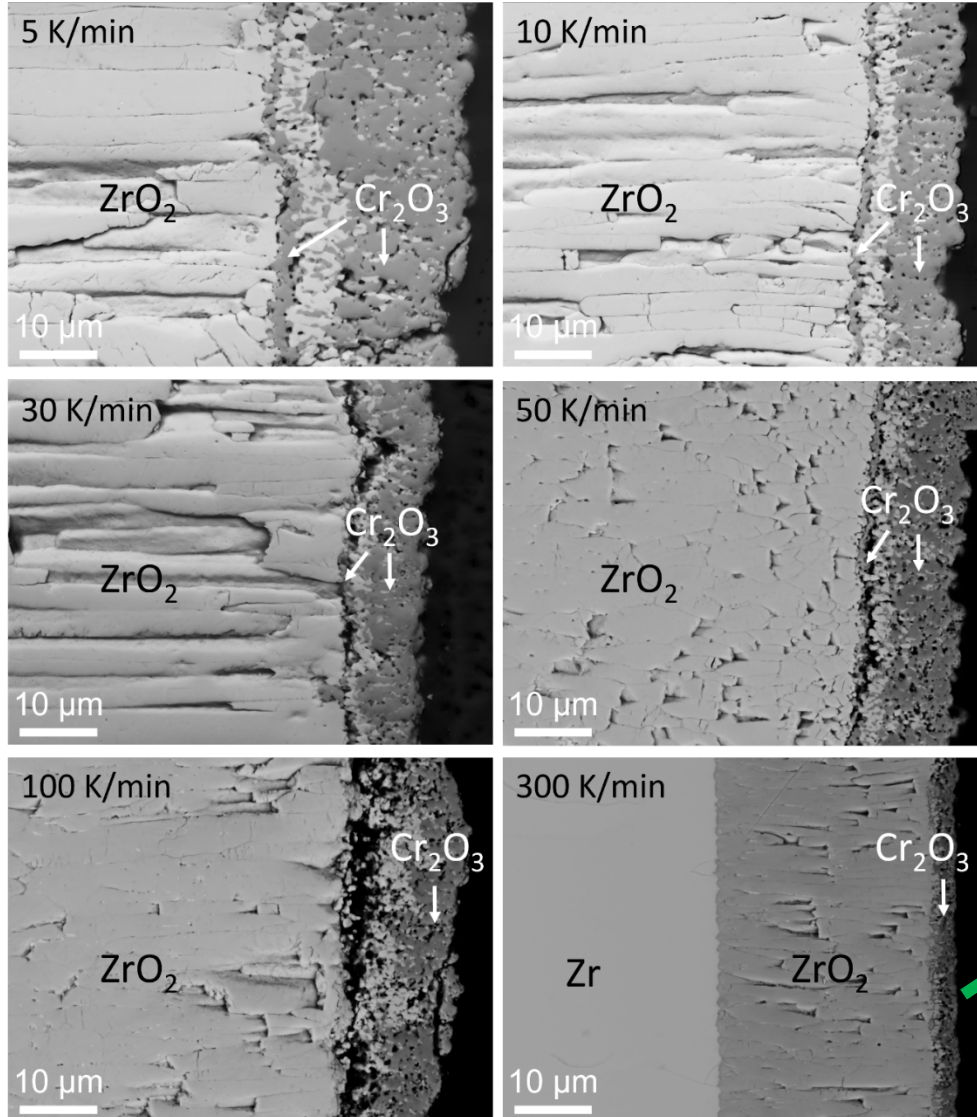
eutectic



# Magnified view of eutectic microstructure



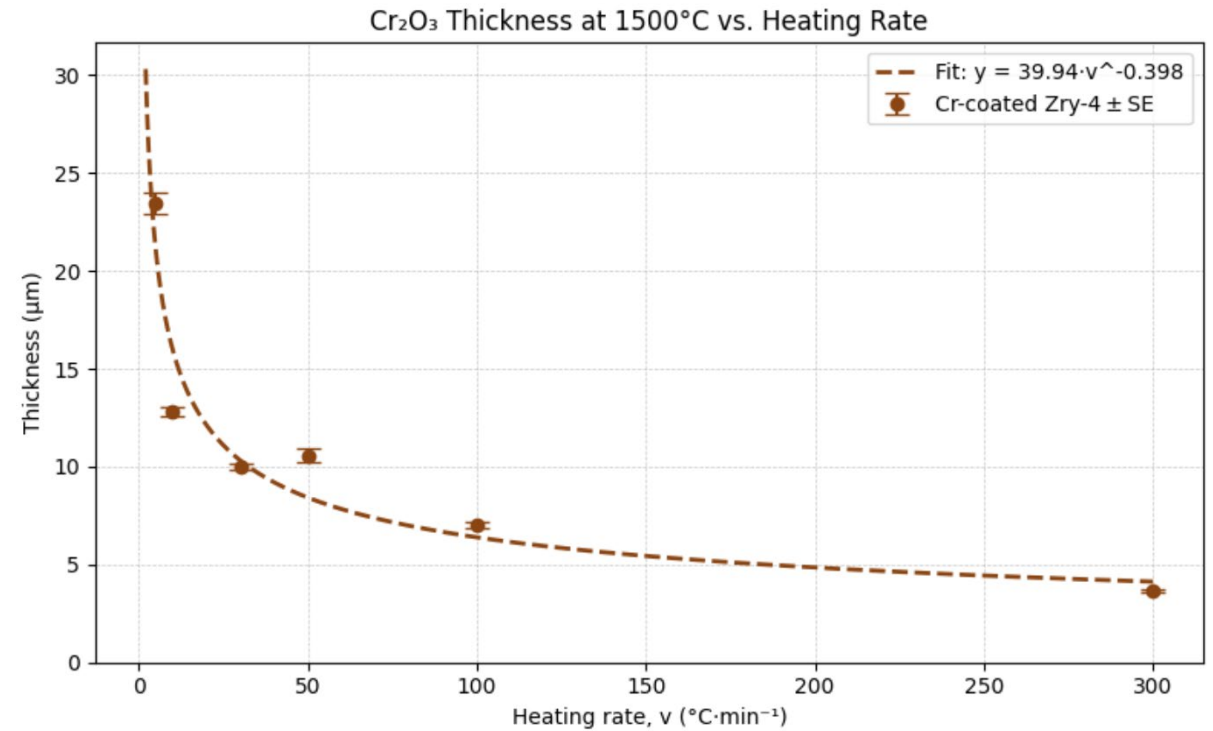
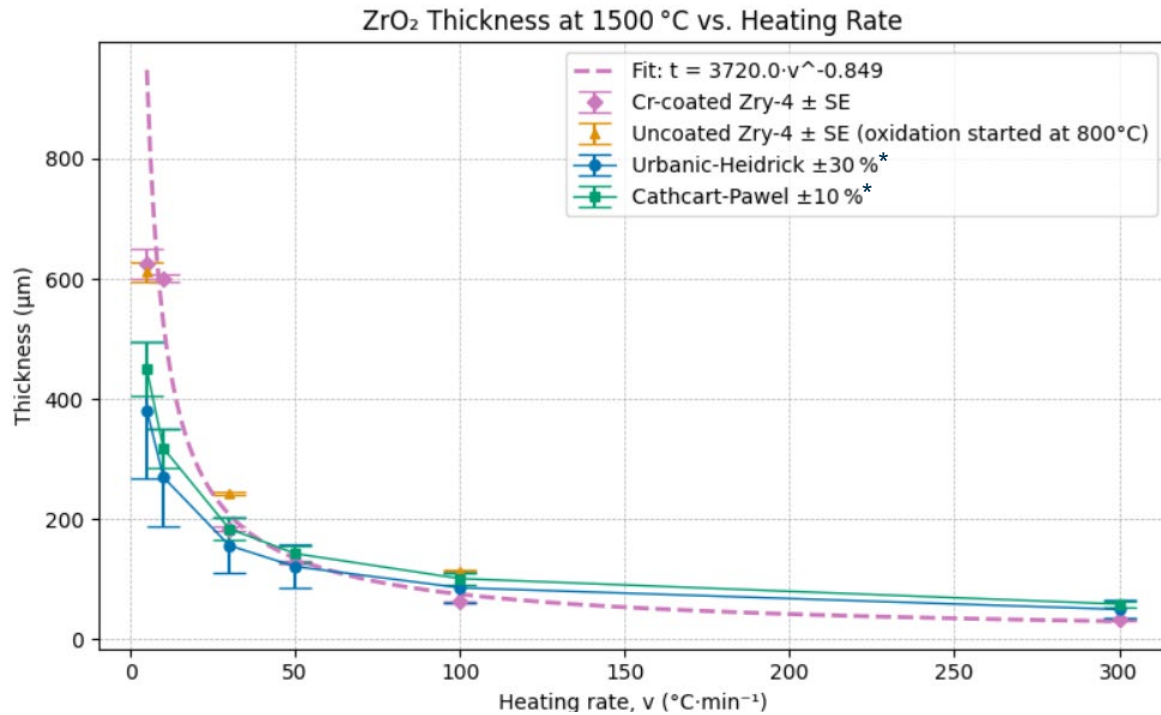
# Oxide layers



EDX

- 1. 61Cr – 32O – 7Zr at.%
- 2. 54O – 43Cr – 2Zr at.%

# Thickness of oxide layers

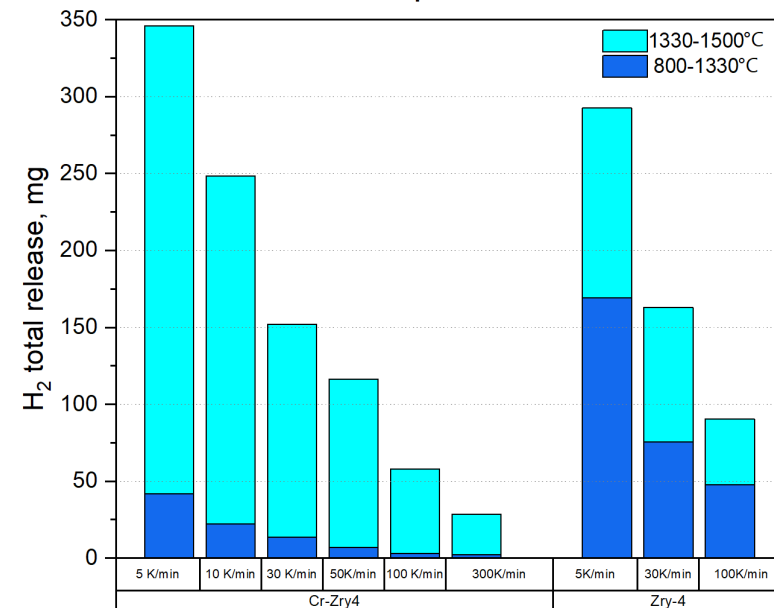
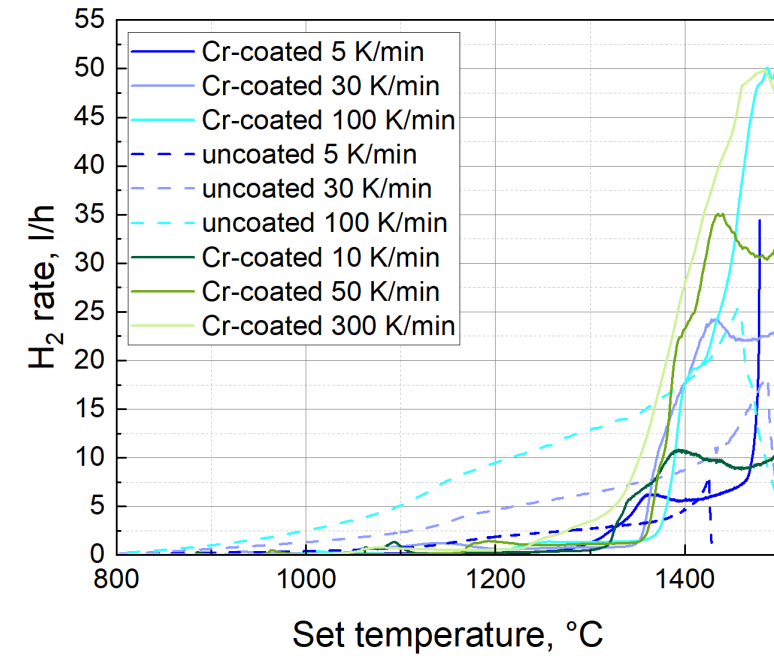
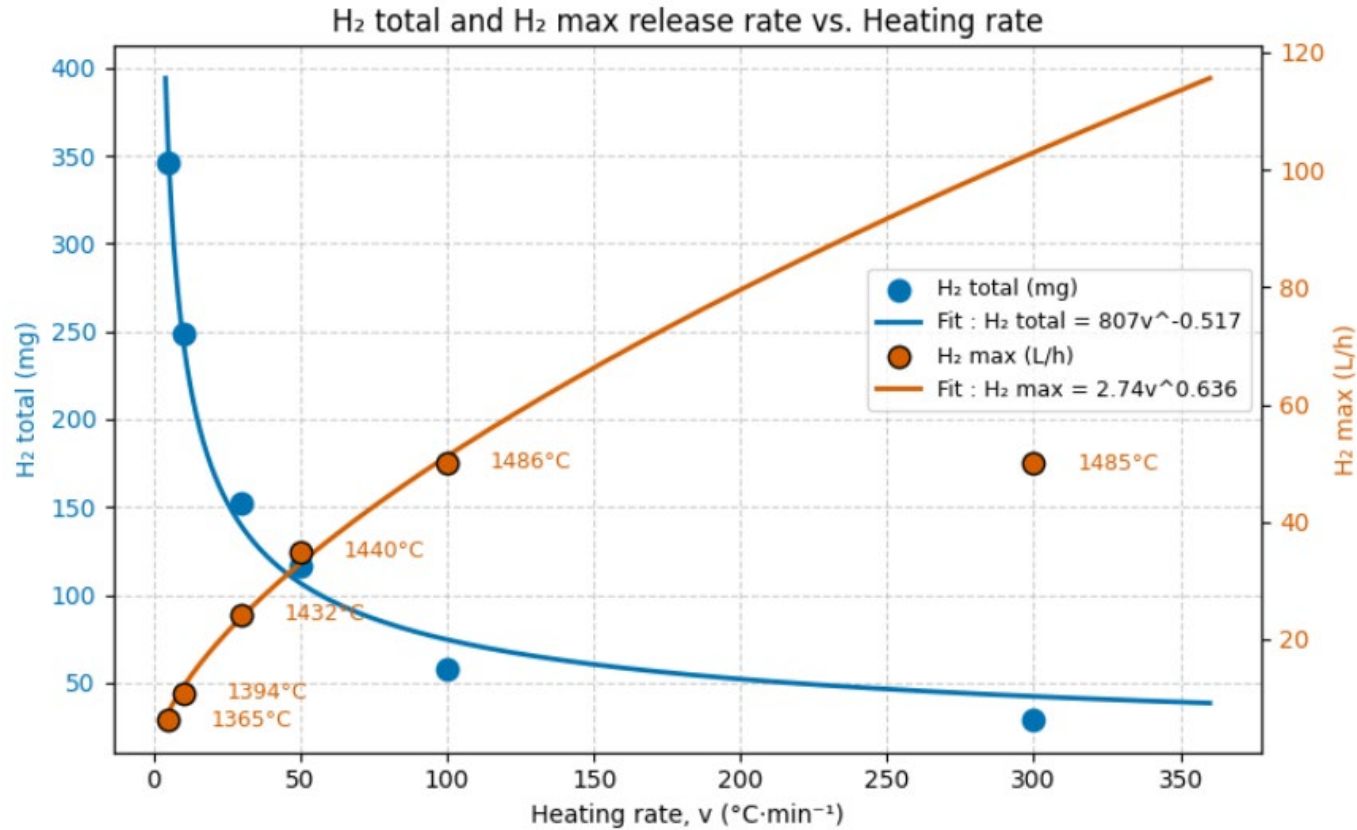


\*Schanz, G., et al. 10.1016/j.nucengdes.2004.02.013



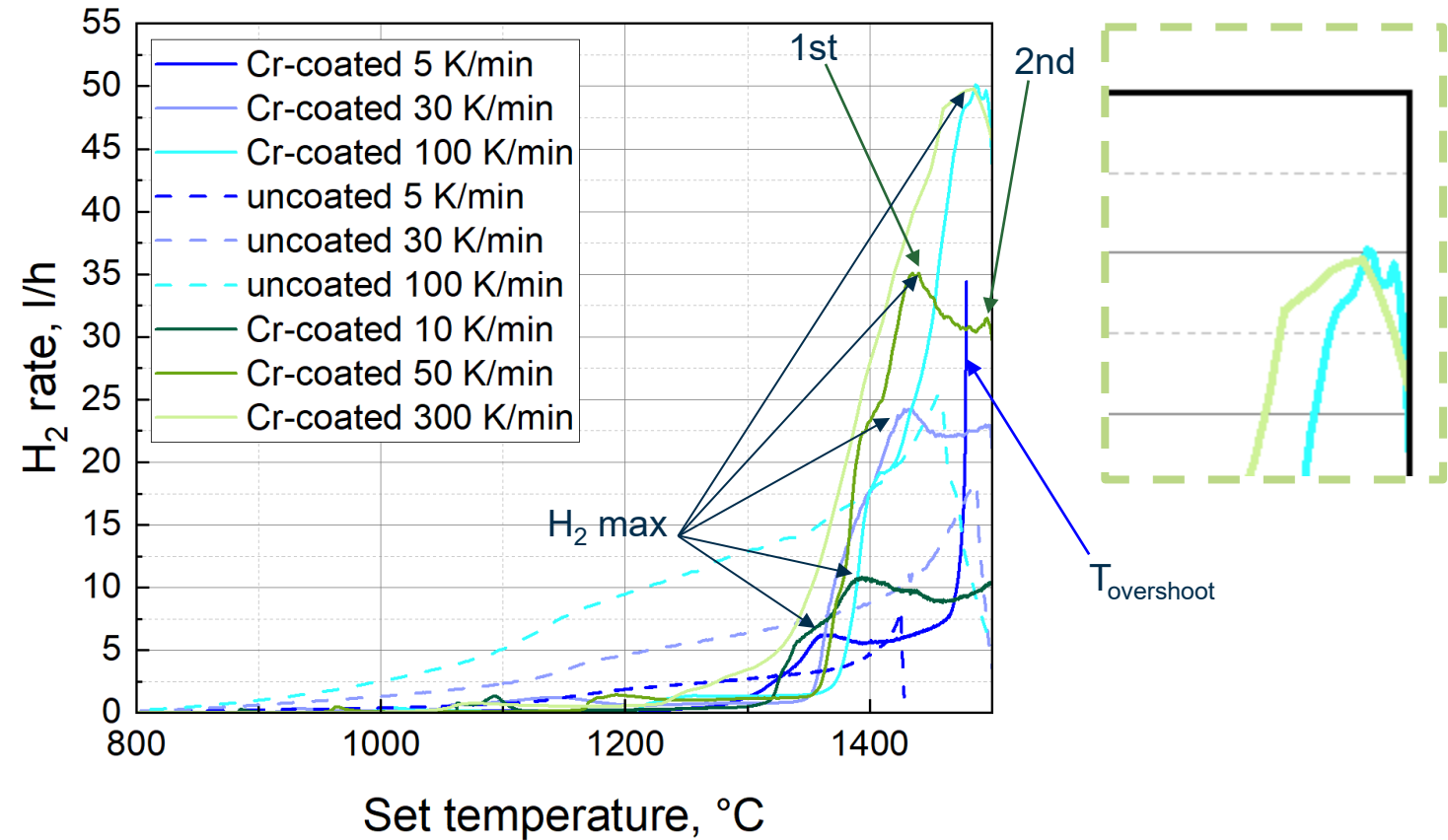
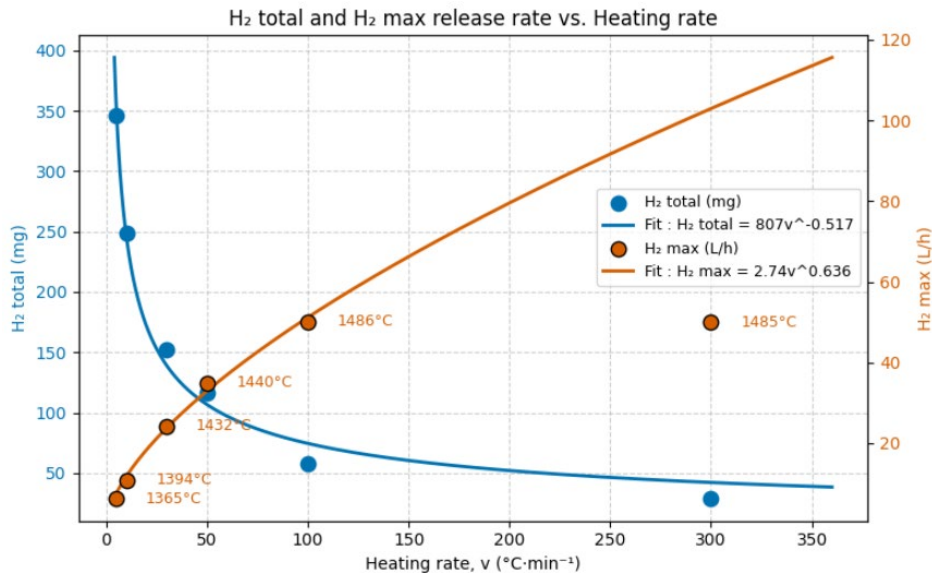
H<sub>2</sub> release

# H<sub>2</sub> release



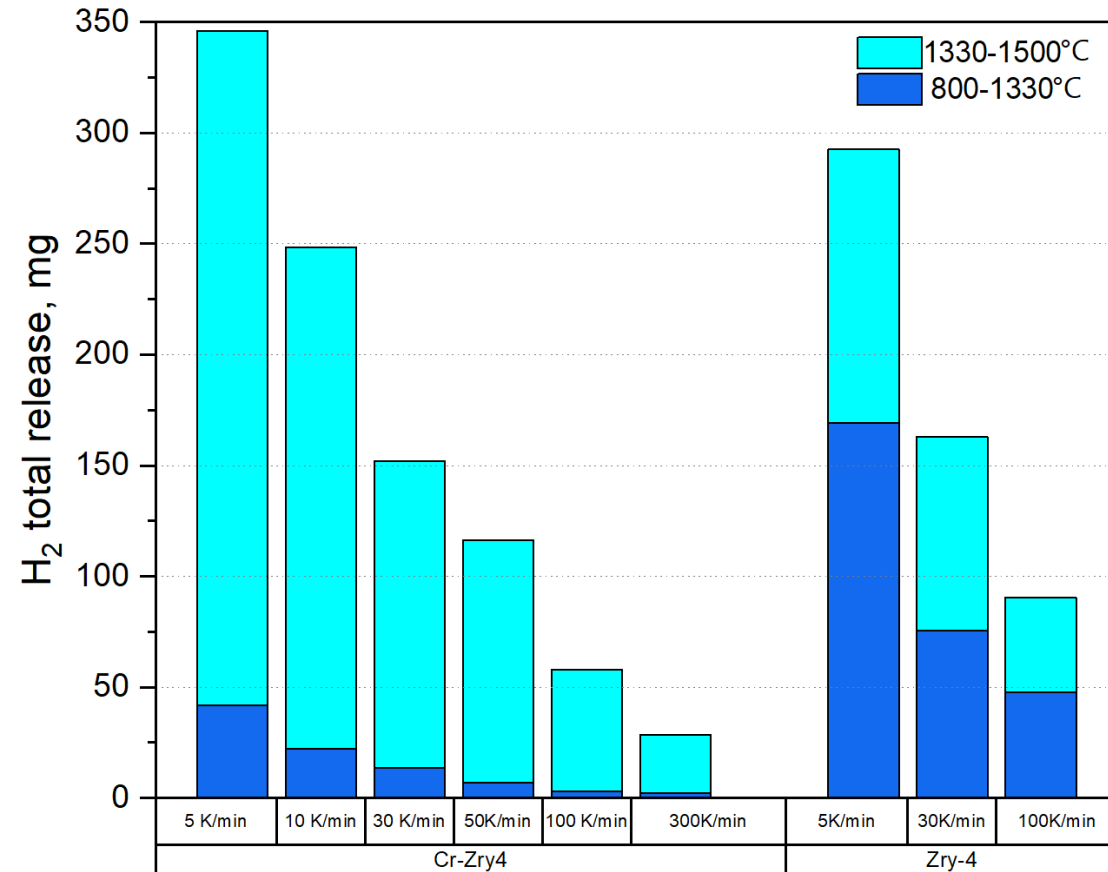
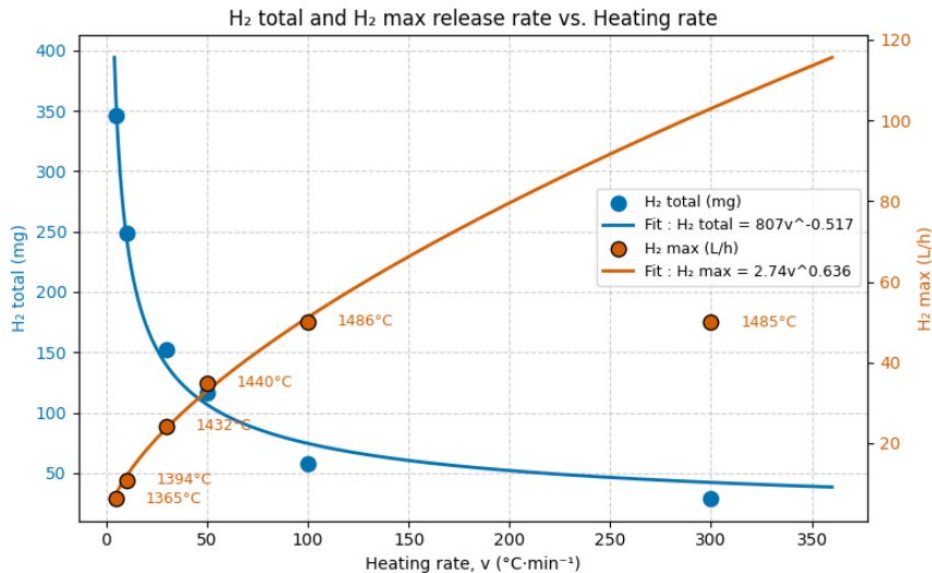


# H<sub>2</sub> release rate



- Two peaks, similar to those observed in tests on plate samples at 10 K/min<sup>1</sup>.
- 2<sup>nd</sup> Second peak corresponds to tetr→cub ZrO<sub>2</sub> transition<sup>2</sup>.
- At 5 K/min 2<sup>nd</sup> peak – T<sub>overshoot</sub>.
- At 300 K/min 2<sup>nd</sup> peak is not visible → max H<sub>2</sub> rate may not have been achieved.
- Max H<sub>2</sub> release rate increases with heating rate.
- All peaks shift to higher temperature as the heating rate increases.

# H<sub>2</sub> total



- Most H<sub>2</sub> is generated after the eutectic reaction.
- Total H<sub>2</sub> release decreases as the heating rate increases.
- At 100 K/min, total H<sub>2</sub> release is already lower than for uncoated Zry-4.



# Highlights

## Highlights

**QUENCH-SR tests of Cr-coated Zry-4 were conducted in steam up to 1500 °C at heating rates of 5, 10, 30, 50, 100, and 300 K/min.**

### Microstructure

- “Crocodile skin” morphology appeared at heating rates  $\geq 10$  K/min.
- A clear eutectic microstructure was first observed at 30 K/min. No correlation between eutectic area and heating rate was observed.
- $\text{ZrO}_2$  and  $\text{Cr}_2\text{O}_3$  oxide thicknesses decreased with heating rate following an inverse power law.

### Hydrogen release

- Total hydrogen release decreased with heating rate, approximately following an inverse square-root trend.
- Cr-coated tubes released less hydrogen than uncoated tubes at 100 K/min.
- Hydrogen release rates increased with heating rate, showing near square-root scaling and peaks shifted to higher temperatures.



**Thank you for your attention!**



**Diana Bachurina**  
**diana.bachurina@kit.edu**



**Tong Liu**

SJTU

## **Multiscale Insights into Embrittling Mechanisms of Cr Coated Zircaloy Cladding under Ultra High Temperature Conditions**

The talk by Tong Liu presented multiscale experimental insights into embrittling mechanisms of Cr-coated Zircaloy cladding under ultra-high-temperature LOCA-like conditions. Using an instrumented visual LOCA furnace with in-situ high-speed imaging and DIC strain mapping, the team tracked surface morphology, eutectic onset and real-time strain evolution during high-temperature steam oxidation and quench. Cr-coated tubes (15  $\mu\text{m}$  magnetron sputtered Cr on 9.5 mm  $\times$  0.57 mm Zircaloy) showed strongly reduced oxide growth (oxide thickness reduced by factors  $\sim$ 20–43 versus uncoated at 1200–1350  $^{\circ}\text{C}$ ) but developed a Cr–Zr eutectic layer with characteristic “crocodile-skin” morphology at higher temperatures. Ring compression tests (RCT) combined with DIC revealed that after 1200  $^{\circ}\text{C}$  HTO+quench Cr-coated cladding tended to fail in a brittle through-thickness mode (offset strain  $<2\%$ ), whereas uncoated material failed by ductile fracture; at 1350  $^{\circ}\text{C}$  the coated cladding exhibited better piecewise integrity (fewer fragments) and a much higher maximum load in some cases. Microstructural analyses linked embrittlement to formation of hard, brittle eutectic and intermetallic phases ( $\text{Cr}_2\text{O}_3$ ,  $\text{ZrCr}_2$ , eutectic layer) and identified the inner wall as the preferred crack-initiation site. The authors concluded that standard RCT methods may not fully capture degradation of Cr-coated cladding and advocated for new mechanical assessment methods and integrated experiment-simulation approaches, as well as exploration of multilayer or alternative coatings to suppress eutectic formation and improve accident tolerance.

# Multiscale Insights into Embrittling Mechanisms of Cr-Coated Zircaloy Cladding under Ultra-High Temperature Conditions

**TONG LIU, SHIJIE WANG**

**SHANGHAI JIAO TONG UNIVERSITY, CHINA**



# Content



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UNITED NATIONS



IAEA  
International Atomic Energy Agency

### IAEA Prediction:

561 GW~992 GW

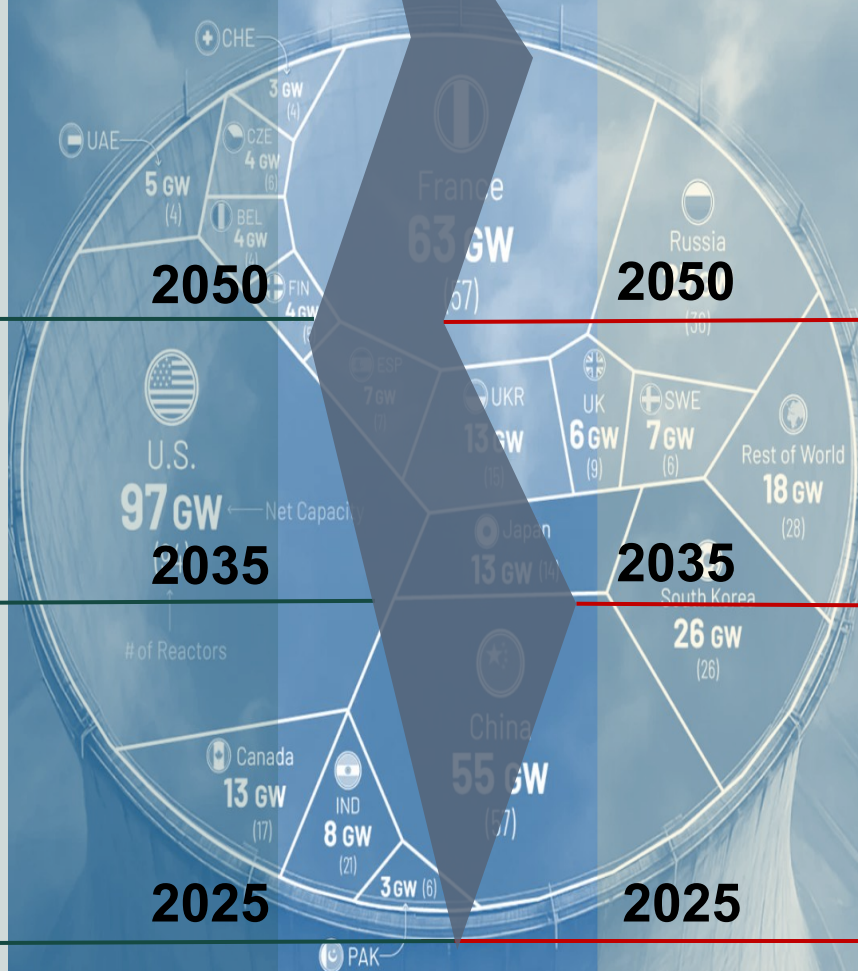
### COP30 Declaration:

33 countries have issued a declaration to **triple nuclear energy** capacity by 2050

### Data of Global Nuclear Power:

376GW operational  
64 GW under construction

# WHERE THE WORLD'S NUCLEAR POWER COMES FROM



### BP Energy Outlook:

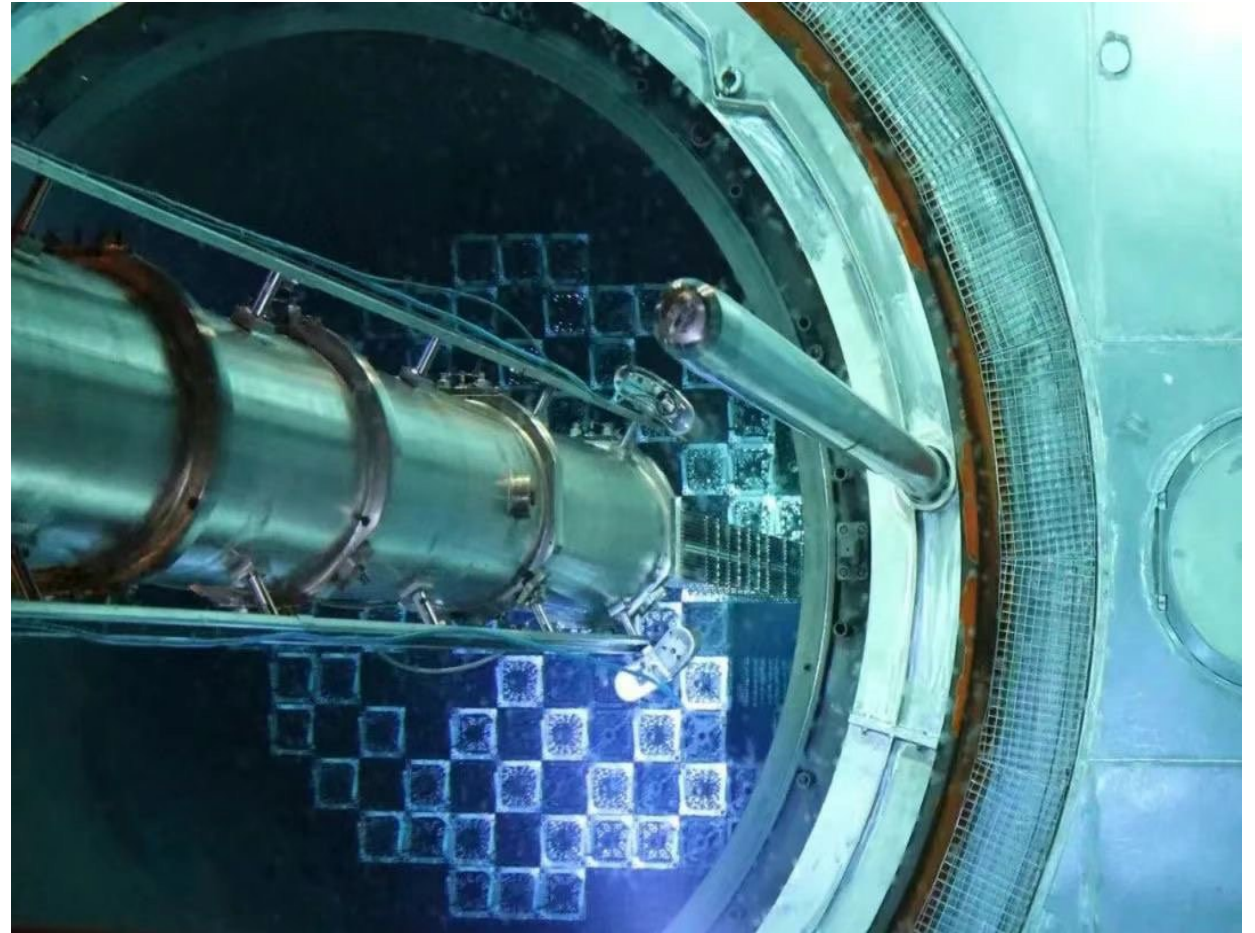
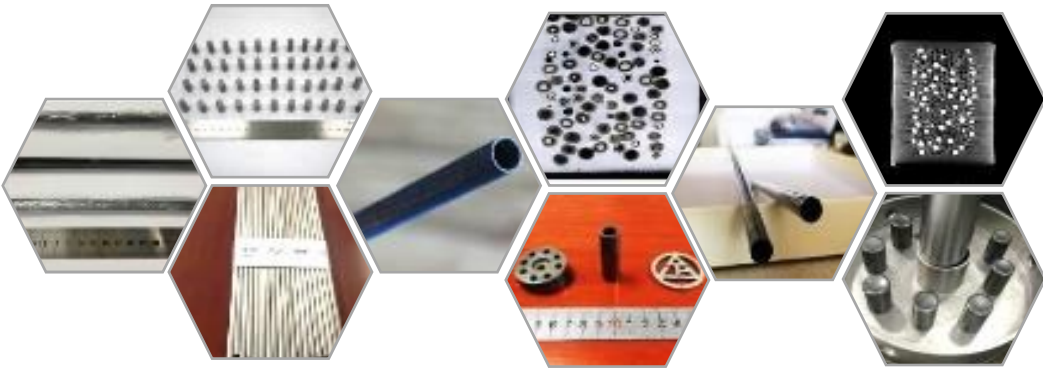
China's nuclear energy production accounts for approximately **40%** of the global total

### China NSSA Prediction:

China's nuclear power capacity in operation and under construction is projected to reach **113 GW**

### Data of Chinese Nuclear Power:

56.3 GW operational  
28.6 GW under construction

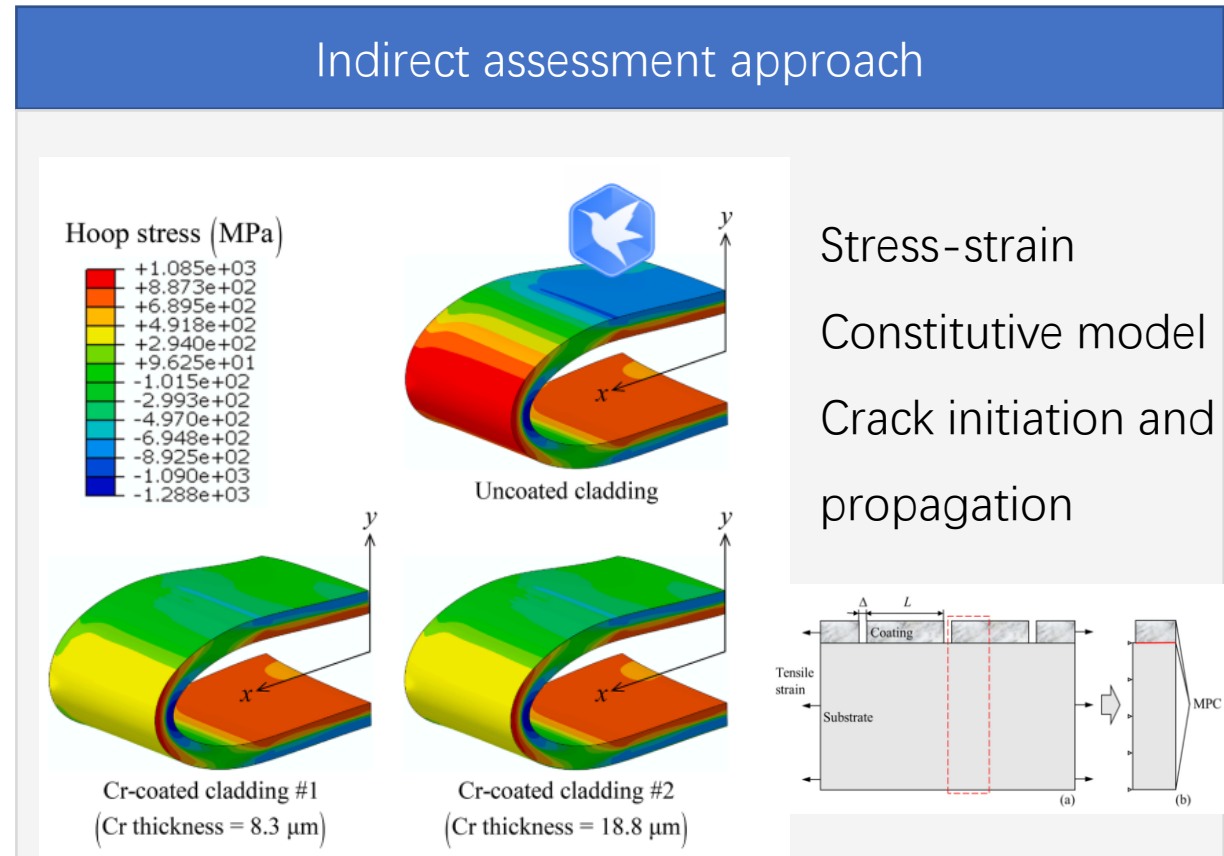
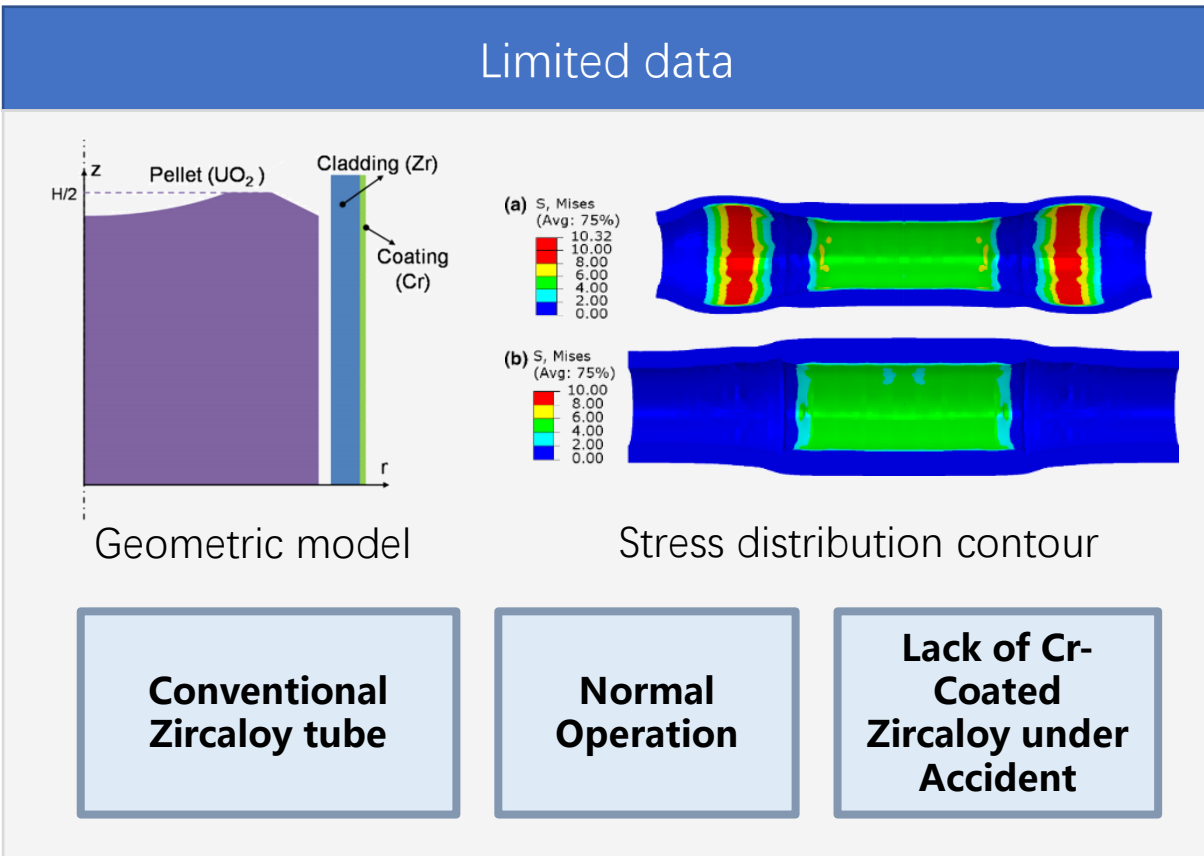


## Chromium-Coated Zircaloy: A Leading ATF Cladding

- Lead Test Assemblies (LTAs) deployed in commercial reactors

# Cladding Performance Analysis-Numerical Simulations

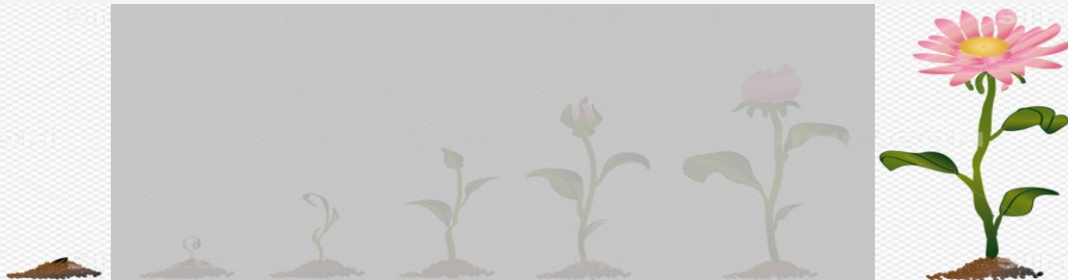
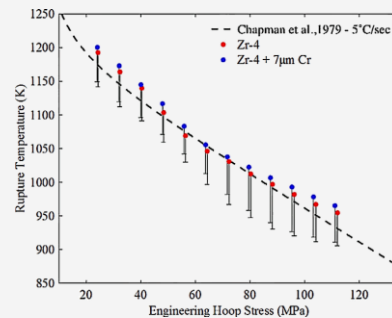
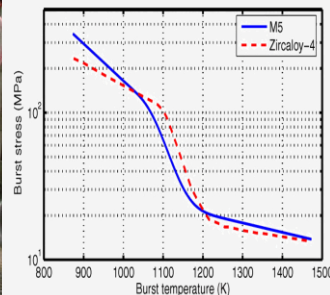
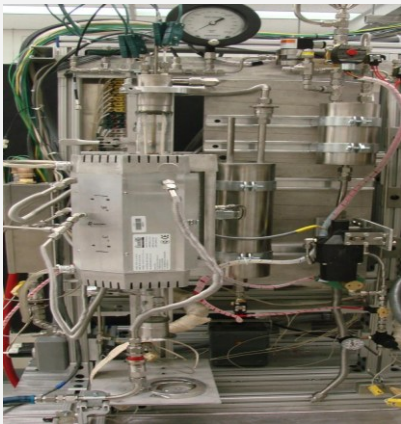
- Despite providing real-time, in-situ data on the cladding's thermo-mechanical response, the accuracy of numerical simulations must be validated.
  - **Absence of experimental validation**



# Cladding Performance Analysis-Traditional Experimental Approach

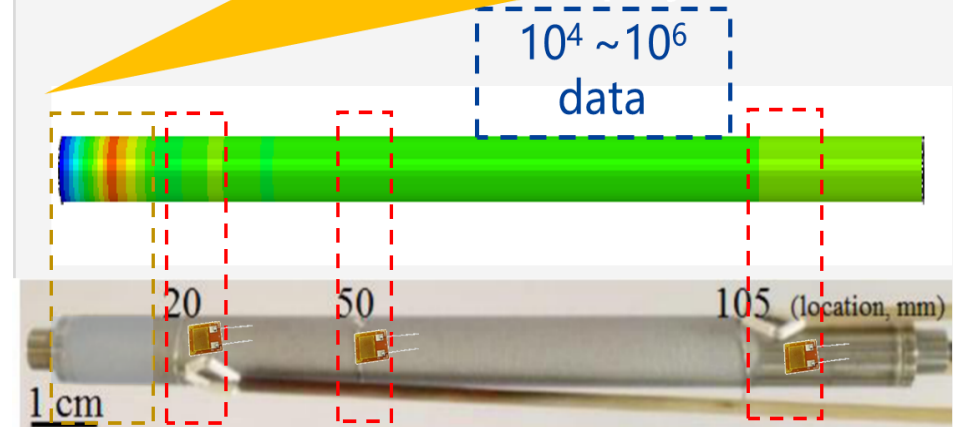
- The intrusive nature of contact-based sensors distorts the intrinsic thermo-mechanical fields of the cladding and fails to capture critical local strain peaks
  - **Compromising the accuracy and reliability of the experimental data**

## Invisible in Closed System



## Interference/ Insufficiency/Undetection

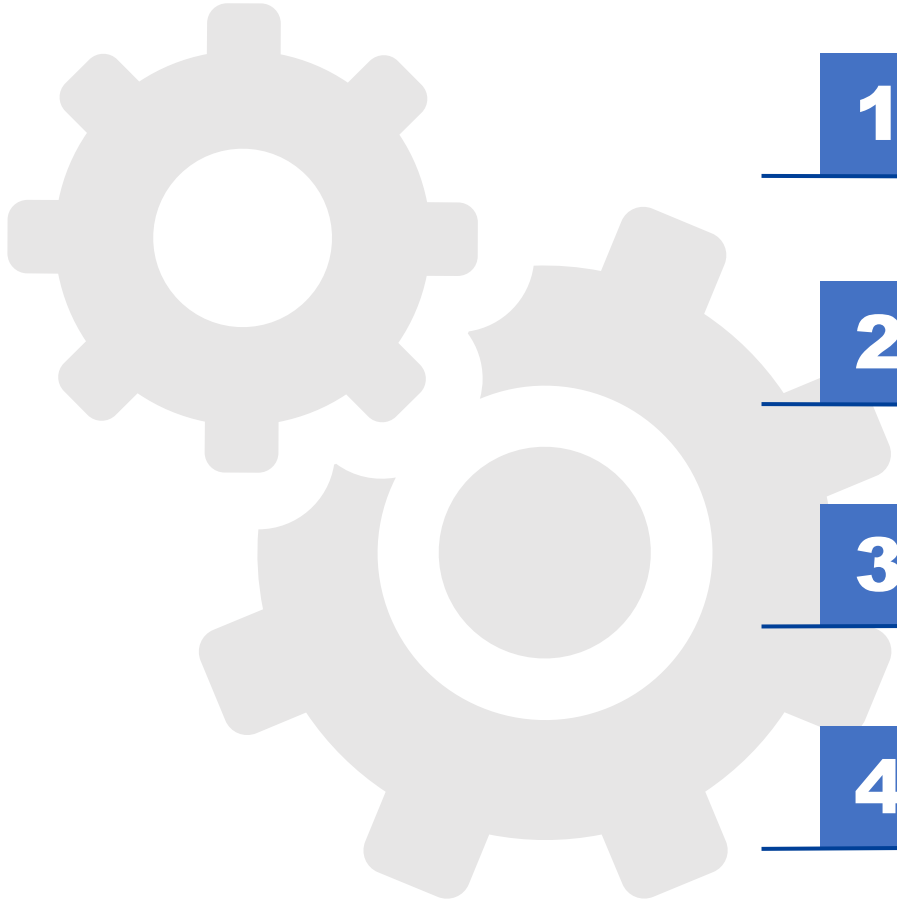
The maximum local strain data is missing due to limited SGs deployment



Numerical simulation

Experimental

Temperature, stress, strain and corrosion of cladding samples are interfered by SGs and TCs



**1**

Introduction & Motivation

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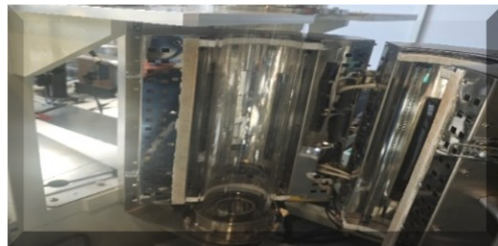
**Summary & Outlook**

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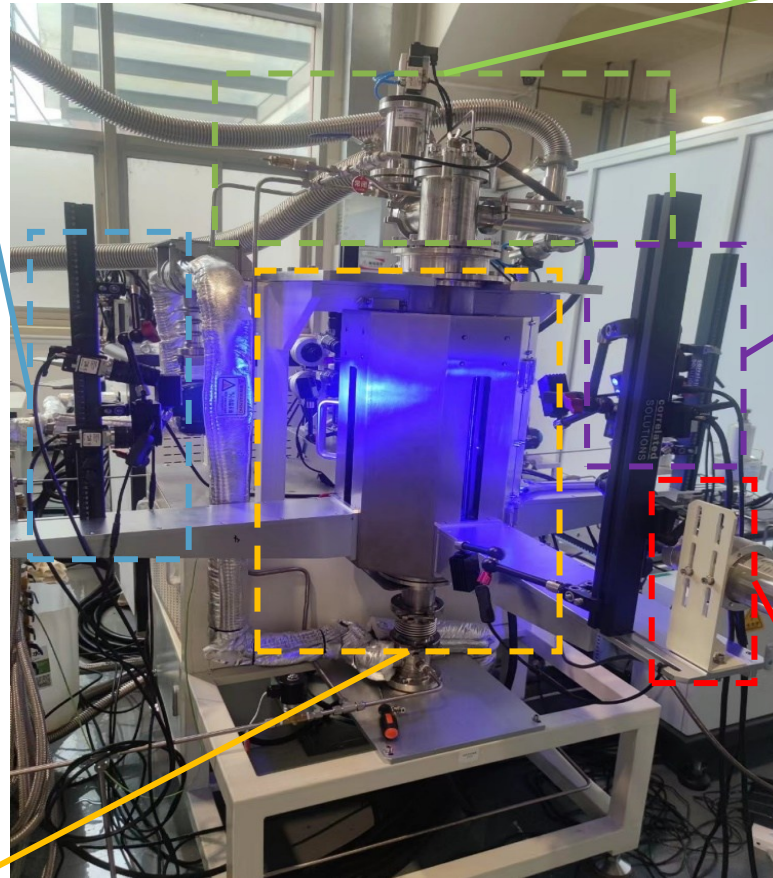
# Visual Experimental Platform

Ultra-high temperature LOCA device with visual system

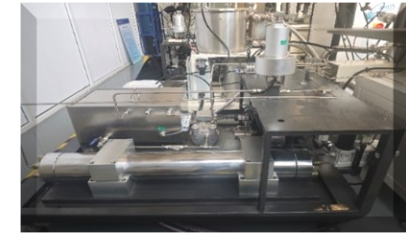
Online Projection Image  
Measuring Instrument



Furnace



Pressure control system



DIC system



Temperature measurement and  
control system



- ✓ Maximum heating temperature **2300 °C**
- ✓ Maximum heating rate **300 °C/s**

## Determining Post Quench Ductility



PRELIMINARY DRAFT  
U.S. NUCLEAR REGULATORY COMMISSION  
OFFICE OF NUCLEAR REGULATORY RESEARCH  
**REGULATORY GUIDE**

Month Year  
Revision 0  
Technical Lead  
M. Bales

Public availability of this draft document is intended to inform stakeholders of the current status of the NRC staff's preliminary draft final rule package and associated documents for § 50.46c of Title 10 of the Code of Federal Regulations (10 CFR). These preliminary draft documents are in support of an October 22, 2015, Category 3 public meeting, and a November 2, 2015, Advisory Committee on Reactor Safeguards (ACRS) subcommittee meeting.

This draft document has not been subject to all levels of NRC management review. Accordingly, it is incomplete and may be error in one or more respects. The document may be subject to further revision before the staff provides the final draft rule language package to the Commission (currently scheduled to be provided to the Commission in February 2016).

### REGULATORY GUIDE 1.223

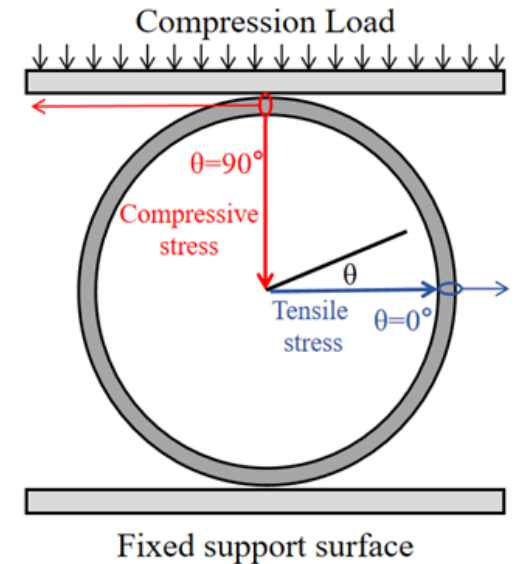
(Draft was issued as DG-1262, dated March 2014)

### DETERMINING POST QUENCH DUCTILITY

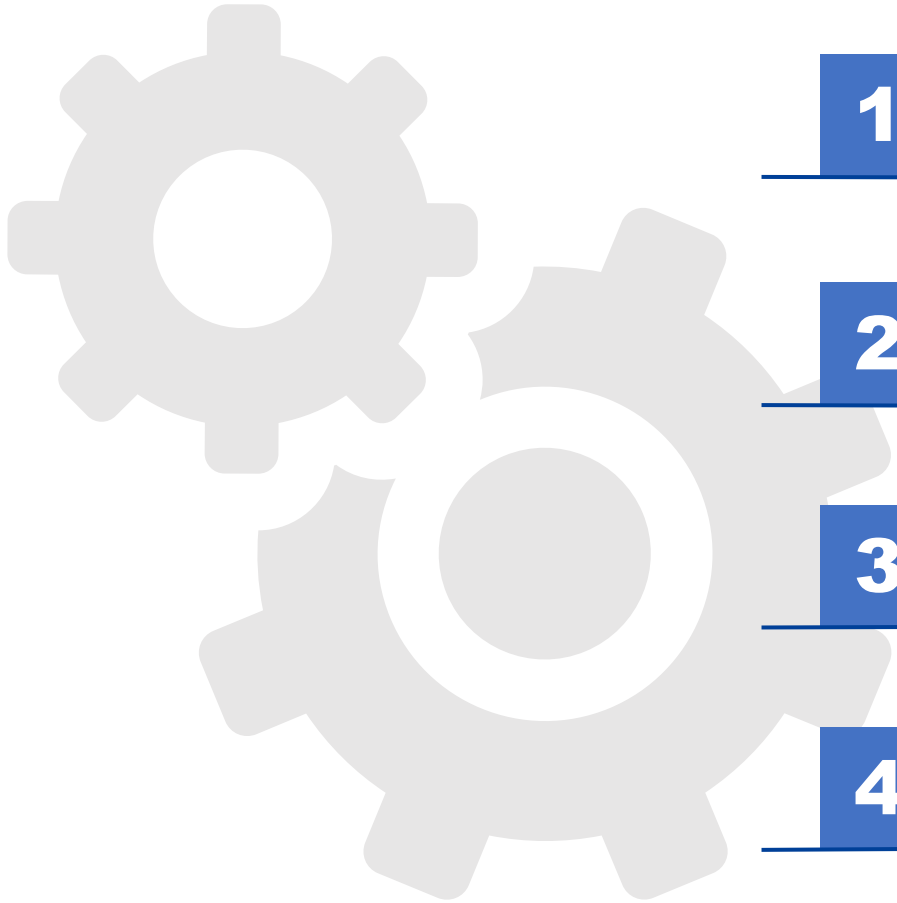
### NRC Regulatory Guide 1.223 Determining Post Quench Ductility (PQD)



Mechanical Test System  
(MTS)



Schematic of simulated Ring  
Compression Test (RCT)



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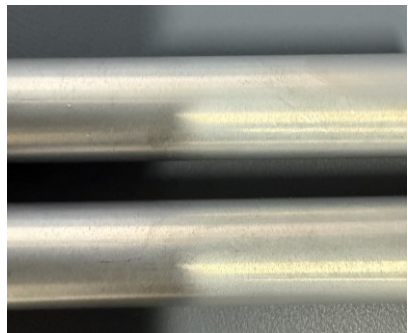
# Experimental materials and conditions

## □ Experimental materials



zircaloy cladding

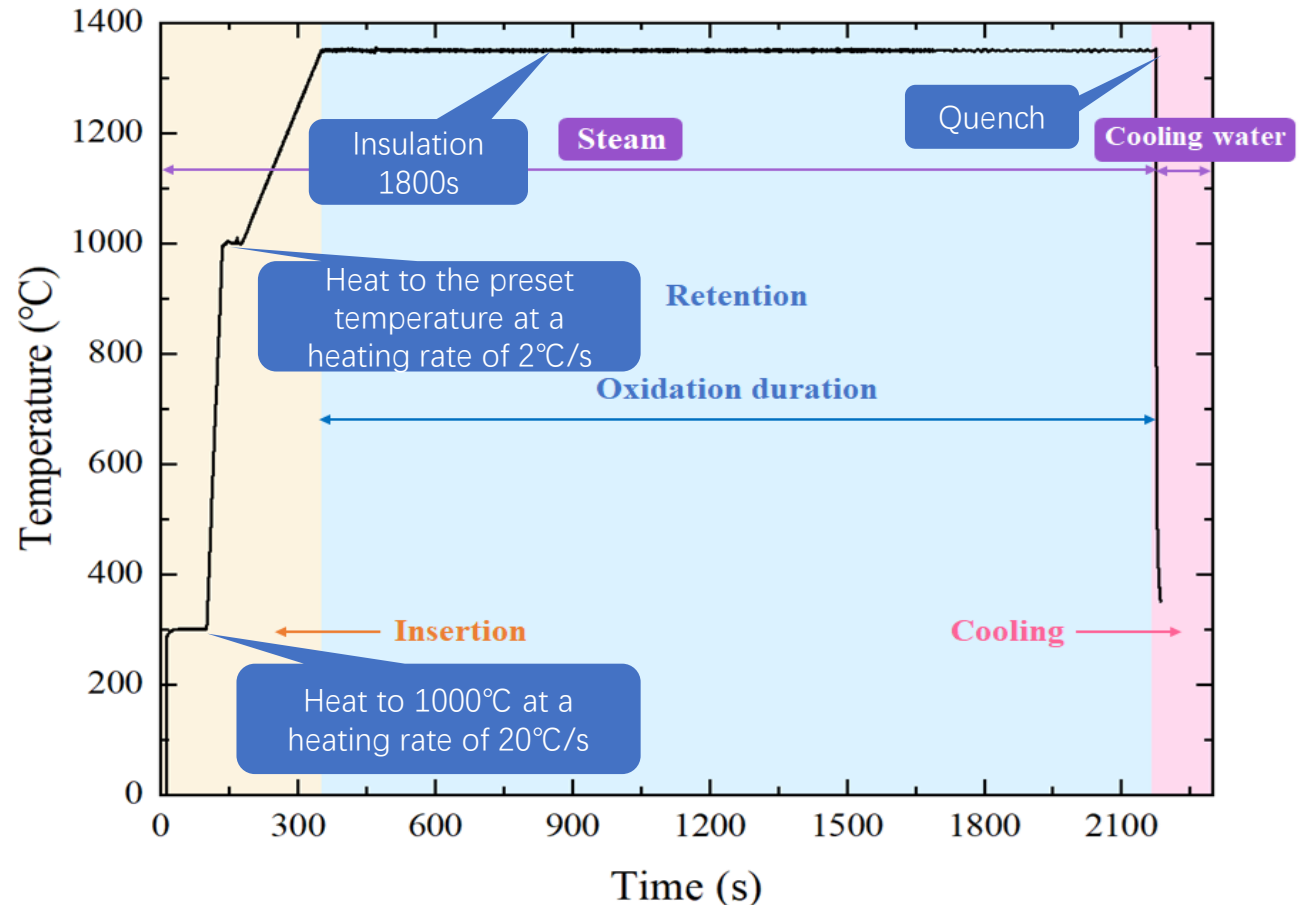
- Diameter  
9.5 mm
- thickness  
0.57 mm



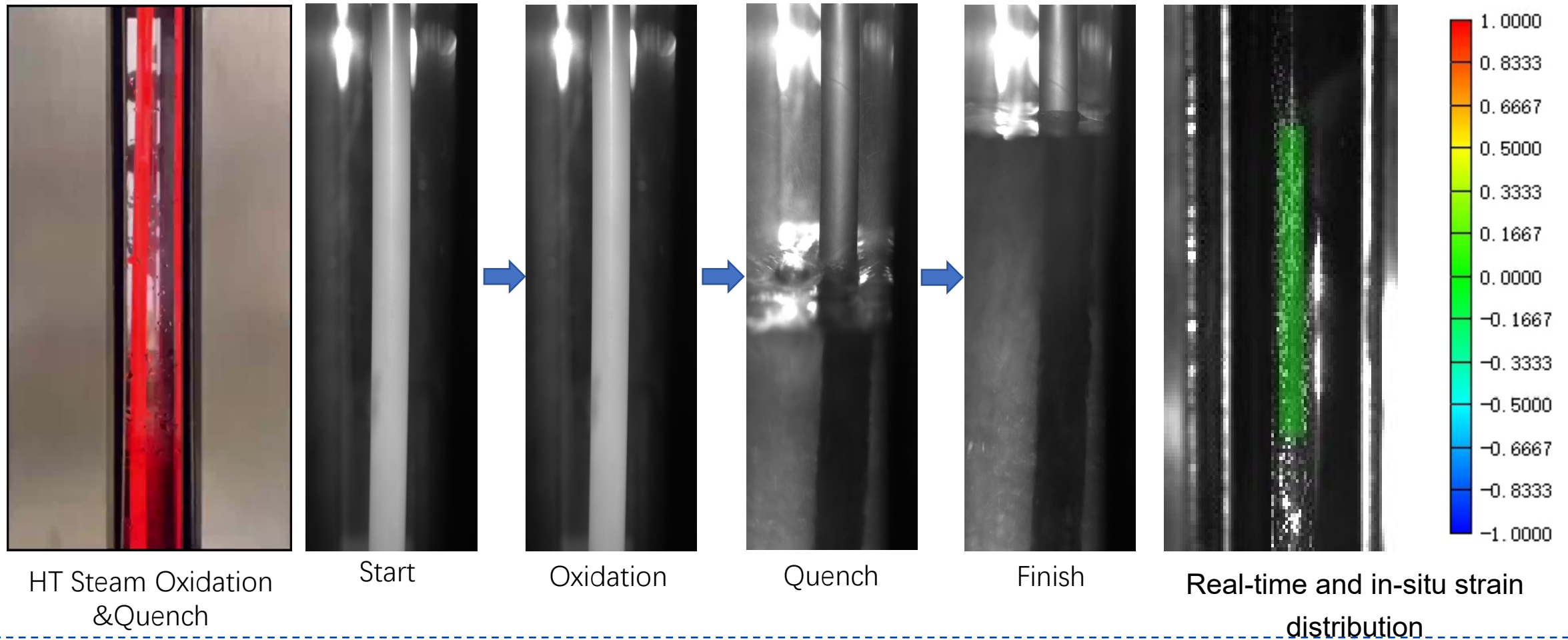
Cr-coated  
cladding

- Magnetron  
sputtering process
- Coating thickness  
15  $\mu\text{m}$

## □ Experimental conditions

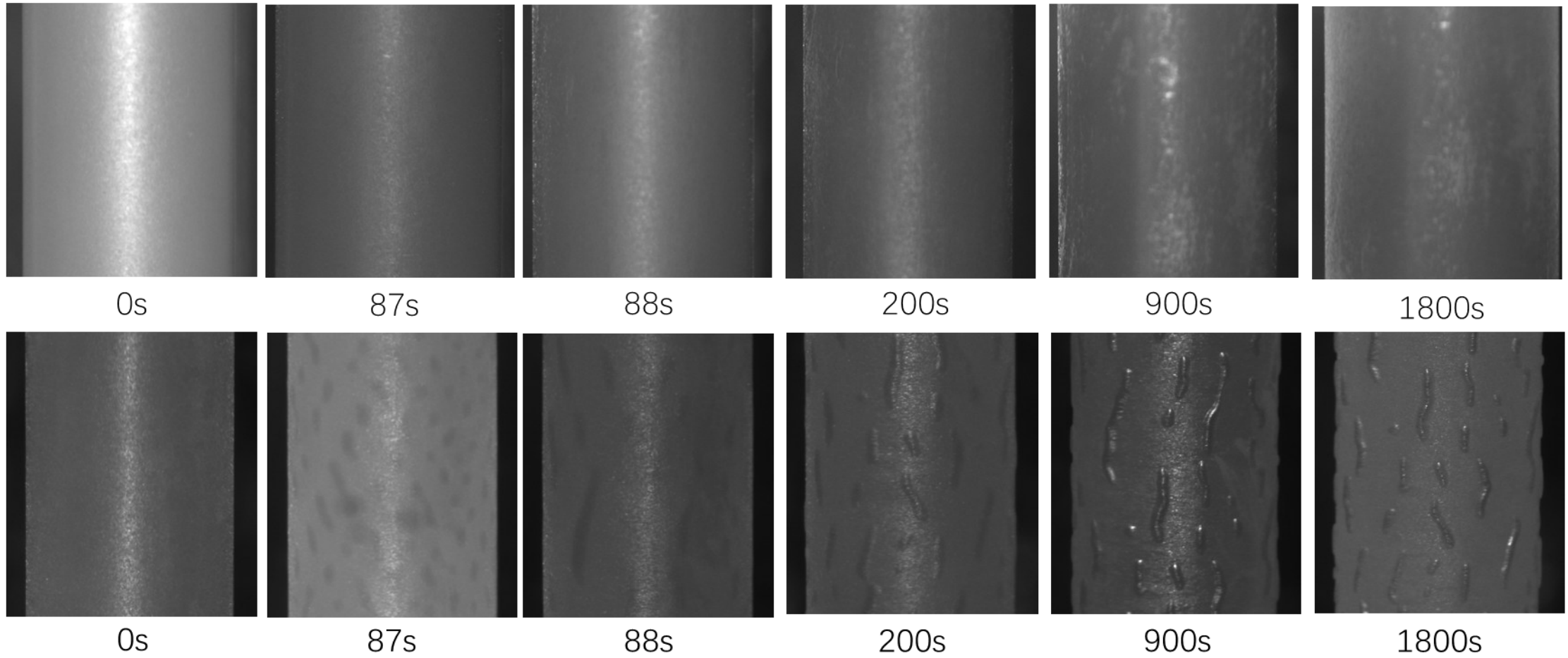


# In-situ Visualization during HTO and Quench









➤ In-situ high speed camera tracks surface morphology during HTO+Q

# Pre-/Post-HT Oxidation Cladding Morphology



**The onset of the chromium-zirconium eutectic reaction and the subsequent evolution of its surface morphology were precisely captured using in-situ high-speed photography.**

# Pre-/Post-HTO+Q Cladding Morphology

Type	As-received	Oxidation at 1200°C 1800s	Oxidation at 1350°C (Trant.) 1800s
Uncoated Zr cladding			
Cr-coated Zr cladding			

- **Uncoated Zr: metallic luster → rough black/brown**
- **Cr-coated Zr: silvery white → dark green; 1350 °C shows eutectic “crocodile-skin” morphology.**

# Pre-/Post-HTO Cladding Microstructure

Type	As-received	Oxidation at 1200 ° C 1800s	Oxidation at 1350 ° C 1800s
Uncoated Zr cladding			
Cr-coated Zr cladding			

➤ The coated cladding exhibited a reduction in oxide layer thickness by factors of **~20** and **~43** at 1200°C and 1350°C as compared to uncoated.

# Pre-/Post-HTO Cladding Composition

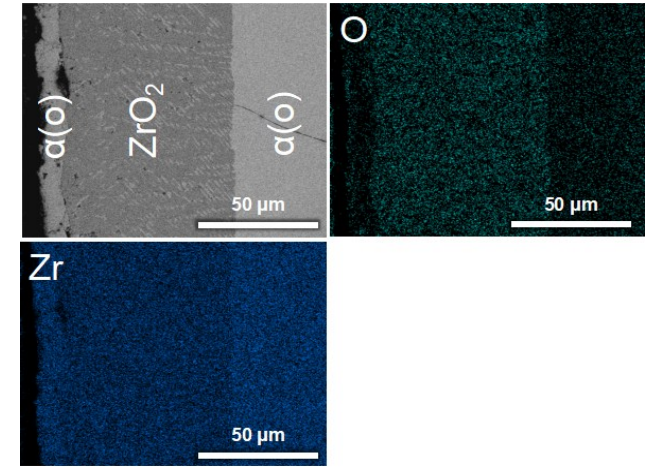
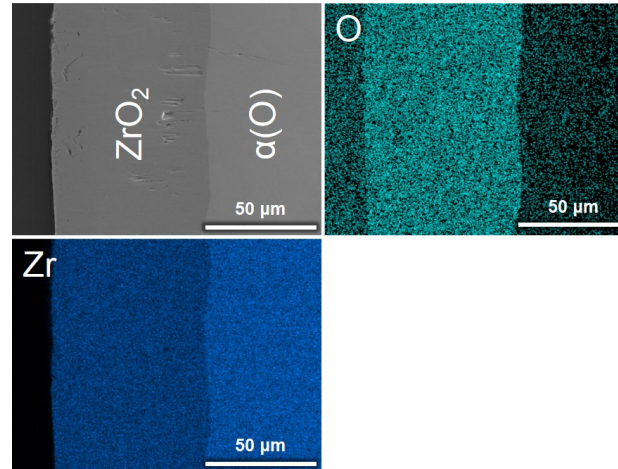
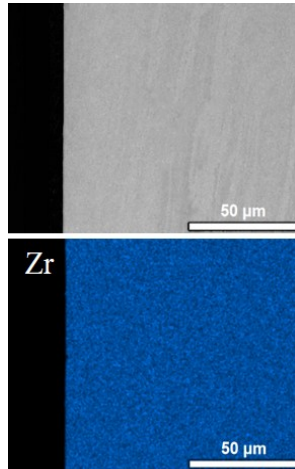
Type

As-received

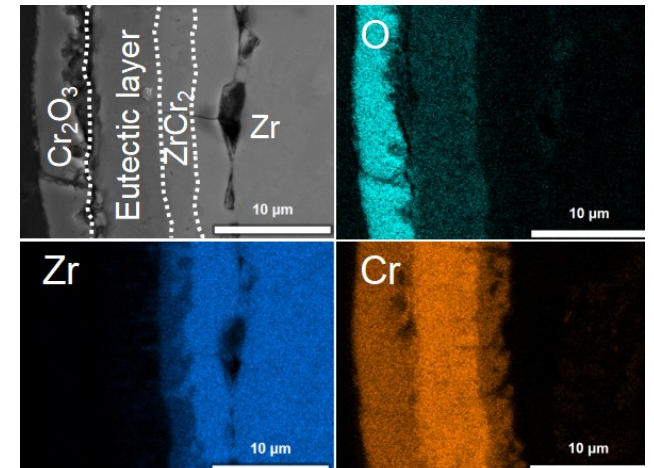
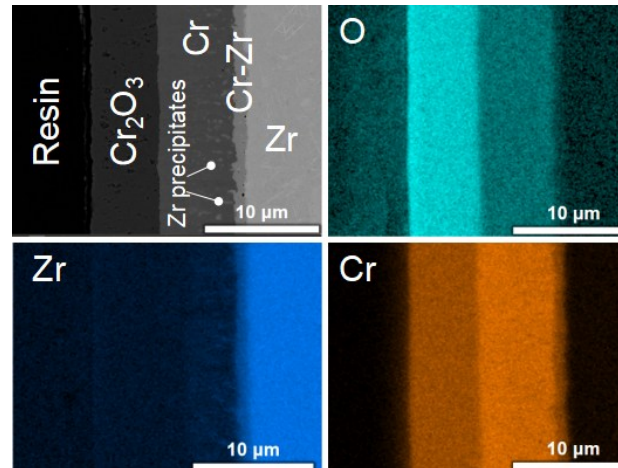
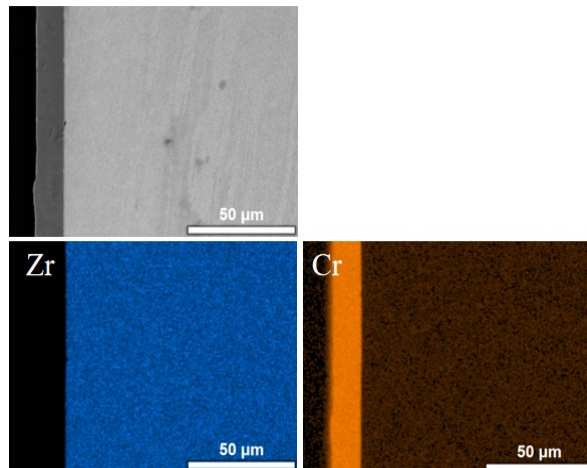
Oxidation at 1200 ° C 1800s

Oxidation at 1350 ° C Tran 1800s

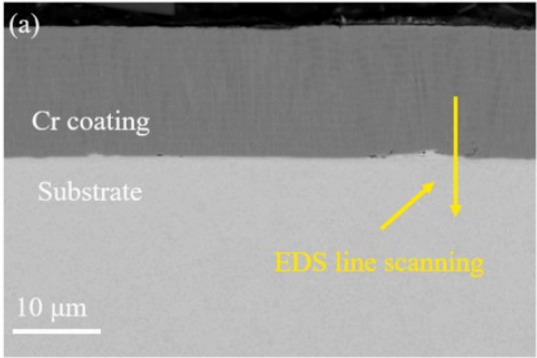
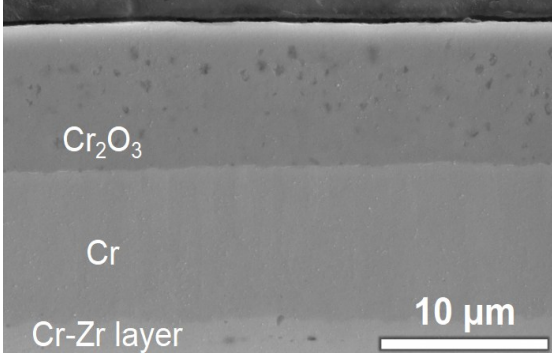
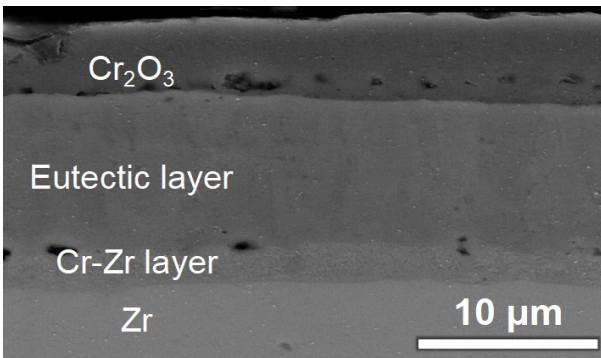
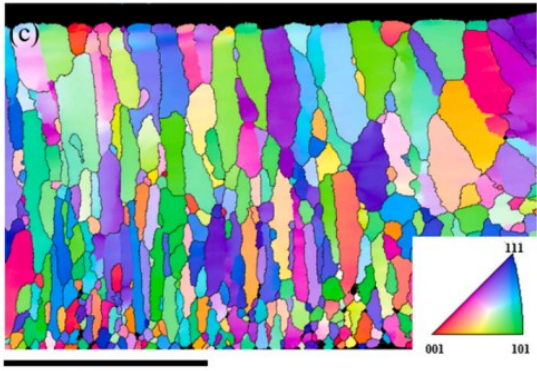
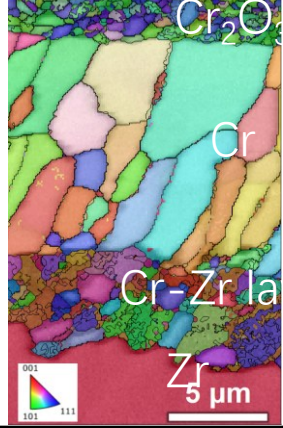
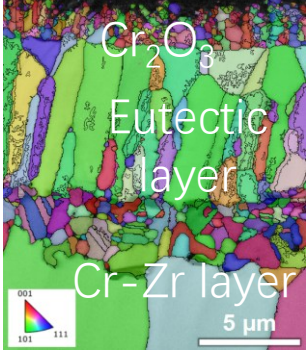
Uncoated Zr  
cladding



Cr-coated Zr  
cladding



# Pre-/Post-HTO Coated Cladding Grain Structure

Type	As-received	Oxidation at 1200°C 1800s	Oxidation at 1350°C 1800s
Cr-coated Zr cladding			
			

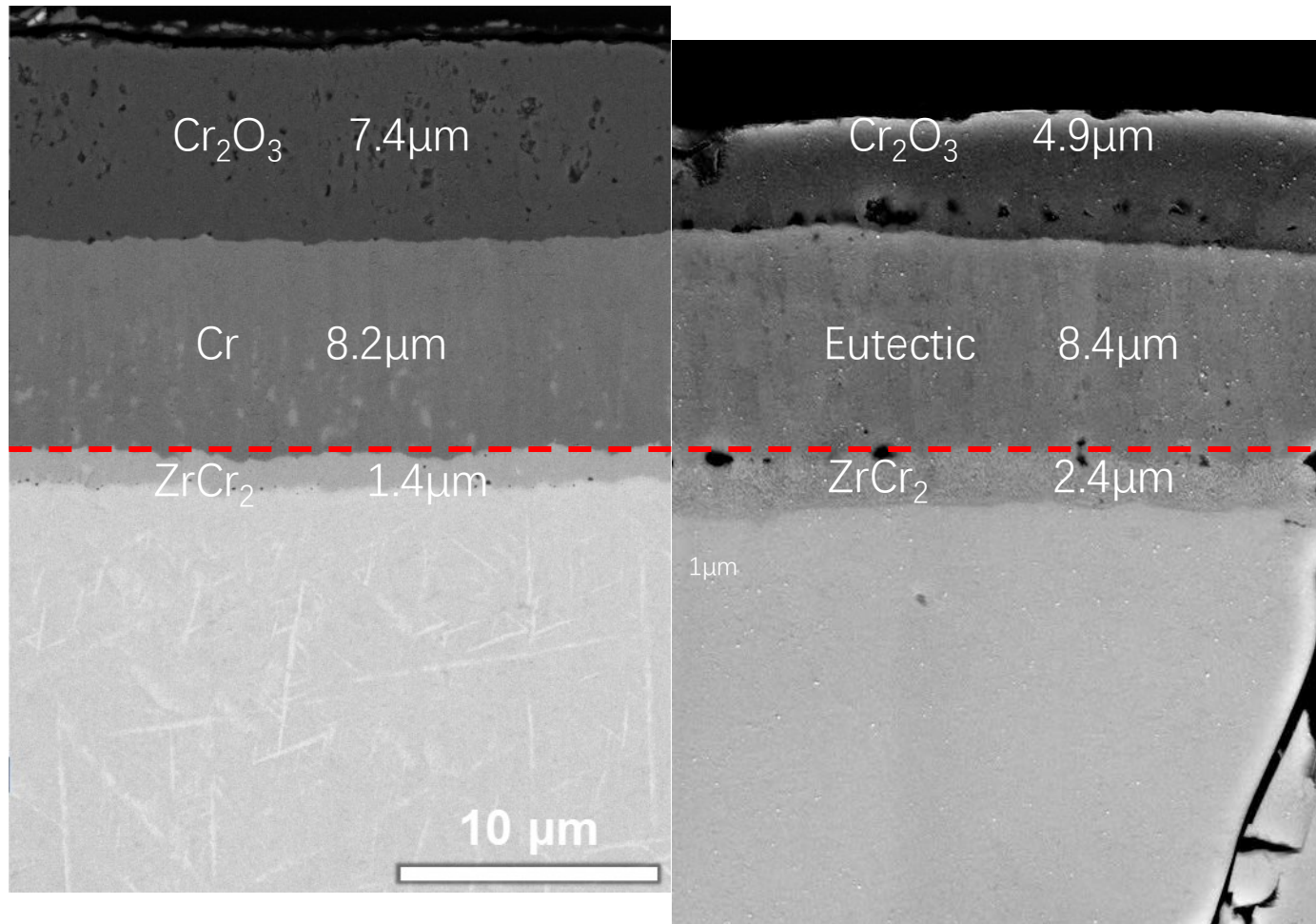
➤ Cr layer:Columnar crystal

- Cr<sub>2</sub>O<sub>3</sub> layer:Equiaxed crystal
- Cr layer:Columnar crystal
- Zr-Cr layer:Equiaxed crystal

- Cr<sub>2</sub>O<sub>3</sub> layer:Equiaxed crystal
- Eutectic layer:Columnar crystal
- Zr-Cr layer:Equiaxed crystal 17

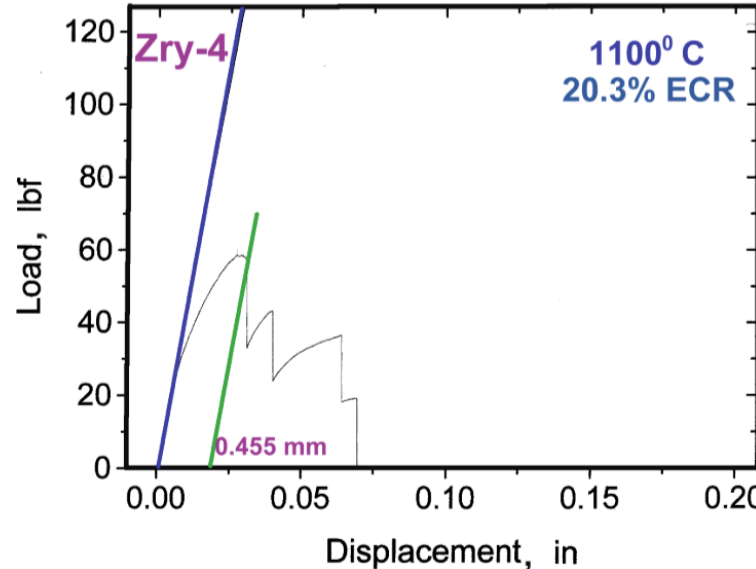
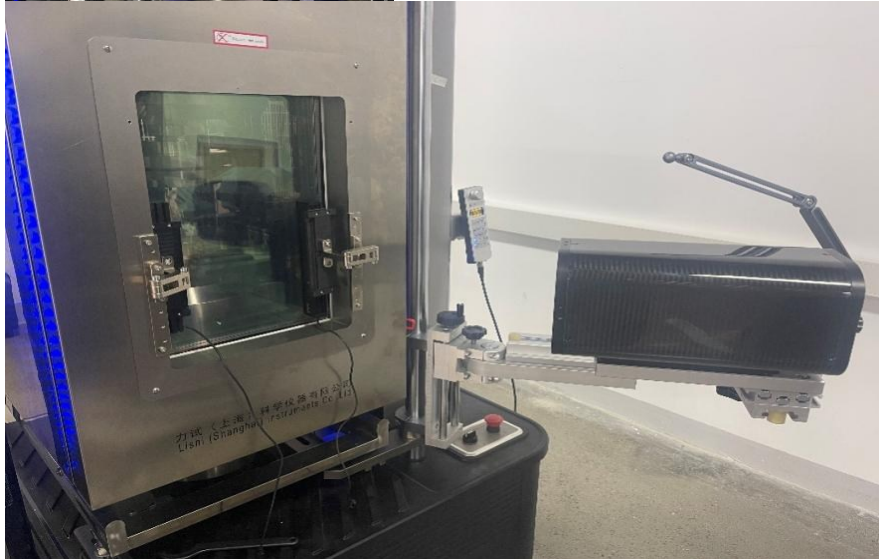
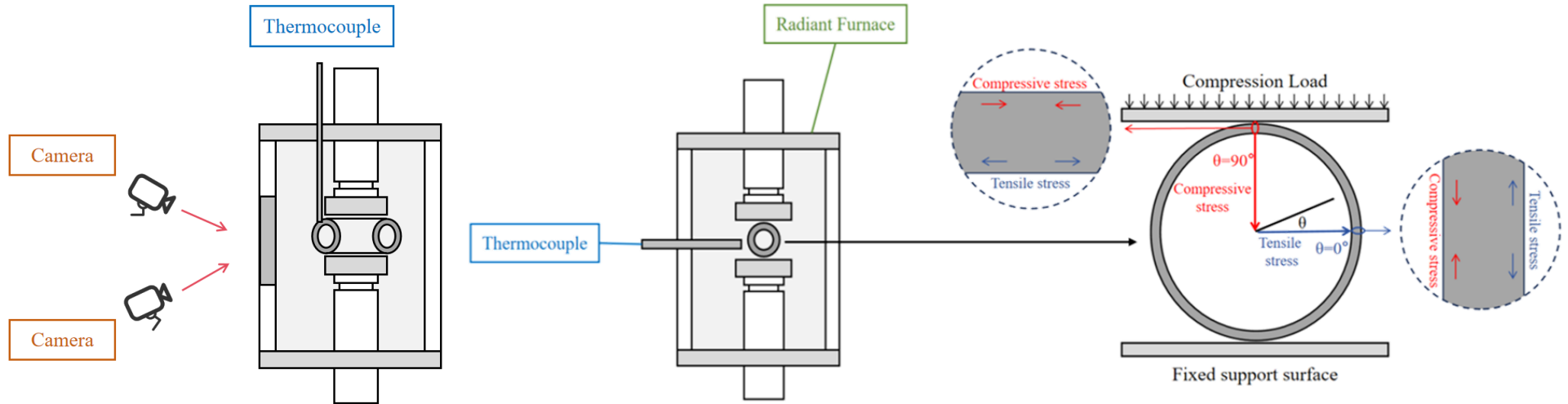
1200°C 30min

1350°C 30min





# Ring Compression Test



Typical load-displacement curve<sup>[1]</sup>

U.S. NRC  
United States Nuclear Regulatory Commission  
Protecting People and the Environment

REPORT A SAFETY CONCERN SEARCH

NUCLEAR REACTORS NUCLEAR MATERIALS RADIOACTIVE WASTE NUCLEAR SECURITY PUBLIC MEETINGS & INVOLVEMENT NRC LIBRARY ABOUT NRC

Home » NRC Library » Document Collections » Regulations (NRC, 10 CFR) » Part Index

**§ 50.46 Acceptance criteria for emergency core cooling systems for light-water nuclear power reactors**

(a)(1)(i) Each boiling or pressurized light-water nuclear power reactor fueled with uranium oxide pellets within cylindrical zircaloy or ZIRLO cladding must be provided with an emergency core cooling system (ECCS) that must be designed so that its calculated cooling performance following postulated loss-of-coolant accidents conforms to the criteria set forth in paragraph (b) of this section. ECCS cooling performance must be calculated in accordance with an acceptable evaluation model and must be calculated for a number of postulated loss-of-coolant accidents of different sizes, locations, and other properties sufficient to provide assurance that the most severe postulated loss-of-coolant accidents are calculated. Except as provided in paragraph (a)(1)(ii) of this section, the evaluation model must include sufficient supporting justification to show that the analytical technique realistically describes the behavior of the reactor system during a loss-of-coolant accident. Comparisons to applicable experimental data must be made and uncertainties in the analysis method and inputs must be identified and assessed so that the uncertainty in the calculated results can be estimated. This uncertainty must be accounted for, so that, when the calculated ECCS cooling performance is compared to the criteria set forth in paragraph (b) of this section, there is a high level of probability that the criteria would not be exceeded. Appendix K, Part II Required Documentation, sets forth the documentation requirements for each evaluation model. This section does not apply to a nuclear power reactor facility for which the certifications required under § 50.82(a)(1) have been submitted.

(ii) Alternatively, an ECCS evaluation model may be developed in conformance with the required and acceptable features of appendix K ECCS Evaluation Models.

(2) The Director of Nuclear Reactor Regulation may impose restrictions on reactor operation if it is found that the evaluations of ECCS cooling performance submitted are not consistent with paragraphs (a)(1)(i) and (ii) of this section.










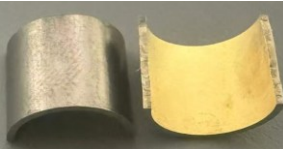

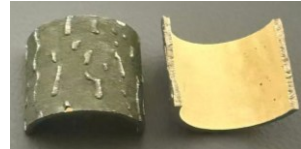
## NRC Fuel safety criteria during LOCA [2]

<2% Brittle failure  
offset strain  
>2% Ductile failure

1] No. NUREG/CR-696. Argonne National Lab.(ANL), Argonne, IL (United States), 2008.; [2] NRC, 10CFR50.46 [3]REGULATORY GUIDE 1.223

# Pre-/Post-RCT Cladding Morphology

➤ Specimen  $8.00 \pm 0.05$  mm (axial length); crosshead rate 0.033 mm/s.

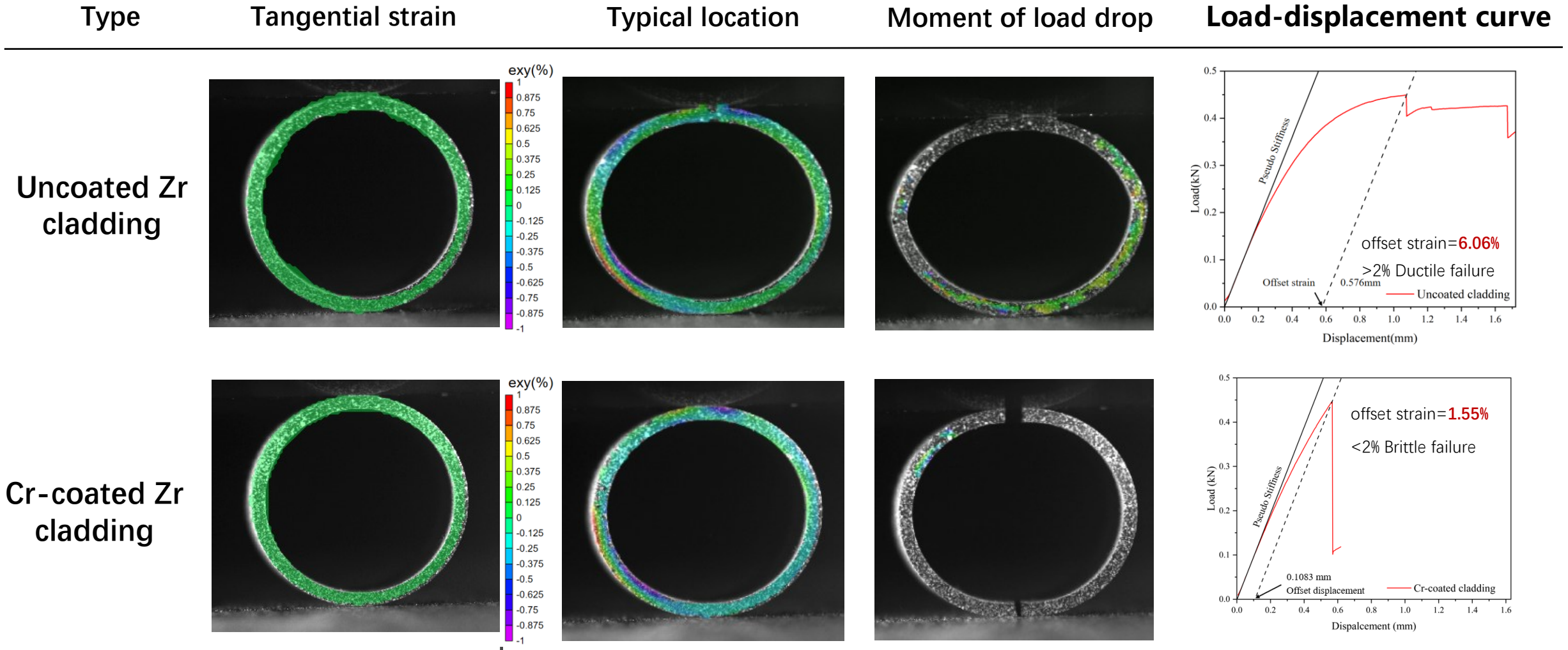
Type	As-received		Oxidation at 1200 ° C 1800s		Oxidation at 1350 ° C 1800s	
Uncoated Zr cladding						
Cr-coated Zr cladding						
	Pre-RCT	Post-RCT	Pre-RCT	Post-RCT	Pre-RCT	Post-RCT

The oxide layer spalls off.

➤ 1200 °C: Uncoated—local/non-penetrating; Cr-coated—through-thickness → weaker fracture resistance.

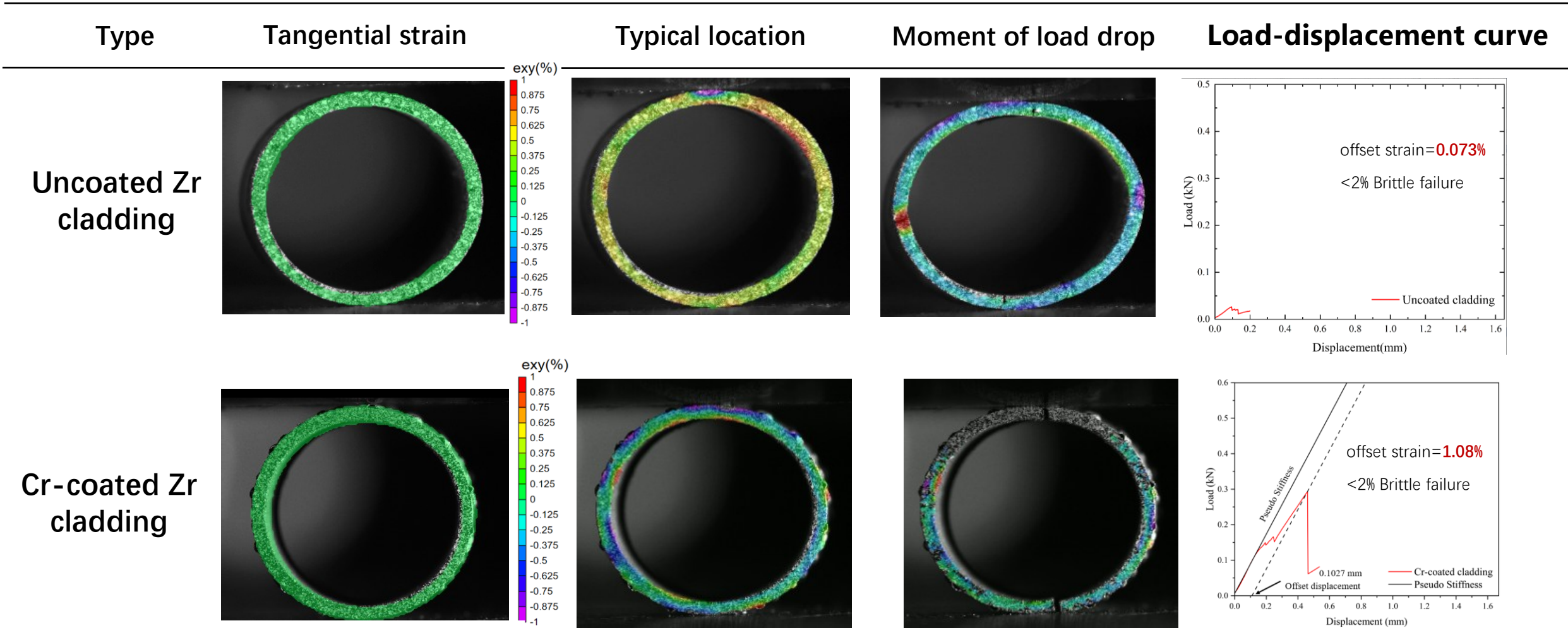
➤ 1350 °C: Uncoated—4 pieces; Cr-coated—2 pieces → superior fracture resistance for Cr-coated.

# DIC mapping during RCT after 1200°C HTO+Quench

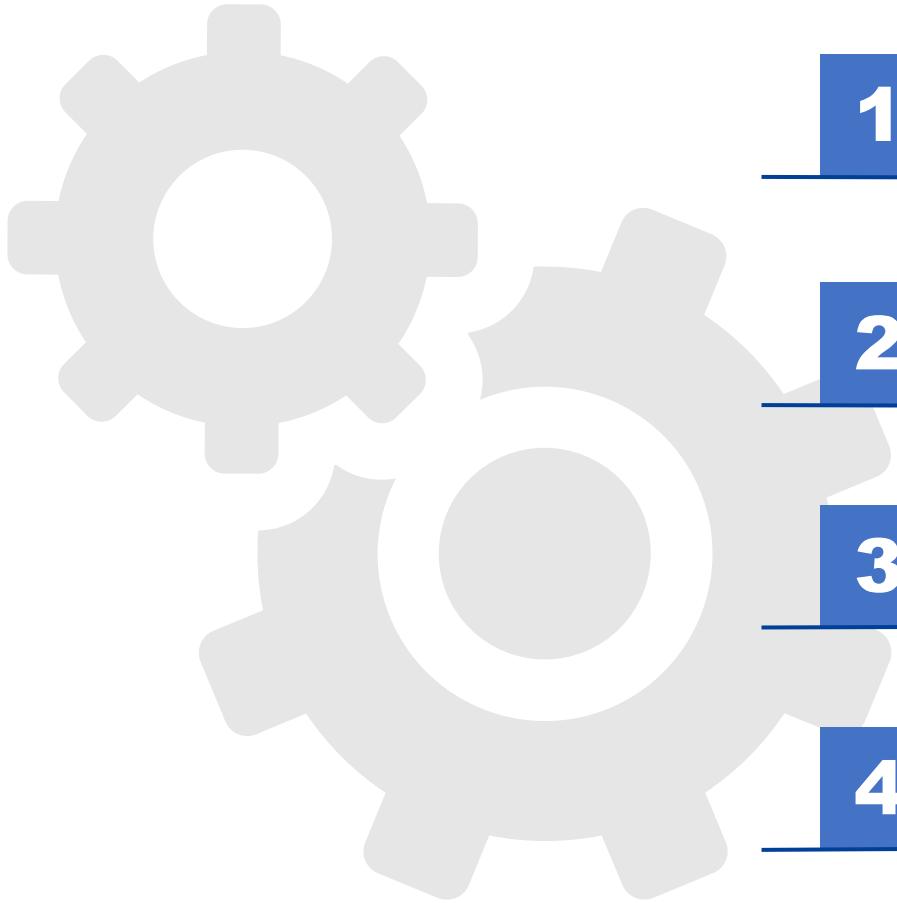


➤ After HTO at 1200 °C, the uncoated cladding fails by ductile fracture, whereas the Cr-coated cladding fails by brittle fracture, with similar maximum load-bearing capacity

# DIC mapping during RCT after 1350°C HTO+Quench



The Cr-coated cladding exhibited an approximately 16.7-times increase in maximum load-bearing capacity. 22



**1**

**Introduction & Motivation**

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**2**

**Methodology & Facilities**

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**3**

**Results & Discussion**

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**4**

**Summary & Outlook**

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# Summary

- **A combined in-situ/ex-situ approach correlated mechanical embrittlement of Cr-coated Zircaloy cladding with its microstructure.**
- **Dynamic monitoring identified the Cr-Zr eutectic onset and associated "crocodile-skin" morphology**
- **The eutectic reaction degrades mechanical properties by creating hard-brittle phases and initiating crack nucleation and growth.**
- **RCT+DIC on single-sided oxidized specimens shows peak tensile stress on the inner wall, identifying it as the preferred crack-initiation site.**
- **RCT following exposure to 1200°C HTO reveal that the chromium coating significantly reduces oxidation; nevertheless, it induces premature brittle fracture of the cladding.**
- **The standard ring compression test may not be suitable for evaluating the mechanical degradation of Cr-coated cladding.**

# Outlook

## ➤ **Mechanical Assessment Methodology**

New mechanical assessment methods in experimental and numerical modeling must be developed to accurately characterize its performance degradation.

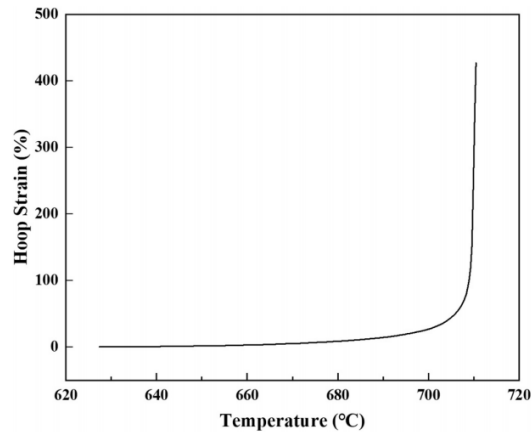
## ➤ **Integration of Experiment and Simulation**

The experimental phenomenology for visualizing extreme-scenario responses provides a critical foundation. Subsequent research will focus on quantitatively correlating these findings with numerical simulations to validate and refine predictive models.

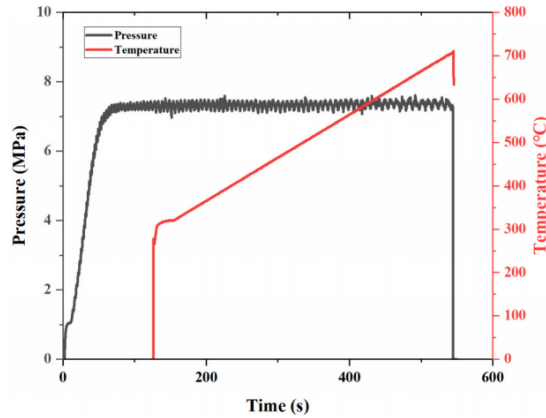
## ➤ **Advanced Coating Systems**

Exploring multi-layer or alternative coating materials could provide pathways to suppress eutectic formation and achieve superior accident tolerance.

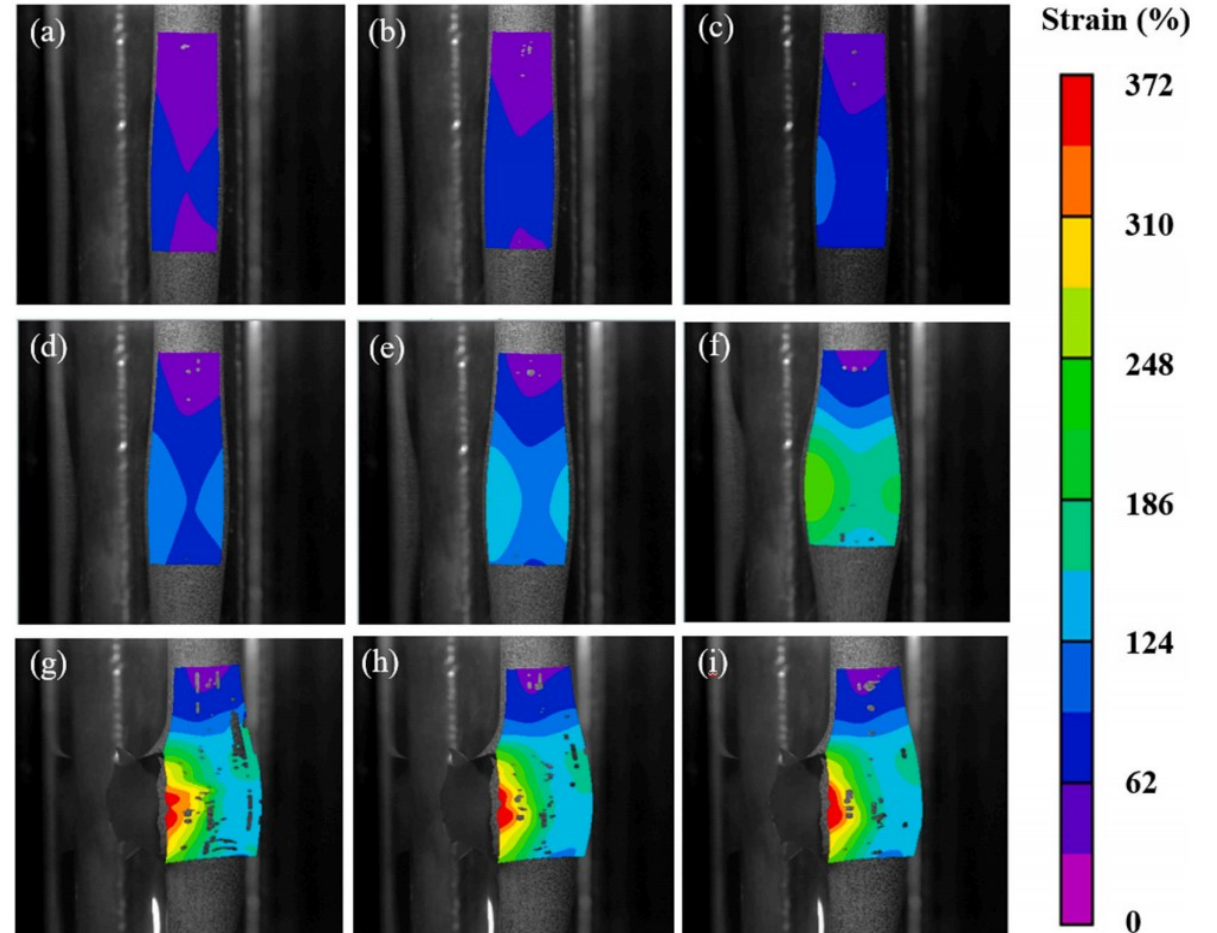
# Ballooning and Burst Test



Hoop Strain vs Temperature



Pressure/Temperature vs Time



Strain distribution mapping on Zry-4 cladding tube during the B&B test

Optical image							
	(a)	(b)	(c)	(d)	(e)	(f)	(g)
Temperature	683.1°C	708.9°C	709.3°C	709.7°C	709.9°C	710.2°C	710.5°C
Strain variations	0	0.007	0.082	0.104	0.149	0.223	0.611

Optical image sequence during the onset of the eutectic reaction

## Ballooning burst experimental curves and strain calculation results<sup>[1]</sup>



# Acknowledgments

Prof. Jun Sun

Prof. Zhongxiao Song

Dr. Martin Steinbruck

Prof. Xiaoqin Zeng

Dr. Yehong Liao

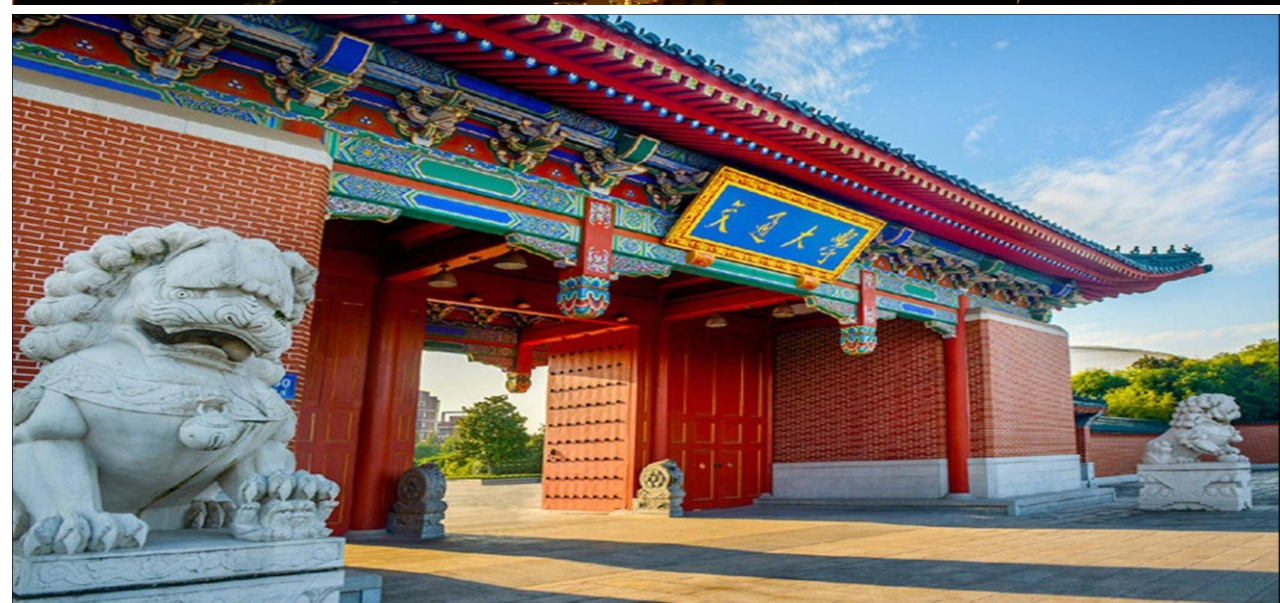
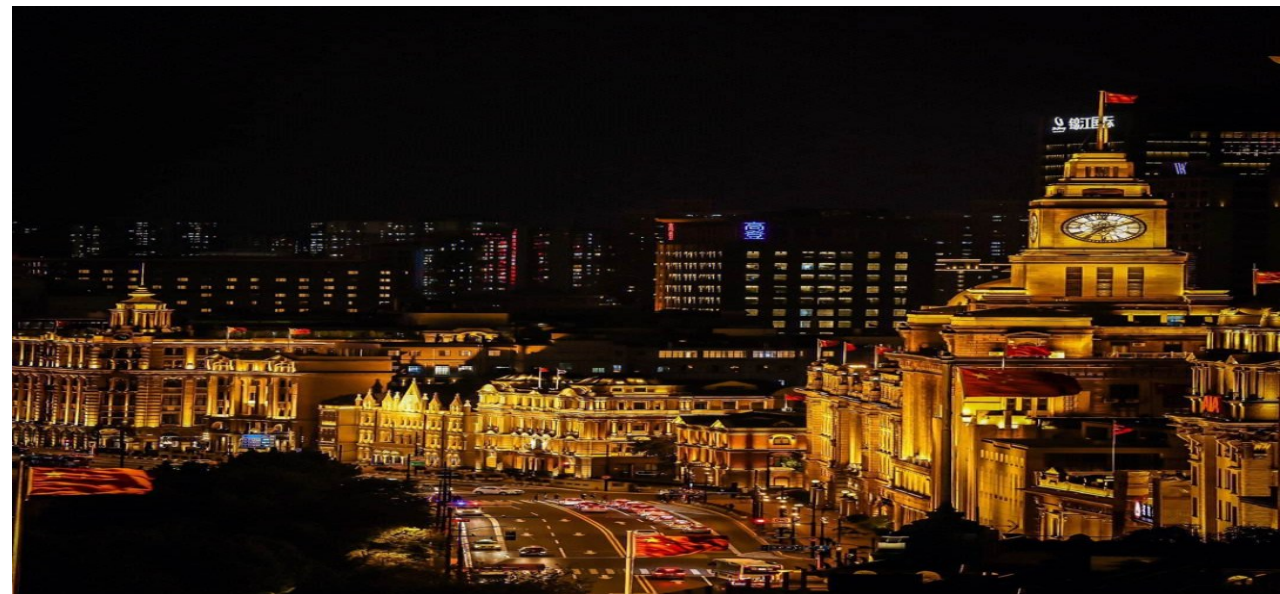
Mr. Shijie Wang

Mr. Yi Li

Ms. Beiqi Wang



# Welcome to Shanghai and SJTU!



# Thank for your attention

[tongliu@sjtu.edu.cn](mailto:tongliu@sjtu.edu.cn)





**Václav Bouček**

UJP

## **Behavior of Fuel Cladding with Cr Coating during LOCA and Study of Oxygen Diffusion into Zr-alloy using Different methods**

The advancement of Accident Tolerant Fuel (ATF) technologies is critical for enhancing the safety of nuclear reactors under accident conditions. Chromium (Cr) coatings on conventional zirconium alloys have been identified as the most promising near-term ATF concept due to their high-temperature resistance to oxidation. However, the presence of Cr influences the solubility of oxygen in the zirconium alloy, which can influence the mechanical properties and potentially lead to fuel cladding failure at unanticipated temperatures.

The presentation deals with the oxidation behavior of damaged Cr-coated claddings under Loss-of-Coolant Accident (LOCA) scenarios, with particular emphasis on the effects of oxygen diffusion into the zirconium substrate. The protective Cr layer was locally removed to simulate coating defects, and the subsequent oxidation behavior of the exposed zirconium substrate was analyzed.

Particular attention was paid to the diffusion of oxygen into the Zr-substrate. The oxygen concentration profiles were determined using various microanalytical and spectroscopic techniques, including Electron Probe Microanalysis (EPMA), Wavelength Dispersive Spectroscopy (WDS), and Inert Gas Fusion (IGF). The results indicate that oxygen diffusion has a complex effect on the cladding microstructure and mechanical integrity.



ujp praha



# Behaviour of Fuel Cladding with Cr Coating during LOCA and Study of Oxygen Diffusion into Zr-alloy using Different methods

A. Endrychová, V. Bouček

UJP PRAHA a.s., Czech Technical University in Prague

30<sup>th</sup> International QUENCH Workshop

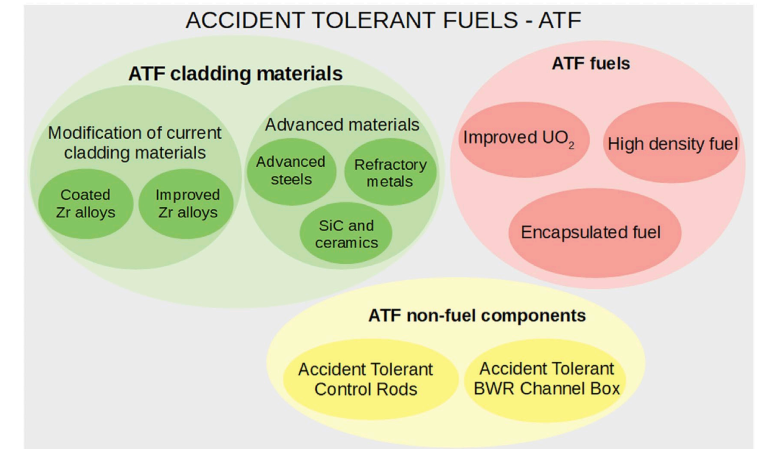
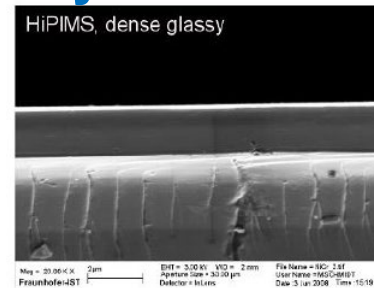
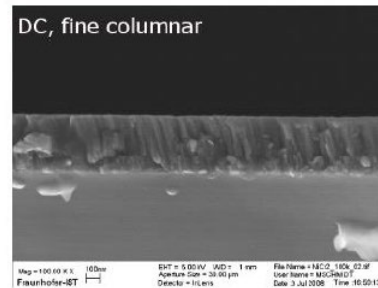
18. 12. 2025

# 1. ATF cladding concepts

- Development and testing of different concepts of **Accident Tolerant Fuels (ATFs)** - 2 concepts:

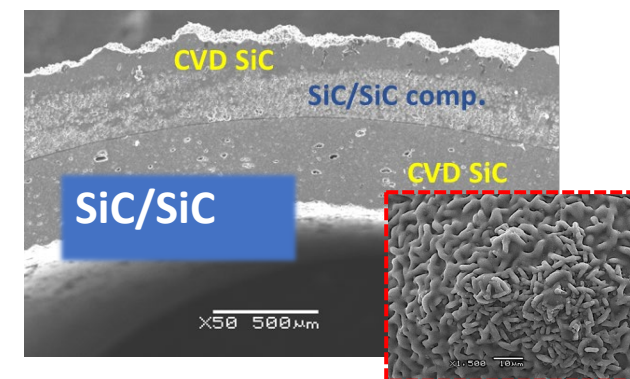
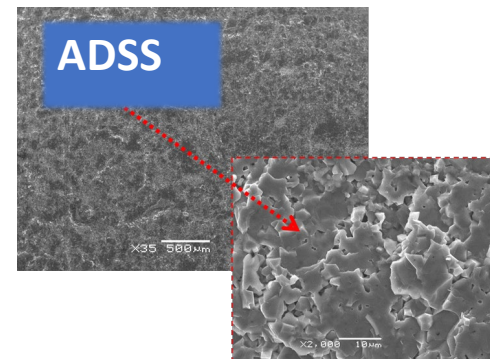
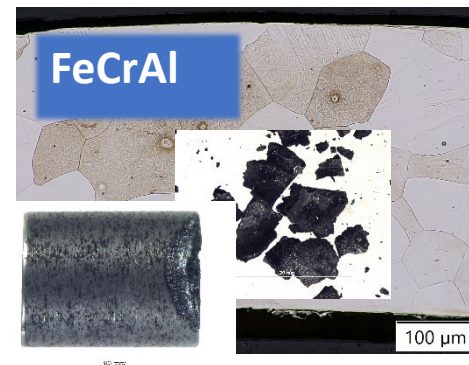
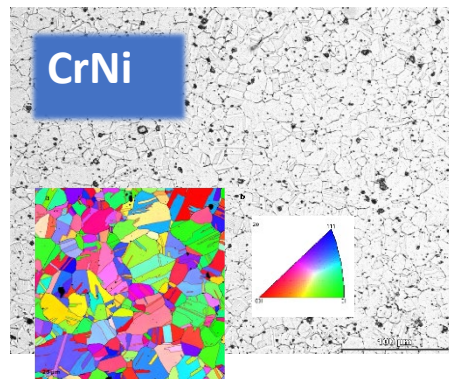
## 1. Protective coatings on zirconium-based alloys (Near Term ATF)

- Cr, CrN, CrNCr, ZrNCr
- CrNb, CrAl



ATF concepts[1]

## 2. „New“ materials (Longer Term ATF)



## 2. Zr-alloy with Cr coating: Diffusion

- Cr coating as **the most promising near-term concept**:
  - Already being tested in commercial reactors in Europe and the USA (Framatome – Gösgen in Switzerland, Westinghouse – Doel 4 in Belgium and Byron 2 in the United States).
- During oxidation at high temperatures (1000–1300 °C), typical for a LOCA accident, **the protective coating is “consumed”** mainly in two ways:

### 1. Formation of Cr<sub>2</sub>O<sub>3</sub> oxide on the outer side of the cladding

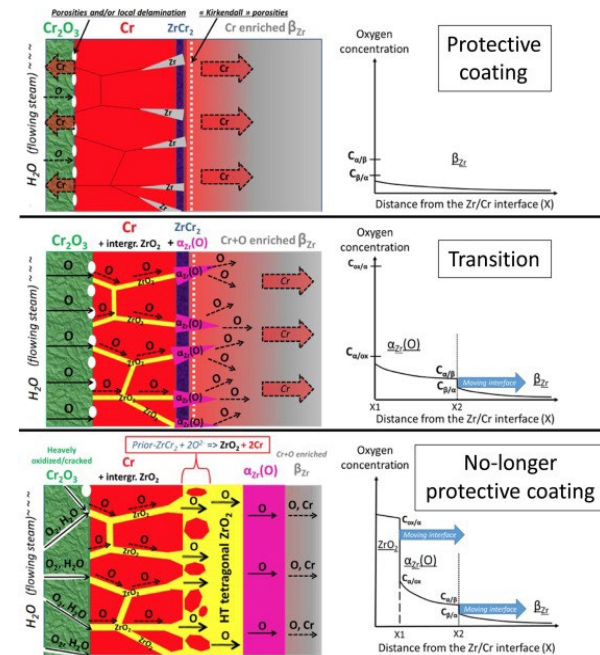
$$\Delta Cr_2O_3 = \sqrt{K_p(Cr_2O_3) \cdot t}$$

### 2. Diffusion of Cr into Zr-alloy

$$\Delta Cr_{(Cr \rightarrow \beta-Zr)} = 8,61 \cdot 10^3 \cdot \exp\left(\frac{-17166}{T}\right) \cdot t^{1/2}$$



Zr-alloy with protective coating - 1200°C/30 min

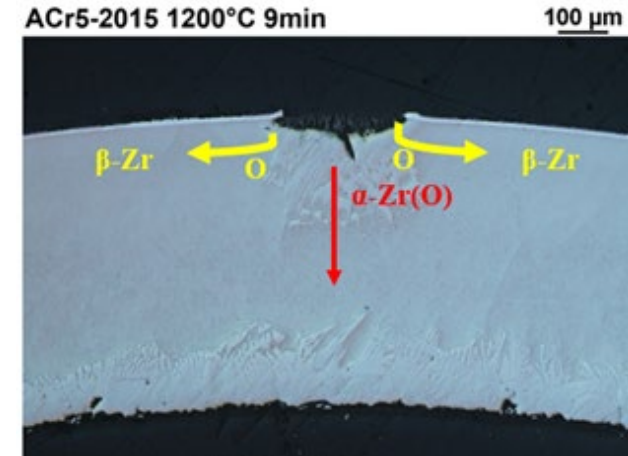
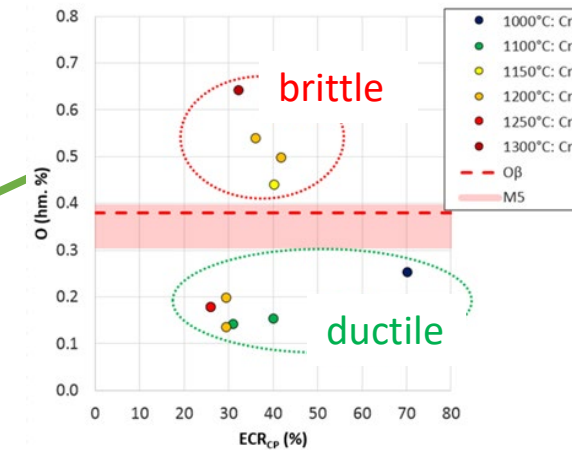


Diffusion of Cr [4]

## 2. Zr-alloy with Cr coating: Diffusion

- **Assumption:** Cr is a  $\beta$ -stabilizer, and oxygen diffusion in  $\beta$ -Zr proceeds significantly faster -> The presence of Cr increases the oxygen solubility limit in  $\beta$ -Zr, which can **negatively impact the ductility and brittleness of the material**
- **Criterion " $O_{\beta}$ " based on the critical oxygen concentration** in the original  $\beta$ -phase, which is crucial for determining the ductility of the samples. (The limit value - 0.38 wt.%)
- Most studies focus on a compact Cr layer, but regarding a **damaged coating:**
  - A new testing methodology for „damaged coating“ will be developed -> monitoring of O and Cr diffusion
  - Pseudobinary phase diagram (Cr-Zr1Nb)-O

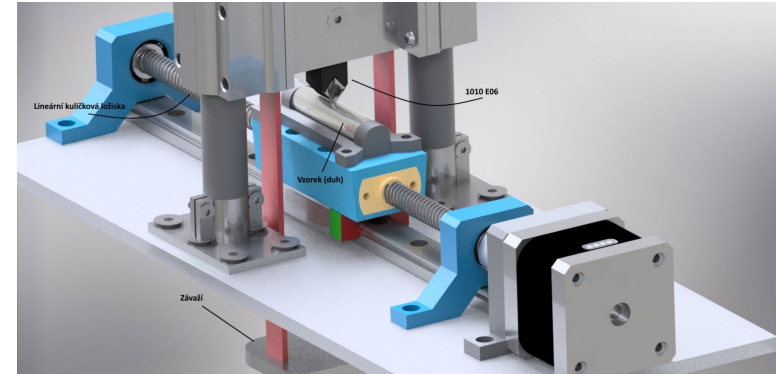
Dependence of oxygen content on ECR[47]





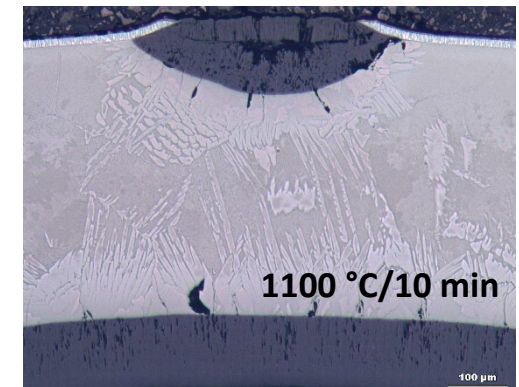
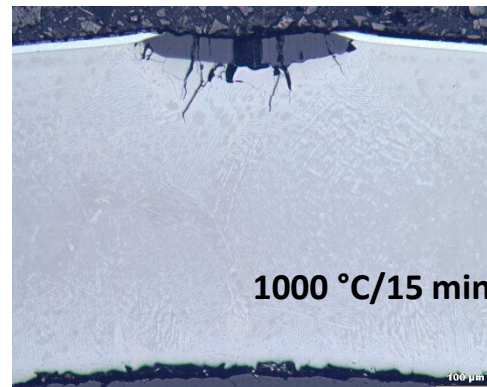
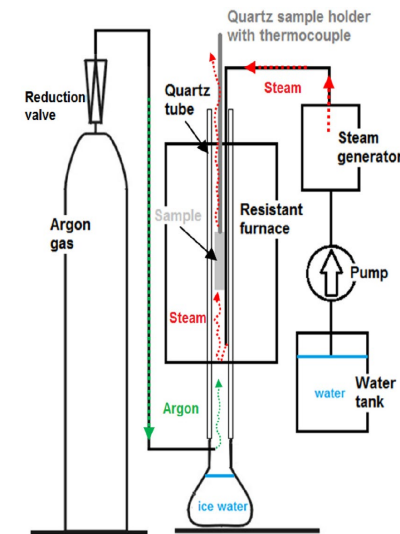
## 3. Construction of diagram (Cr-Zr1Nb)-O: Method

1. Introduce a controlled defect into the Cr-coated sample
2. Partially dissolve the Cr layer into the substrate
3. Perform the high-temperature oxidation test
4. Measure oxygen equilibrium concentrations using WDS (EPMA)
5. Optionally analyze oxygen concentration using SIMS or IGF (TEA)
6. Use the obtained concentrations to estimate phase boundaries
7. Construction of (Cr+Zr1Nb)-O diagram



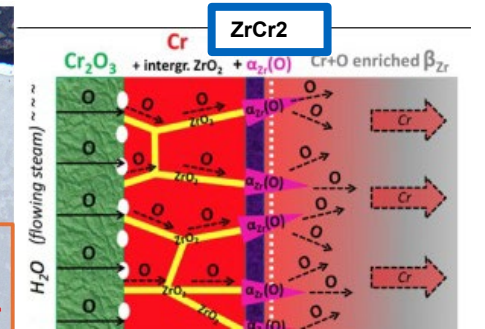
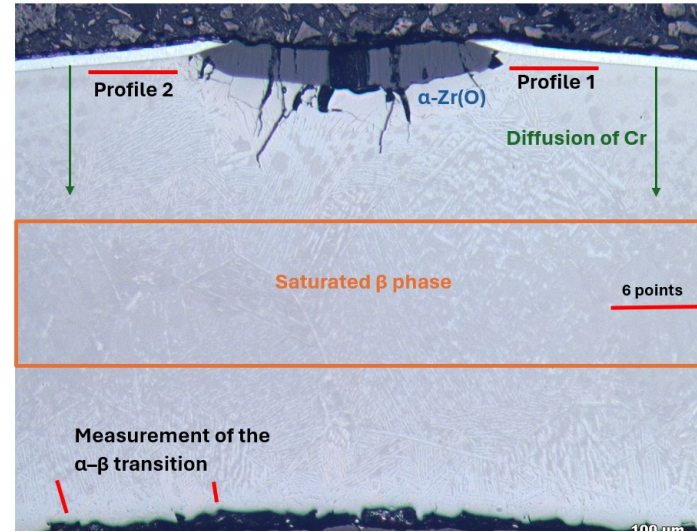
## 3. Construction of diagram (Cr-Zr1Nb)-O: Method

1. Introduce a controlled defect into the Cr-coated sample
2. **Partially dissolve the Cr layer into the substrate (1200 °C/4,5 min, Ar)**
3. **Perform the high-temperature oxidation test (1000, 1100, 1200 °C Ar + steam)**
4. Measure oxygen equilibrium concentrations using WDS (EPMA)
5. Measurement of oxygen concentration using IGF (TEA)
6. Use the obtained concentrations to estimate phase boundaries
7. Construction of (Cr+Zr1Nb)-O diagram



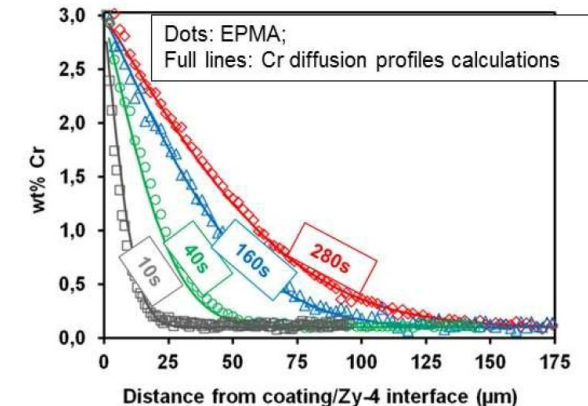
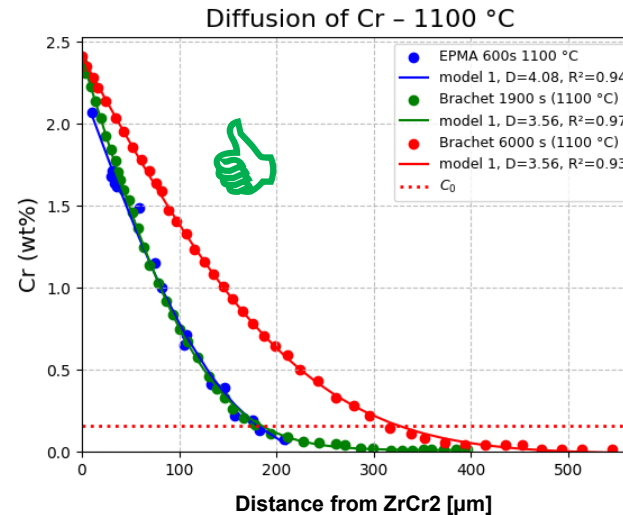
### 3. Construction of diagram (Cr-Zr1Nb)-O: Method

1. Introduce a controlled defect into the Cr-coated sample
2. Partially dissolve the Cr layer into the substrate
3. Perform the high-temperature oxidation test
4. **Measure oxygen equilibrium concentrations using WDS (EPMA, SEM-WDS)**
5. Measurement of oxygen concentration using IGF (TEA)
6. Use the obtained concentrations to estimate phase boundaries
7. Construction of (Cr+Zr1Nb)-O diagram



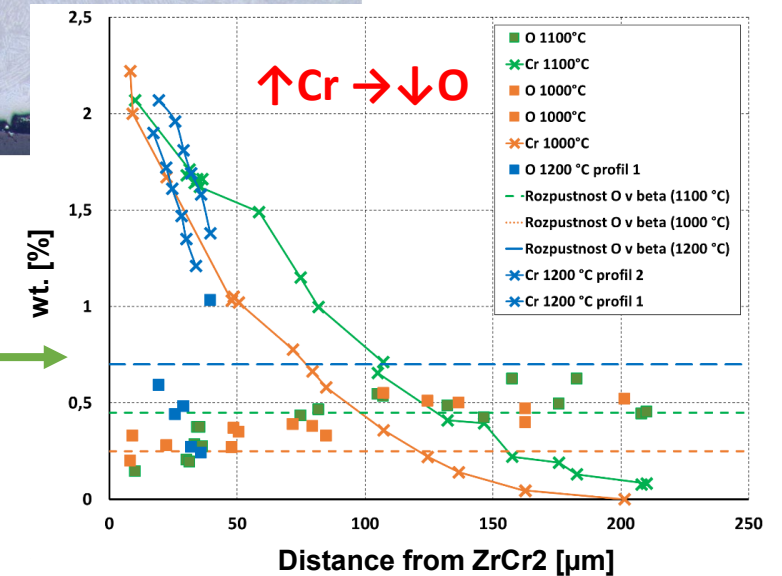
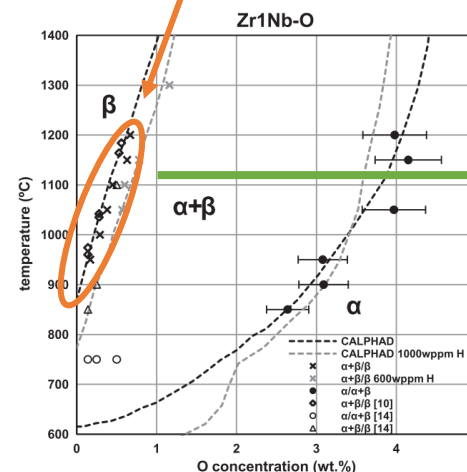
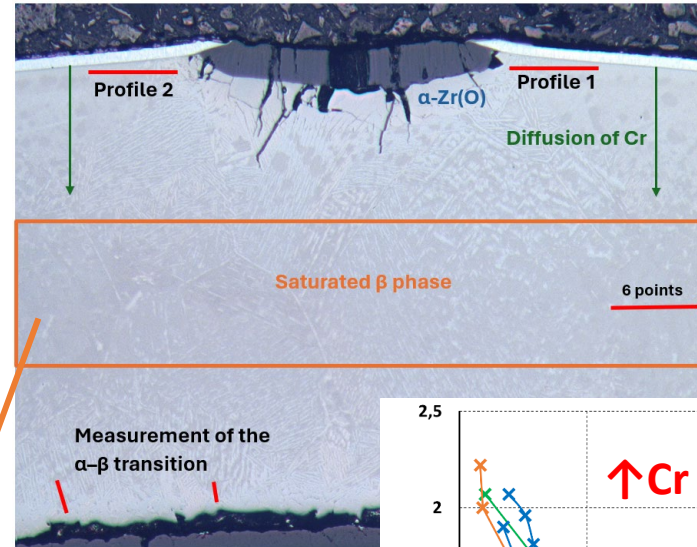
$$\frac{C(x, t) - C_0}{C_s - C_0} = 1 - \operatorname{erf}\left(\frac{x}{2\sqrt{Dt}}\right) \quad [3]$$

$$D = D_0 \cdot \left(-\exp\left(\frac{Q}{RT}\right)\right)$$



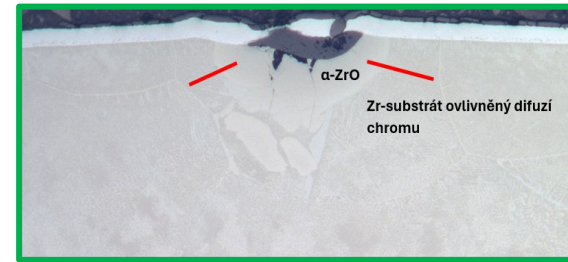
# 3. Construction of diagram (Cr-Zr1Nb)-O: Method

1. Introduce a controlled defect into the Cr-coated sample
2. Partially dissolve the Cr layer into the substrate
3. Perform the high-temperature oxidation test
4. **Measure oxygen equilibrium concentrations using WDS (EPMA, SEM-WDS)**
5. Measurement of oxygen concentration using IGF (TEA)
6. Use the obtained concentrations to estimate phase boundaries
7. Construction of (Cr+Zr1Nb)-O diagram



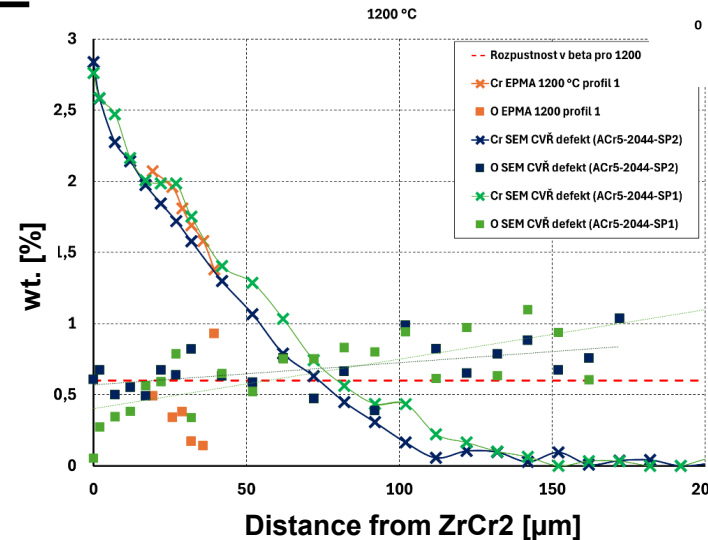
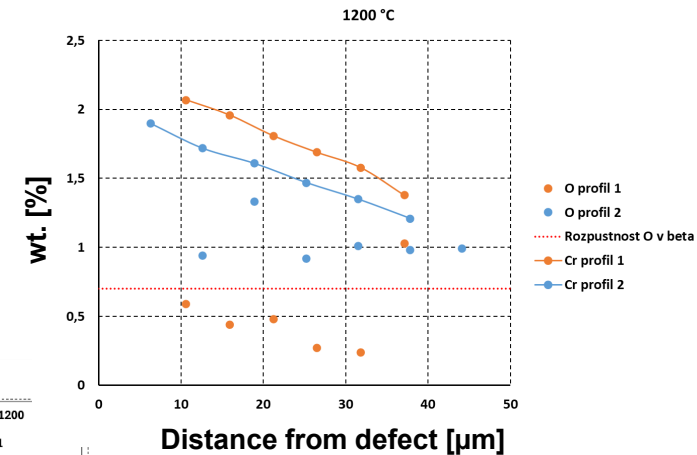
### 3. Construction of diagram (Cr-Zr1Nb)-O: Method

1. Introduce a controlled defect into the Cr-coated sample
2. Partially dissolve the Cr layer into the substrate
3. Perform the high-temperature oxidation test



#### 4. Measure oxygen equilibrium concentrations using WDS (EPMA, SEM-WDS)

5. Measurement of oxygen concentration using IGF (TEA)
6. Use the obtained concentrations to estimate phase boundaries
7. Construction of (Cr+Zr1Nb)-O diagram



↑Cr → ↓O

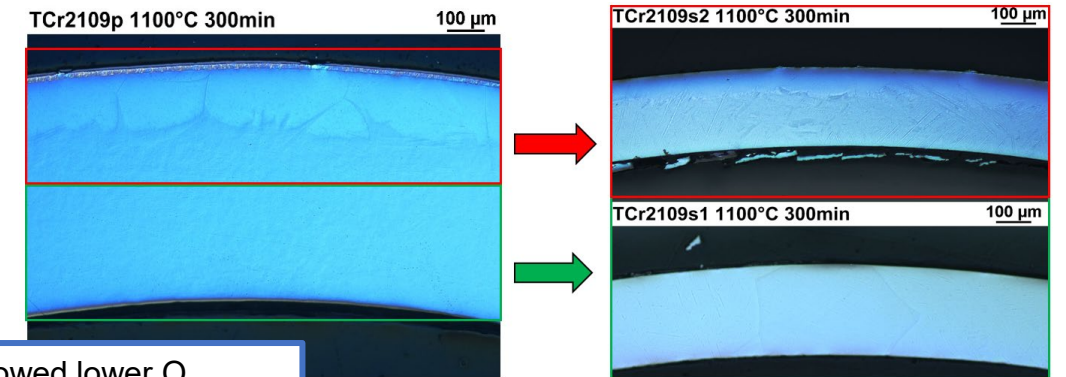
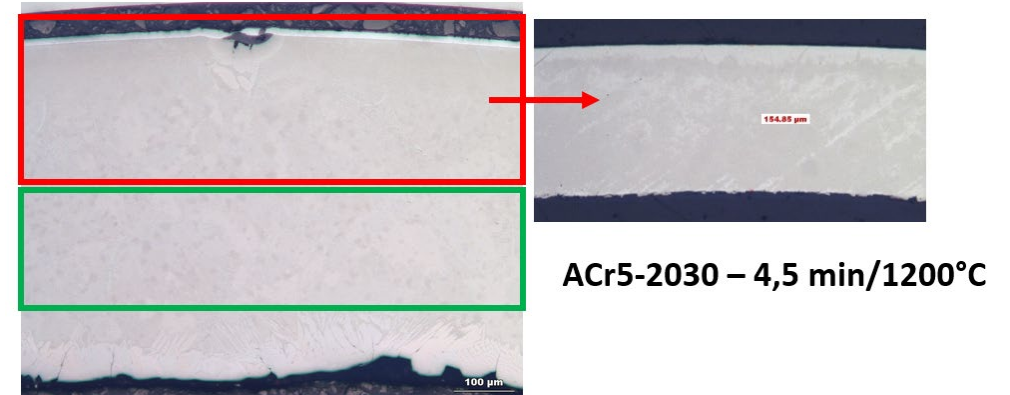
Reduced mobility of interstitial oxygen in the presence of diffused chromium, which inhibits diffusion and increases the activation energy of the diffusion process.

### 3. Construction of diagram (Cr-Zr1Nb)-O: Method

1. Introduce a controlled defect into the Cr-coated sample
2. Partially dissolve the Cr layer into the substrate
3. Perform the high-temperature oxidation test
4. Measure oxygen equilibrium concentrations using WDS (EPMA, SEM-WDS)

#### 5. Measurement of oxygen concentration using IGF (TEA)

6. Use the obtained concentrations to estimate phase boundaries
7. Construction of (Cr+Zr1Nb)-O diagram



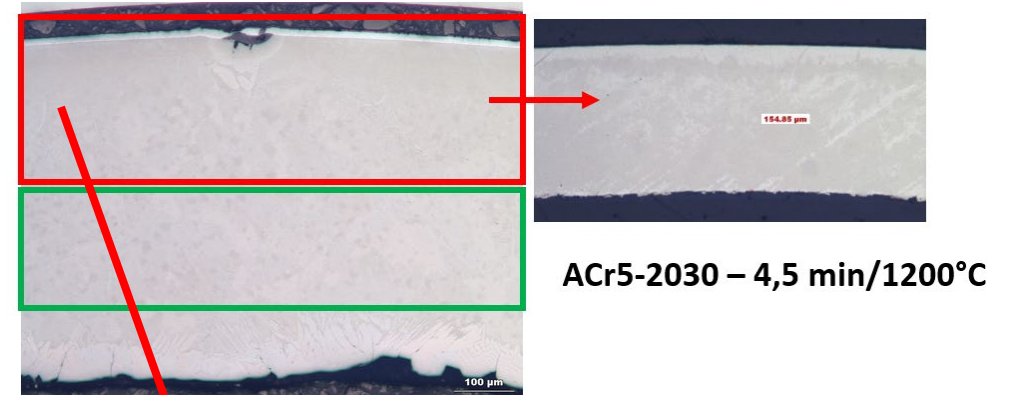
IGF results showed lower O concentrations and higher variability than EPMA, strongly dependent on **machining quality** and removal of oxide/ $\alpha$ -Zr(O)

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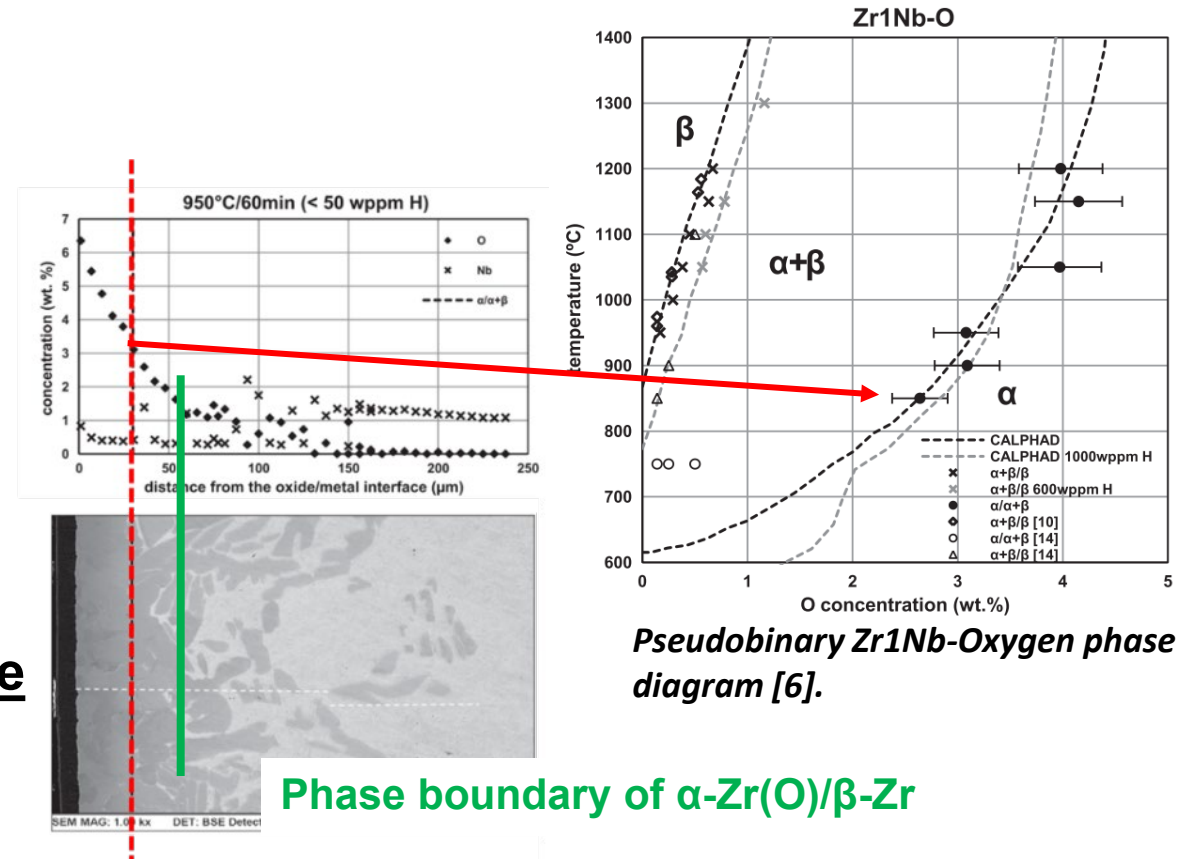


Temp [°C]	IGF [wt. %]	IGF STD	EPMA [wt. %]	EPMA STD	Diff	Eq. Conc. [wt. %]
1000	0,156	0,010	0,322	0,058	-0,166	0,25
1000	0,159	0,006	0,322	0,058	-0,163	0,25
1200	0,299	0,024	0,406	0,132	-0,107	0,70
1200	0,277	0,038	0,406	0,132	-0,128	0,70
1200	0,156	0,003	–	–	–	0,70
1200	0,338	0,012	–	–	–	0,70

IGF results showed lower O concentrations and higher variability than EPMA, strongly dependent on **machining quality** and removal of oxide/ $\alpha$ -Zr(O)

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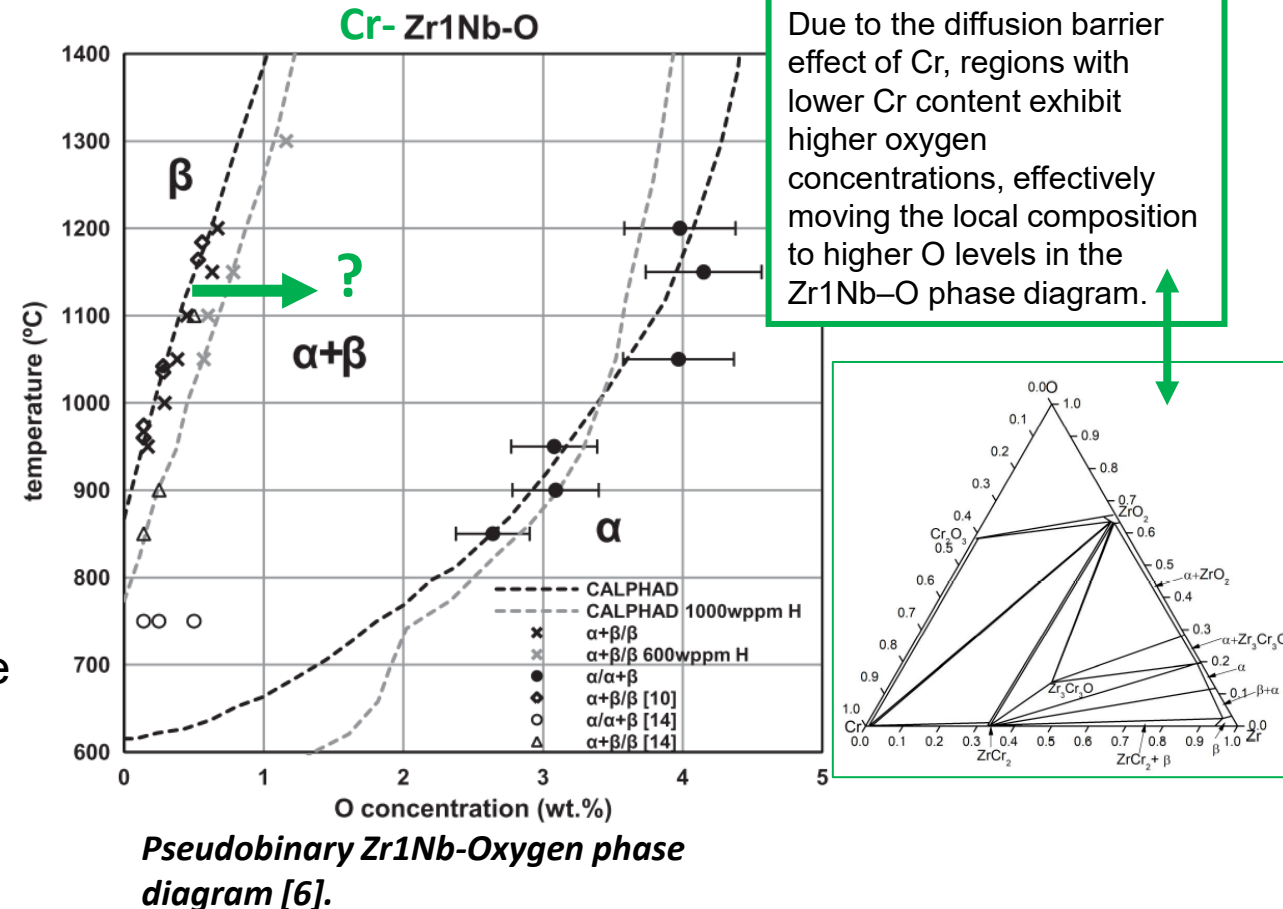




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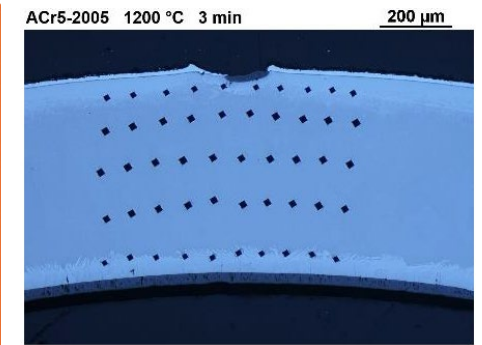
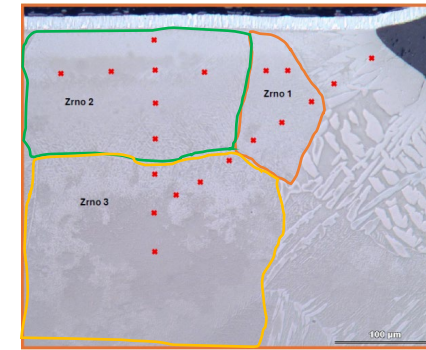
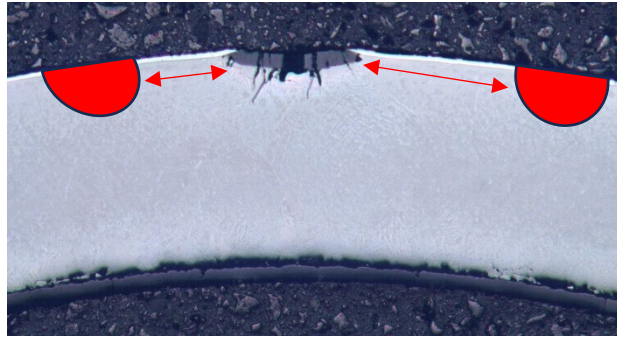
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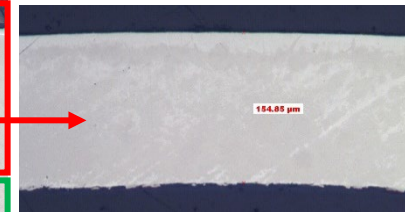
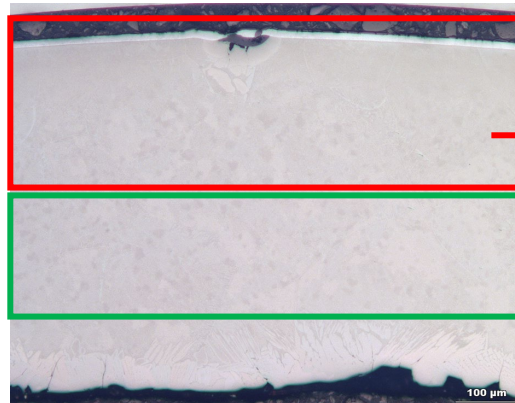


## 4. Future work

- Study of the influence of multiple defects (varying the distance between them) and potential effect of grain orientation on oxygen concentration (EBSD analysis) + microhardness measurement



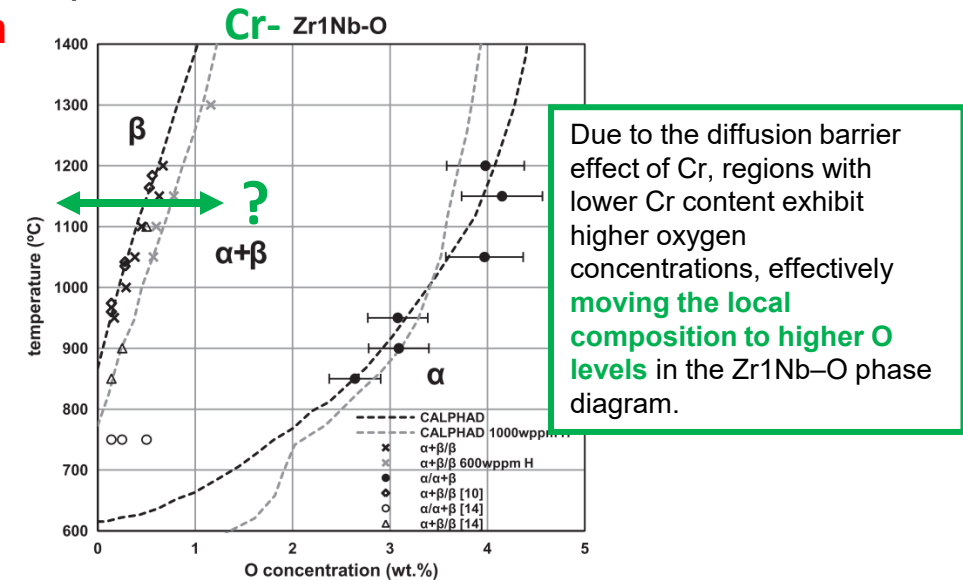
- Refinement of the IGF methodology and machining of rings with various diameters to obtain oxygen-concentration data at different depths corresponding to different Cr-concentration levels + **perform one-side high-temperature oxidation**



ACr5-2030 – 4,5 min/1200°C

## 5. Conclusion

- **WDS measurements** showed that decreasing Cr content leads to locally increased O concentration, indicating reduced O mobility and higher diffusion activation energy in the presence of diffused Cr.
- According to  $\alpha$ - $\beta$  phase-transformation theory in Zr-alloys, O strongly stabilizes the  $\alpha$  phase, while Cr stabilizes  $\beta$   $\rightarrow$  Observed **local O enrichment in low-Cr regions may shift the effective  $\alpha/\beta$  transformation conditions**, potentially promoting earlier  $\alpha$  formation inside the cladding wall during high-temperature transients.
- **IGF results** showed lower O concentrations and higher variability than EPMA, strongly dependent on **machining quality** and removal of oxide/ $\alpha$ -Zr(O) - the method is suitable mainly for comparative use.
- **For IGF, improved and standardized mechanical sample preparation** is essential—particularly control of removed-layer thickness and elimination of oxide and  $\alpha$ -Zr(O) - measurements should be conducted on samples with **varying Cr/O diffusion depths**.
- **Given the strong influence of Cr on O diffusion, this effect should be incorporated into oxygen-transport models near defects and phase boundaries**
- **Additional tests across a broader range of temperatures are required to fully evaluate the coupled Cr-O influence on diffusion and phase stability.**





**Thank you for your  
attention**

# Sources

- [1] ŠEVEČEK, Martin, Anil GURGEN, Arunkumar SESHADRI, Yifeng CHE, Malik WAGIH, Bren PHILLIPS, Victor CHAMPAGNE a Koroush SHIRVAN. Development of Cr cold spray-coated fuel cladding with enhanced accident tolerance. Nuclear Engineering and Technology [online]. 2018, 50(2), 229–236. ISSN 17385733. Dostupné z: doi:10.1016/j.net.2017.12.011
- [2] TERRANI, Kurt A. Accident tolerant fuel cladding development: Promise, status, and challenges. Journal of Nuclear Materials [online]. 2018, 501, 13–30. ISSN 00223115. Dostupné z: doi:10.1016/j.jnucmat.2017.12.043
- [3] BRACHET, Jean-Christophe, Isabel IDARRAGA-TRUJILLO, Marion Le FLEM, Matthieu Le SAUX, Valérie VANDENBERGHE, Stephane URVOY, Elodie ROUESNE, Thomas GUILBERT, Caroline TOFFOLON-MASCLET, Marc TUPIN, Christian PHALIPPOU, Fernando LOMELLO, Frédéric SCHUSTER, Alain BILLARD, Gihan VELISA, Cédric DUCROS a Frédéric SANCHETTE. Early studies on Cr-Coated Zircaloy-4 as enhanced accident tolerant nuclear fuel claddings for light water reactors.
- [4] BRACHET, Jean-Christophe, Thomas GUILBERT, Stéphane URVOY, Elodie ROUESNE, Marion PEYRET, Thierry VANDENBERGHE, Cédric PROU, Thai LE HONG a Didier HAMON. Some practical methodologies to assess the overall high temperature (one-sided) steam oxidation protectiveness of chromium-based coatings on a zirconium-based substrate, as Enhanced – Accident tolerant (Nuclear) fuels (E-ATF) claddings. Journal of Nuclear Materials [online]. 2025, 606, 155620. ISSN 00223115. Dostupné z: doi:10.1016/j.jnucmat.2025.155620
- [5] ČERVENKA, Petr, KREJČÍ, Jakub, CVRČEK, Ladislav, ROZKOŠNÝ, Vojtěch, MANOCH, František, RADA, David and KABÁTOVÁ, Jitka. EXPERIMENTAL STUDY OF DAMAGED CR-COATED FUEL CLADDING IN POST-ACCIDENT CONDITIONS. *Acta Polytechnica CTU Proceedings*. Online. 1 December 2020. Vol. 28, p. 1–7. [Accessed 8 August 2023]. DOI 10.14311/APP.2020.28.0001.
- [6] NÉGYESI, M., J. BURDA, V. KLOUČEK, J. LORINČÍK, J. SOPOUŠEK, J. KABÁTOVÁ, L. NOVOTNÝ, S. LINHART, T. CHMELA, J. SIEGL a V. VRTÍLKOVÁ. Contribution to the study of the pseudobinary Zr1Nb-Oxygen phase diagram by local oxygen measurements of Zr1Nb fuel cladding after high temperature oxidation. Journal of Nuclear Materials [online]. 2012, 420(1–3), 314–319. ISSN 00223115. Dostupné z: doi:10.1016/j.jnucmat.2011.10.022
- [7] BRACHET, Jean-Christophe, ROUESNE, Elodie, RIBIS, Joël, GUILBERT, Thomas, URVOY, Stéphane, NONY, Guillaume, TOFFOLON-MASCLET, Caroline, LE SAUX, Matthieu, CHAABANE, Nihed, PALANCHER, Hervé, DAVID, Amandine, BISCHOFF, Jérémy, AUGEREAU, Julien and POUILLIER, Edouard. High temperature steam oxidation of chromium-coated zirconium-based alloys: Kinetics and process. Corrosion Science. Online. May 2020. Vol. 167, p. 108537. [Accessed 21 August 2023]. DOI 10.1016/j.corsci.2020.108537.
- [8] GOLDNER, FRANK J., MCCAUGHEY, W, WACHS, DANIEL M., KAMERMAN, D, JENSEN, COLBY, HAYES, STEVE L., NELSON, ANDREW, HARP, JASON, CAPPS, NATHAN, LINTON, KORY, PETRIE, CHRISTIAN, SALEH, TARIK A., and WHITE, JOSHUA T. Accident Tolerant Fuels Program — Update on a National Initiative. In : *TopFuel*. Online. United States, 2021. Available from: <https://www.osti.gov/servlets/purl/1873835>.
- [9] CHUNG, H. M. a T. F. KASSNER. PSEUDOBINARY ZIRCALOY-OXYGEN PHASE DIAGRAM. Journal of Nuclear Materials. 1979, 84, 327–339.



## Acknowledgements

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- Project No. TN02000012, TS01020133



**Brock Nowak**

Queen's University

## **High-Temperature Oxidation of Cr Coated Claddings with Interdiffusion Barrier & Solute (Al, Si) Additions**

Accident Tolerant Fuels (ATFs) are a proposed advanced reactor technology that aims to increase safety margins during anticipated operational occurrences (AOOs), and severe loss-of-coolant accidents (LOCA). Coated zirconium alloy claddings (CZACs) are one class of ATF that aim to enhance oxidation performance while minimizing the neutronic penalty (reduced keff). Two parameters are of interest: (i) coating thickness (5 to 20  $\mu\text{m}$ ), and (ii) coating composition (Cr, MoCr, MoCrAl, MoCrSi) with or without a 150 nm Mo diffusion barrier. Coatings were deposited on Zircaloy-4 tube sections ( $h = 400\text{-}450 \mu\text{m}$ ) using magnetron sputtering. Transient and isothermal tests were performed in steam at temperatures up to 1400 °C to observe coating performance under design-basis (DBA) and beyond design-basis accident (BDBA) conditions. Oxidation rates were tracked using mass gain (microbalance, TG) up to 1250 °C or using mass spectrometry (MS) to measure hydrogen gas evolution. Results indicate reduced protection for coatings less than 10  $\mu\text{m}$  and those containing Al, and improved protection in Cr coatings doped with Si until coating breakdown occurs at 1200 °C.

# High-Temperature Oxidation of Cr Coated Claddings with Interdiffusion Barrier & Solute (Al, Si) Additions

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Brock Nowak

Ph.D. Candidate  
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E: [brock.nowak@queensu.ca](mailto:brock.nowak@queensu.ca)

Supervision:  
Suraj Y. Persaud & Zhongwen Yao







### Our Group:

Mark Daymond



Suraj Y. Persaud



Yanwen Zhang



Levente Balogh



Laurent Beland

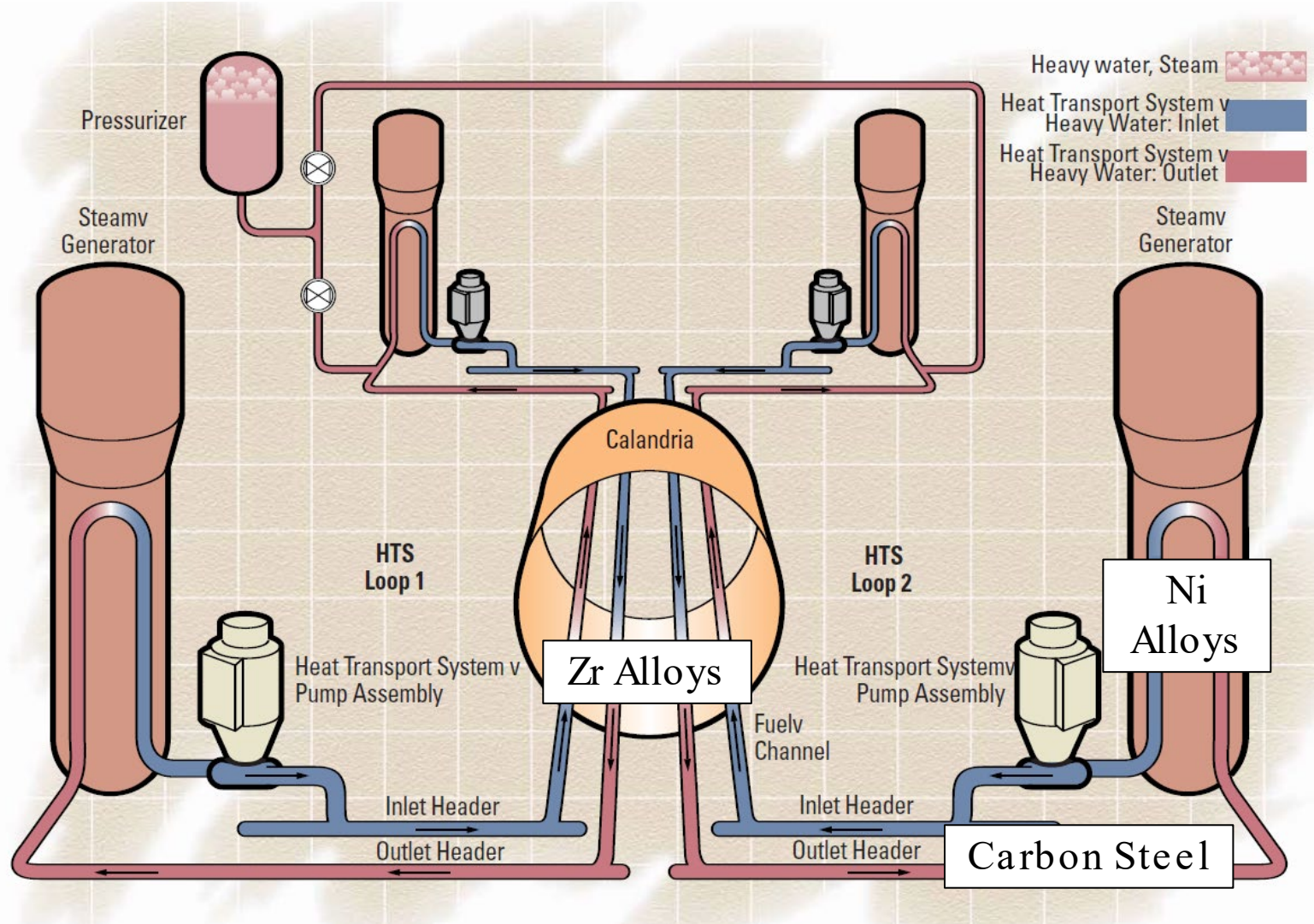


Zhongwen Yao

### Research Areas:

- Mechanics of Materials
- Corrosion Control
- Simulation & Modelling
- Irradiation Effects
- Focus on CANDU Support
- + SMR/GenIV (MSR, HTGR)

# The CANDU<sup>®</sup> Reactor



## CANDU<sup>®</sup> (PHWR) Properties

Primary Coolant: D<sub>2</sub>O (280-310 °C), 10 MPa

Chemistry: pH = ~10.2 (LiOH)

Moderator: D<sub>2</sub>O (~70 °C)

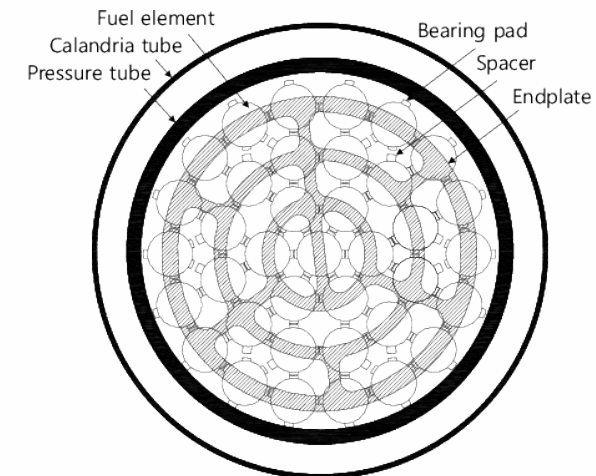
Fuel: UO<sub>2</sub> (0.71% U-235, NU)\*\*

Cladding: Zry-4 (0.4 mm) - Bundles

Pressure Tube: Zr-2.5Nb

Calandria Tube: Zry-2

Power Output: 500 – 900 MWe



CANDU<sup>®</sup> primary heat transfer system, from the CANDU<sup>®</sup>6 Technical Summary

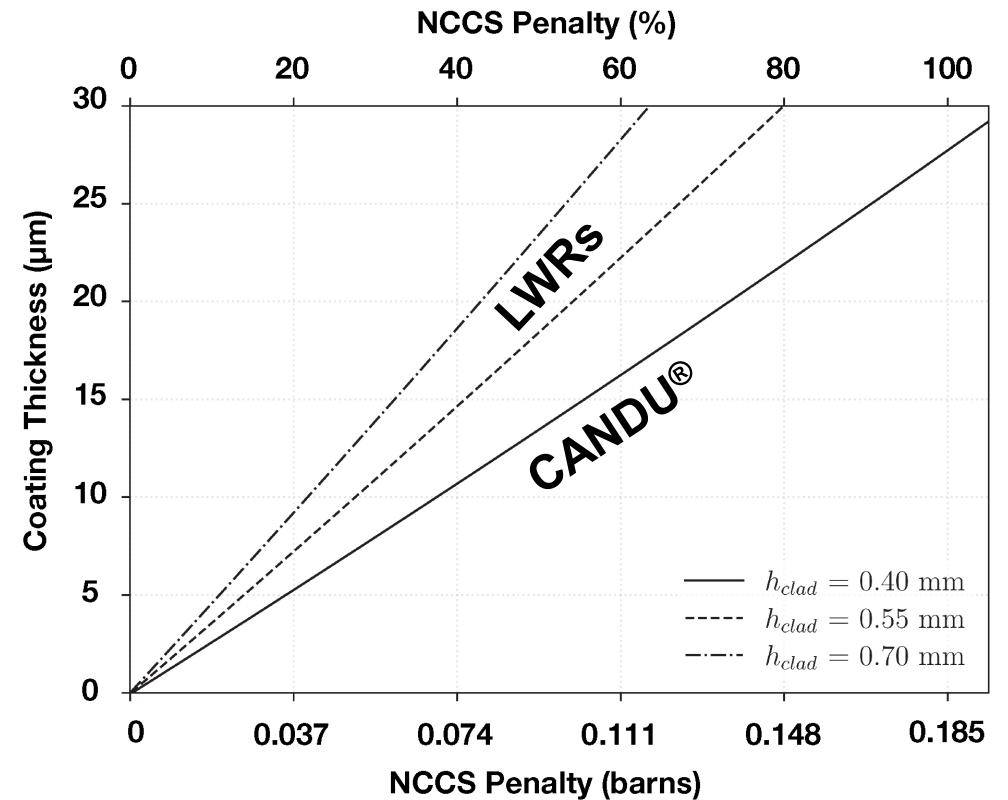
\*\* Designed with CANFlex fuel cycle flexibility

# Research Question

Can we optimize coating protectiveness vs. neutronics penalty?

## Why?

- CANDU<sup>®</sup> reactors operate on natural uranium (NU) but were designed with other fuel cycles in mind
- CANDU<sup>®</sup> fuel sheaths are 0.4 mm thick, and therefore have less cladding volume to react before failure
- Reducing the neutronic impact increases the viability for use in future CANDU<sup>®</sup> iterations

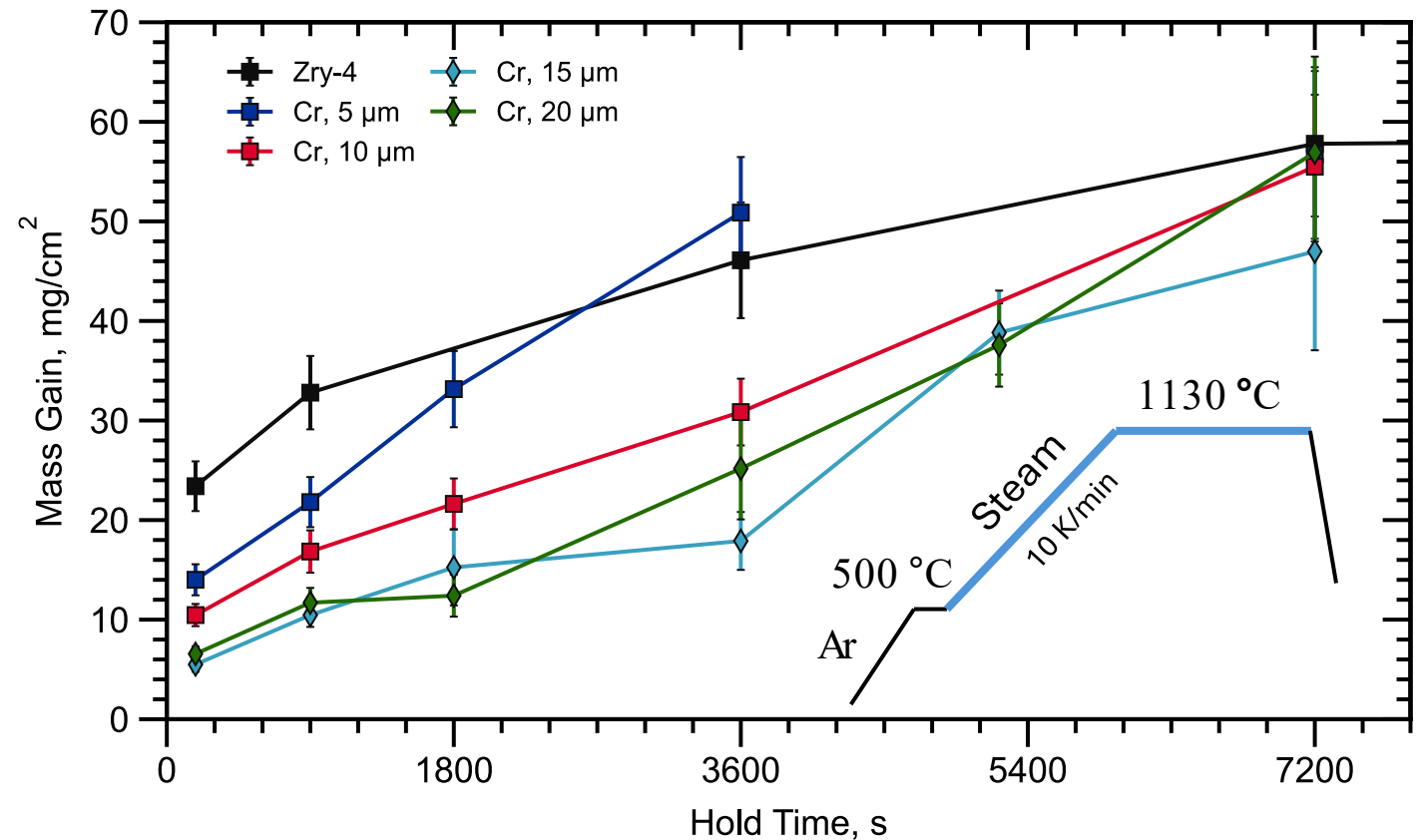
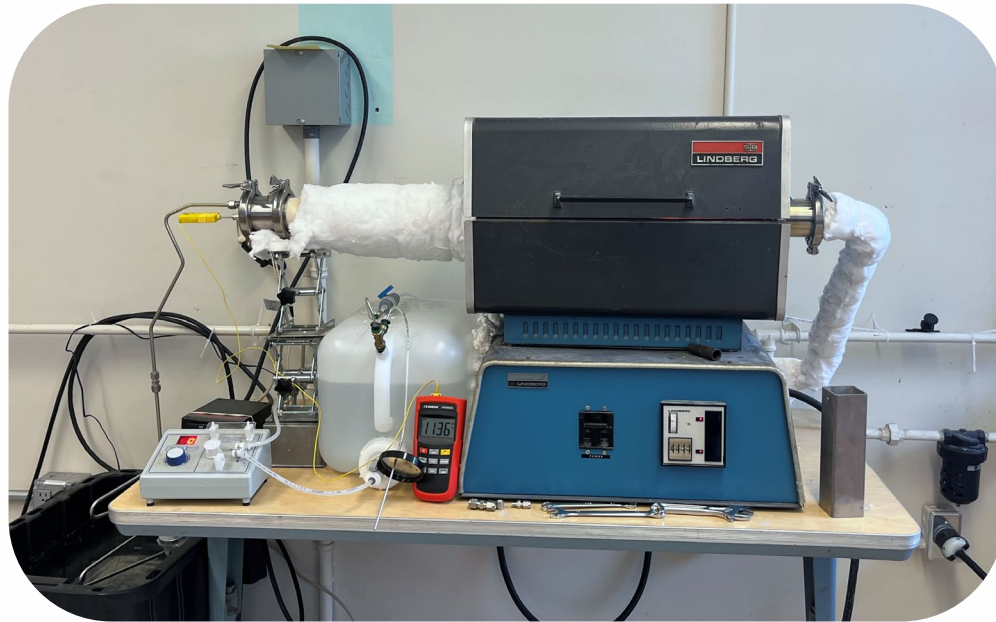


Weighted neutron capture penalty for Cr coating thickness.

# Prior study - minimum effective coating thickness

Tube Furnace 2 – TF2

Steam flow: 75 g/h (air/steam mixture)



Minimum Effective Thickness = ~10 μm

# Sample Fabrication

CSA N285.6, ASTM B350/B350M, UNS R60804

Zr	Sn	Fe	Cr	O	V
Bal.	1.2-1.7	0.18-0.24	0.07-0.13	0.09-0.16	<0.005

## 1. Materials

Zry-4 tube (15 mm OD) from Canadian Nuclear Laboratories (CNL).

## 2. Sectioning

Tubing sectioned into quadrants. Mounting hole installed.

## 3. Surface Refinement

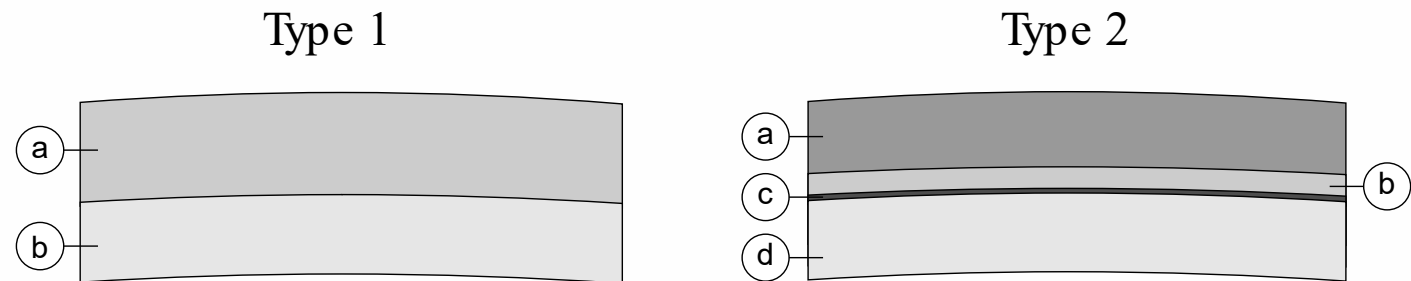
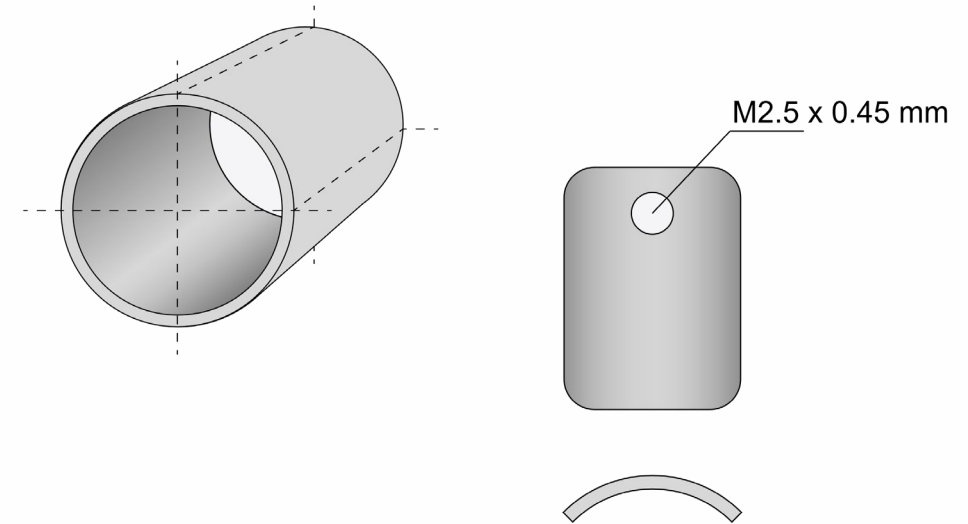
Two-stage surface refinement in vibratory tumbler:

- 1) 400 grit SiC + 600 grit Al<sub>2</sub>O<sub>3</sub>, 18 hours
- 2) 40 mesh walnut shells + diamond polish, 24 hours

## 4. Coating Process

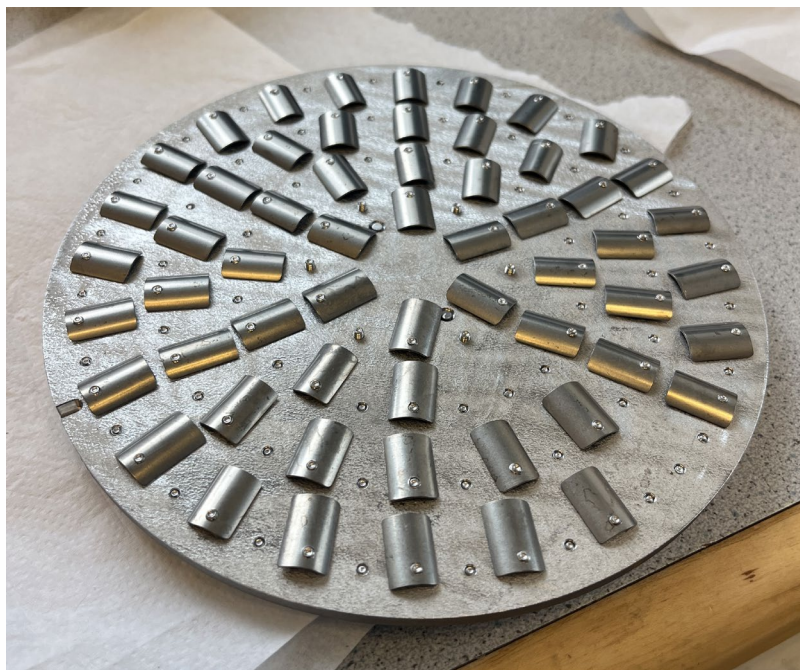
Four coating architectures, 10 μm thick:

- 1) Cr (Type 1)
- 2) Mo/Cr/Cr (Type 2)
- 3) Mo/Cr/CrAl (Type 2)
- 4) Mo/Cr/CrSi (Type 2)



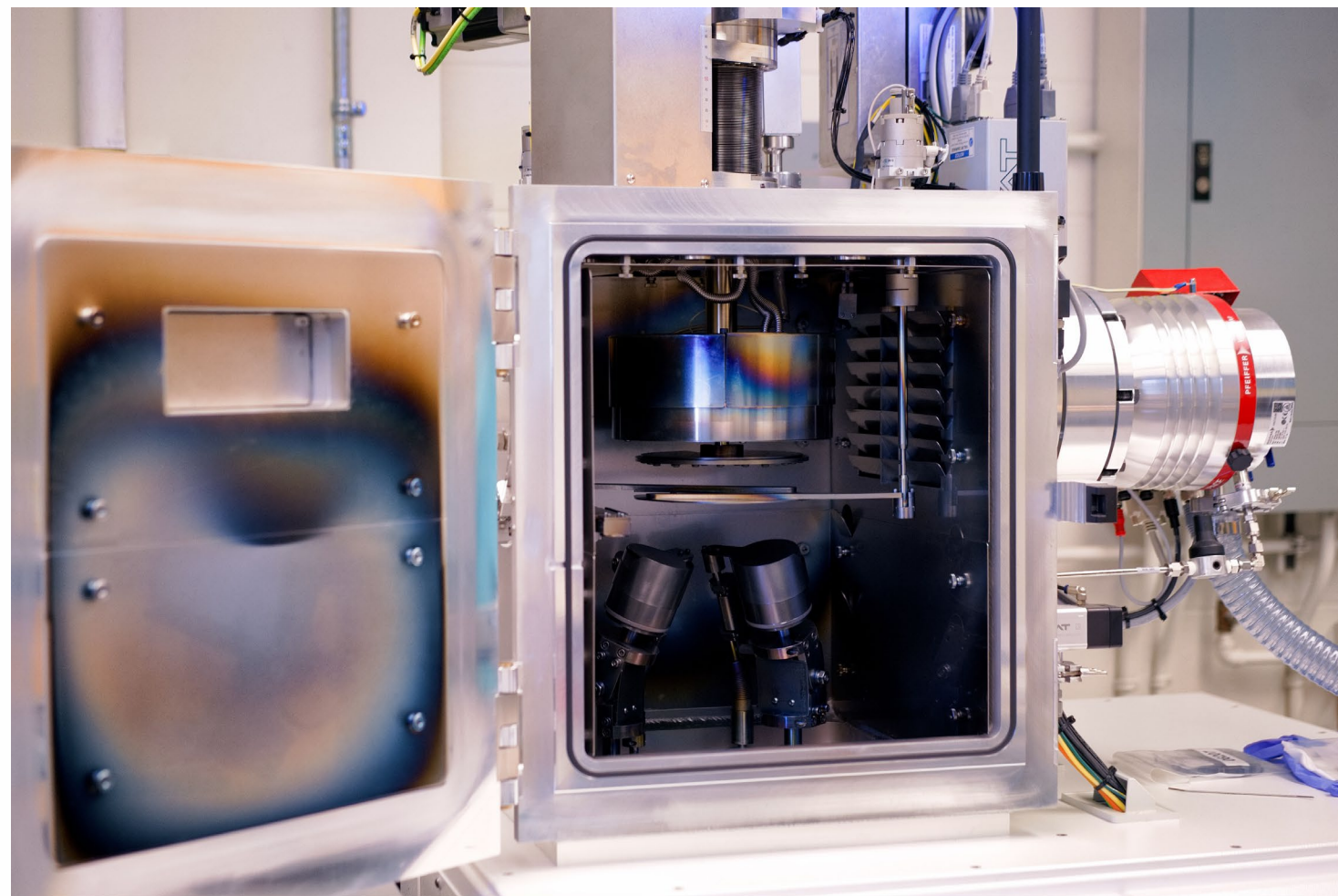
# Sample Fabrication

Dual cathode (DC, RF) magnetron sputtering  
381 °C, 5 mTorr, -60 V stage bias  
Base pressure =  $10^{-6}$  Torr



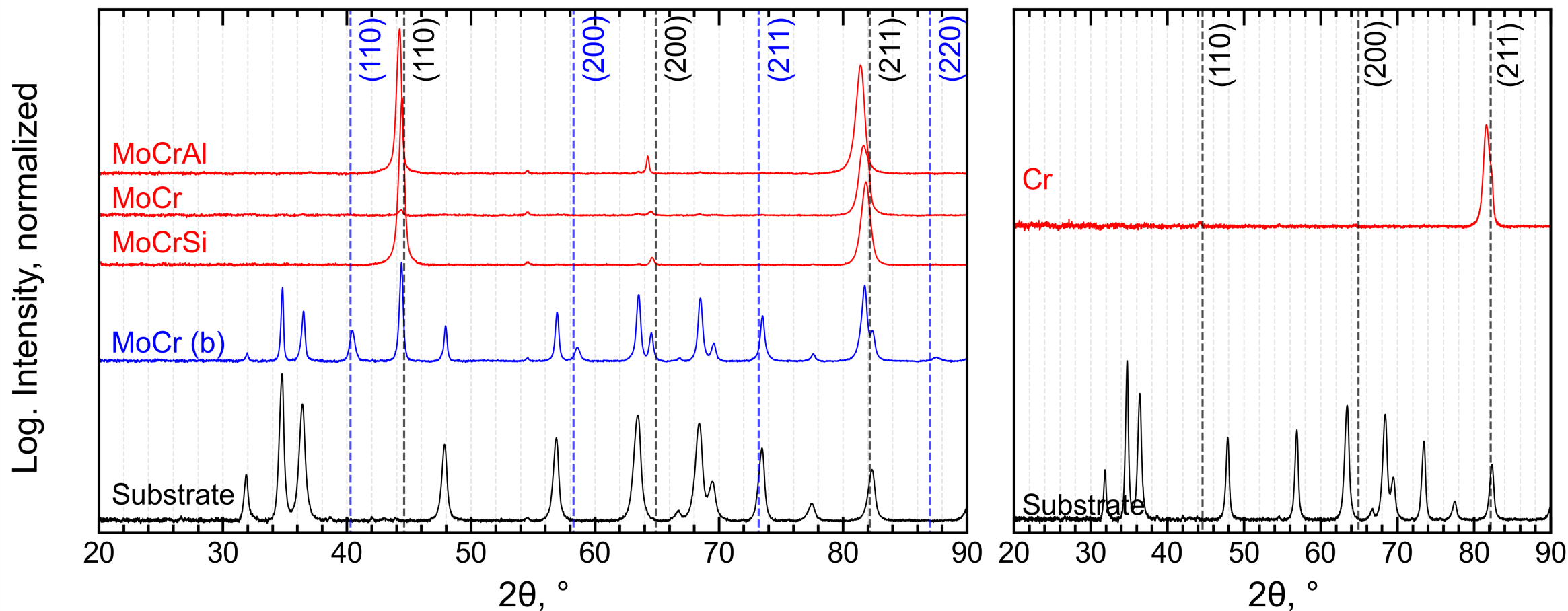
Custom Substrate Holder Plate

Angstrom Engineering NexDep, MS-PVD Chamber



# Effect of Solute Additions and Interdiffusion Barrier

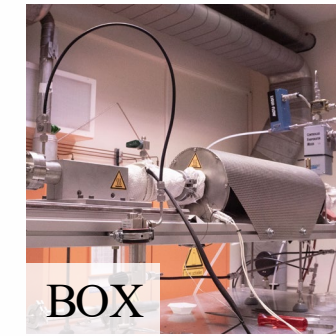
Al additions, left shift (stretched lattice) – Si additions, right shift (compressed lattice)



XRD, Rigaku SmartLab 9 kW,  $\text{CuK}\alpha_1 = 0.1506 \text{ nm}$ , parallel beam,  $20^\circ$  incidence

# Testing Matrix

- CAT1 – Isothermal Steam Oxidation (STA)
- CAT2 – Transient Steam Oxidation (STA/BOX)
- CAT3 – Transient + Hold Steam Oxidation (STA)



	Test	Zry-4	Cr	MoCr	MoCrAl	MoCrSi
CAT 1	1000 °C, 90 min	27	2.7	2.4	8.2	1.3
	1100 °C, 60 min	43	7.1	6.8	14	3.1
	1200 °C, 60 min	45	42	45	50	27
CAT 2	500-1175 °C	18	2.4	2.1	5.1	1
	500-1200 °C	21	<b>2.2</b>	2.5	6	<b>1.2</b>
	500-1225 °C	24	2.2	9	11	1.9
	500-1250 °C	25	6.9	10	16	7.2
	800-1300 °C	30	5.6	7.1	9.9	5.3
	800-1325 °C	30	7.2	9.1	15.7	12
	800-1350 °C	30	14	15	20	17
	800-1400 °C	37	26	25	30	29
CAT 3	500-1150 °C, 60 min	31	15	11	20	11
	500-1200 °C, 10 min	25	<b>6.9</b>	7.3	12	<b>1.8</b>

Mass gain – mg/cm<sup>2</sup>

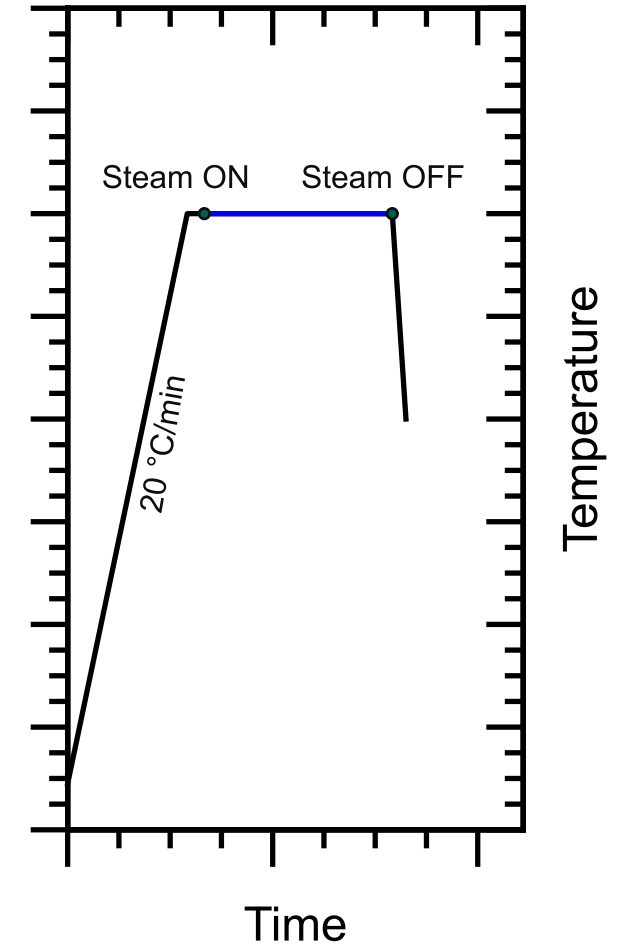
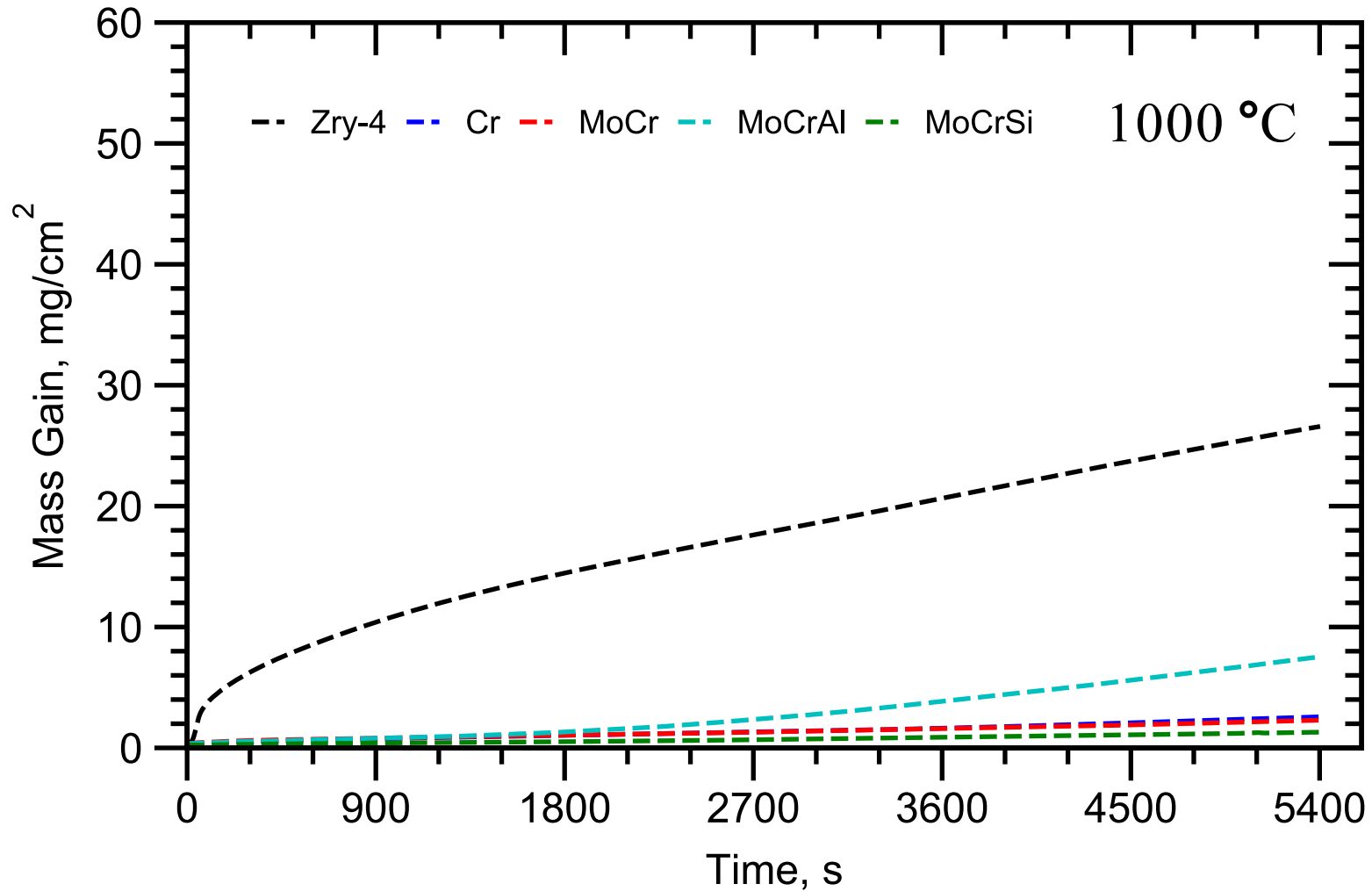


# CAT1 – Isothermal Steam Oxidation (STA)

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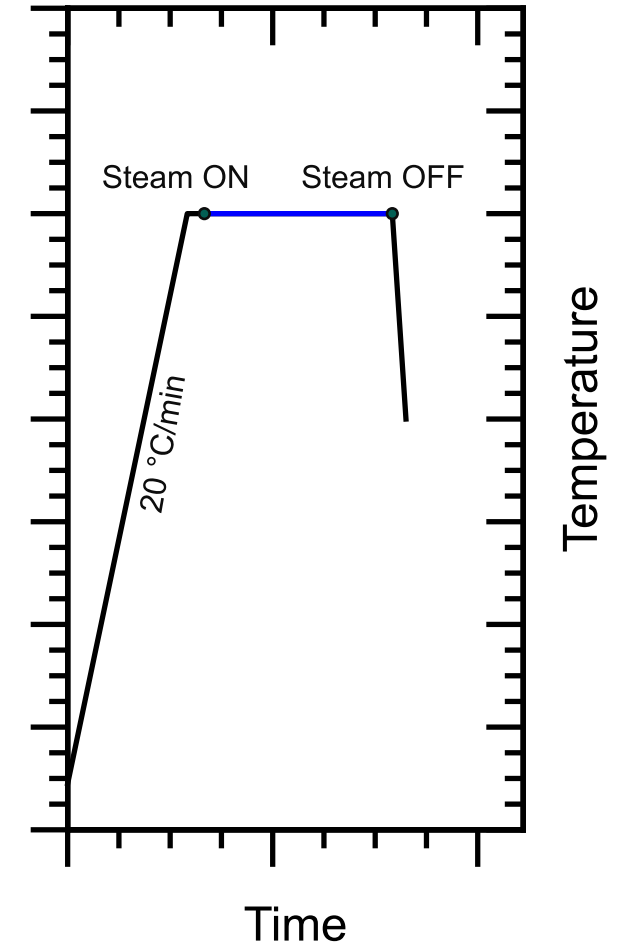
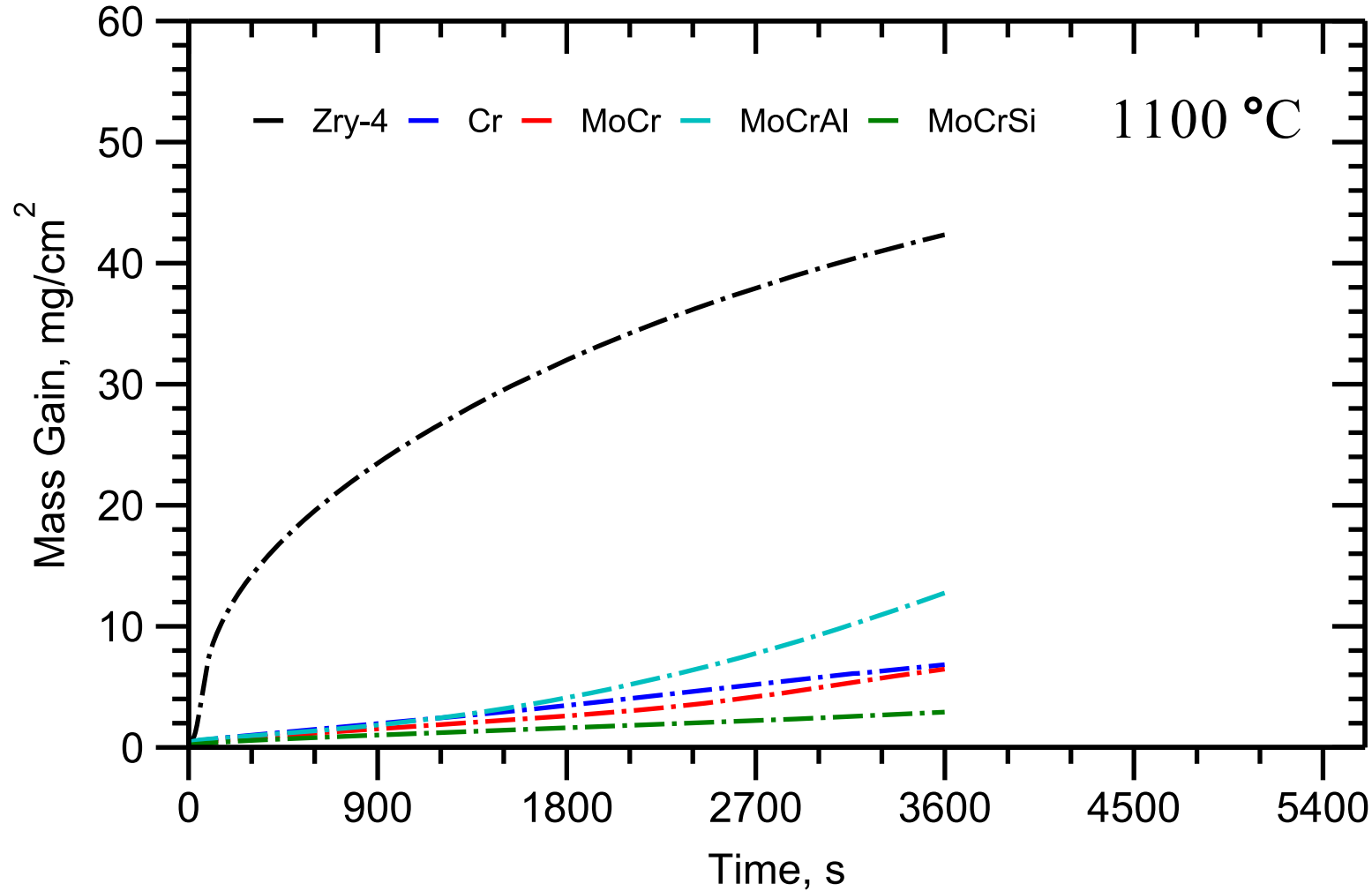
# Effect of Solute Additions and Interdiffusion Barrier

CAT1 – Isothermal Steam Oxidation (STA)



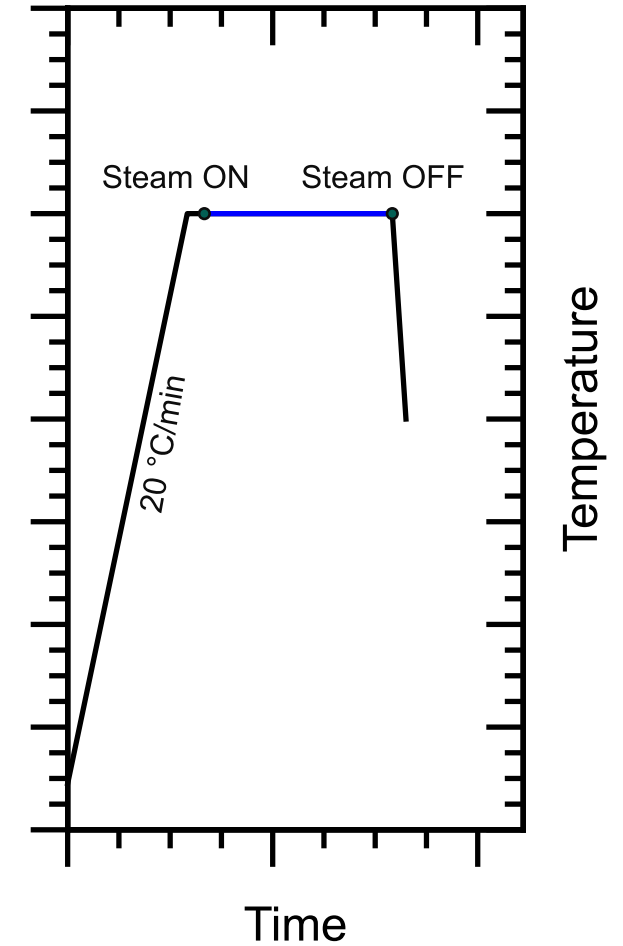
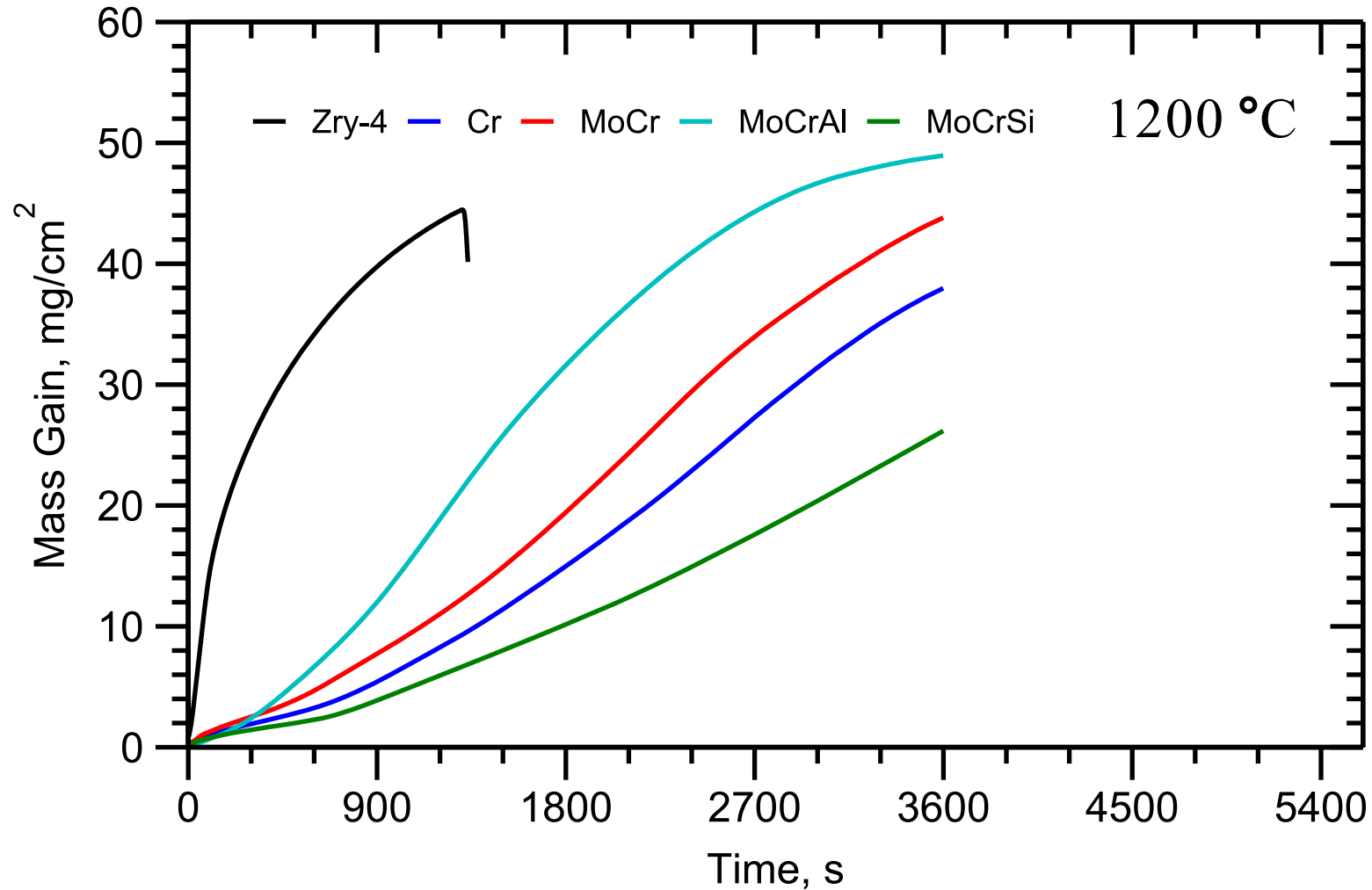
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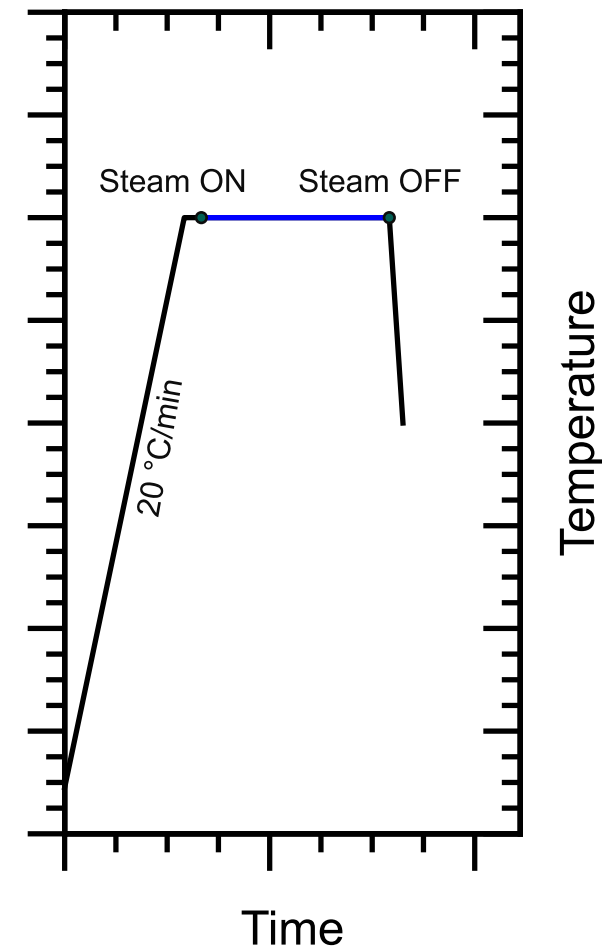
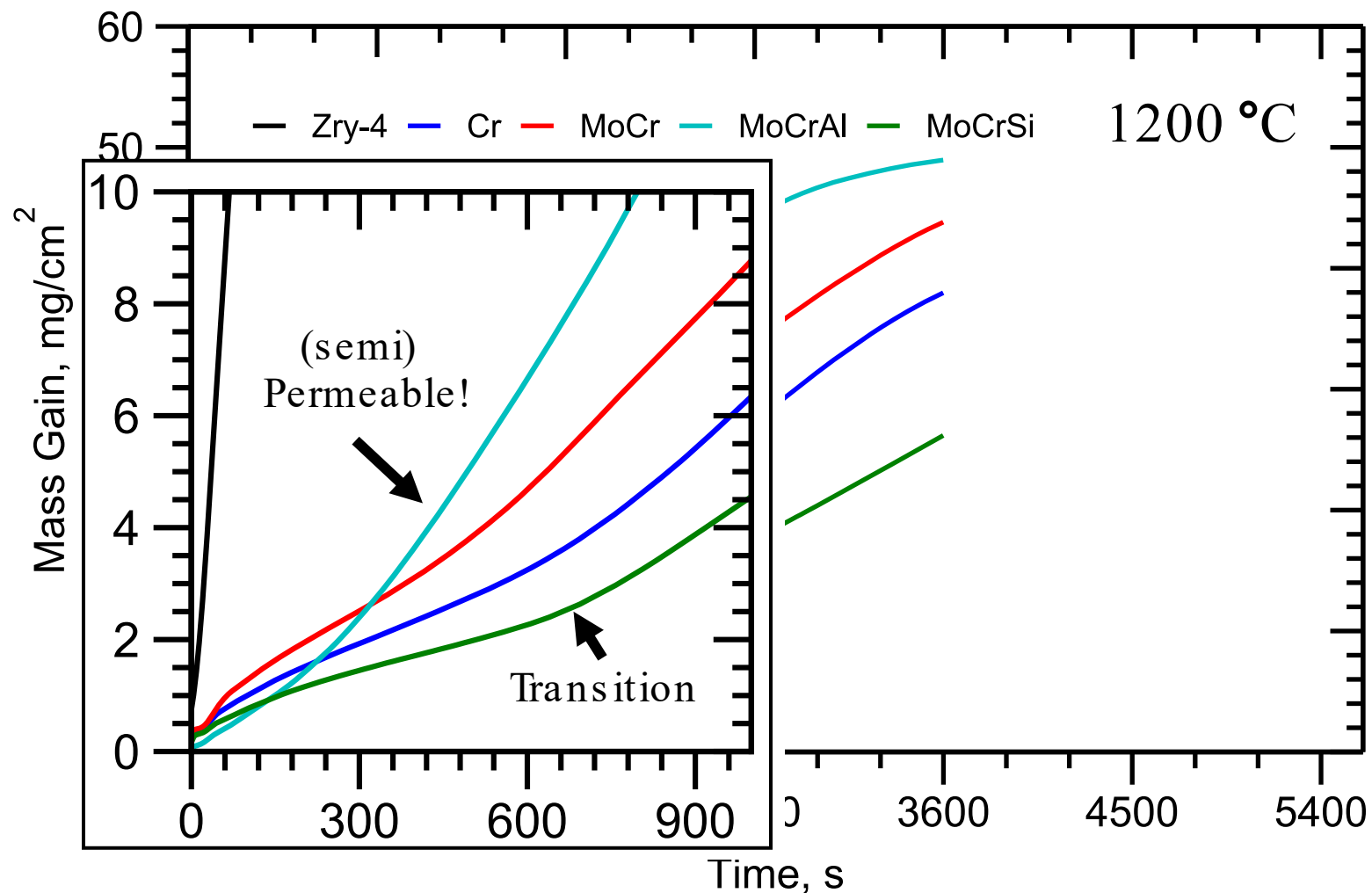
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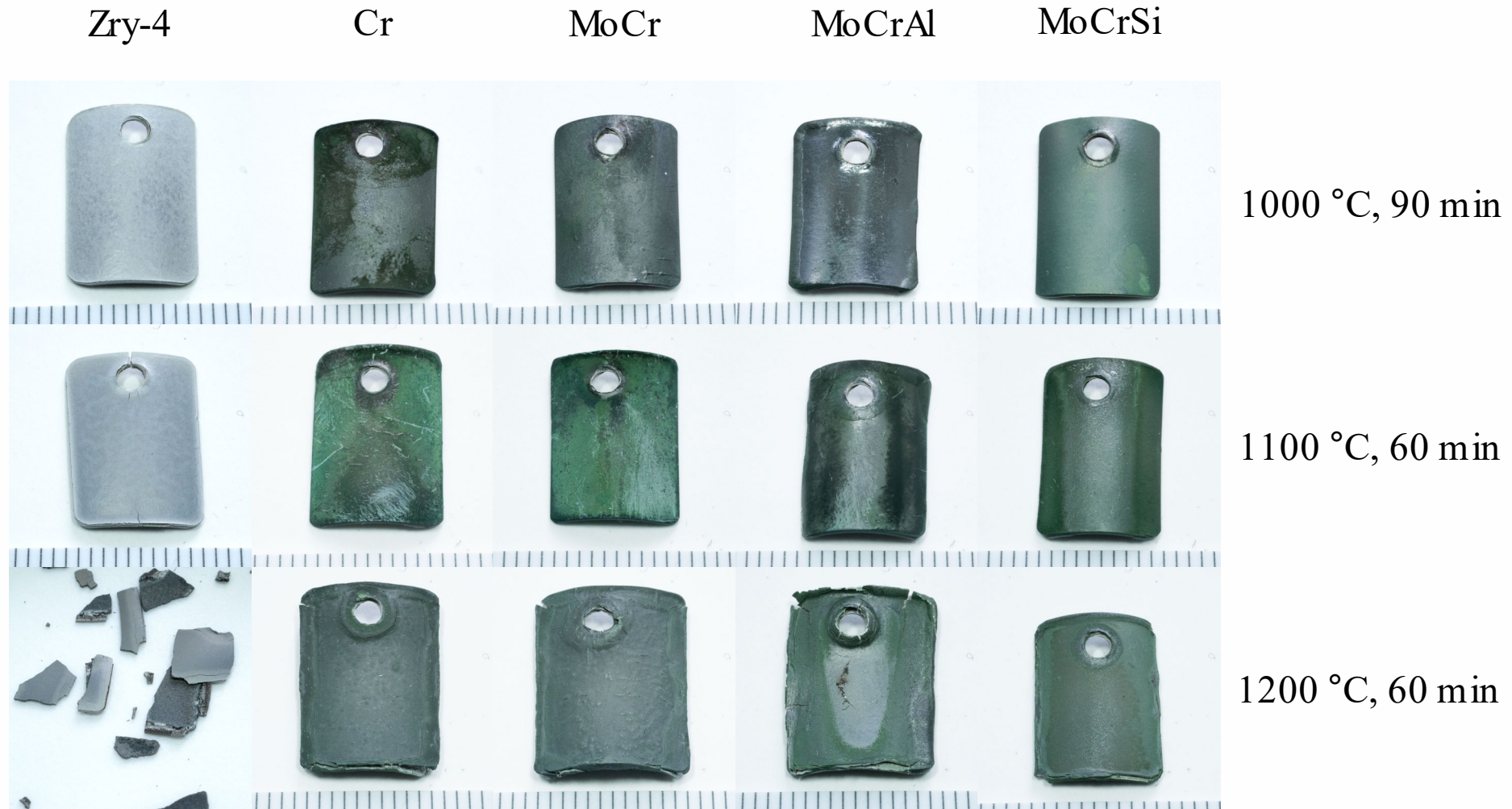
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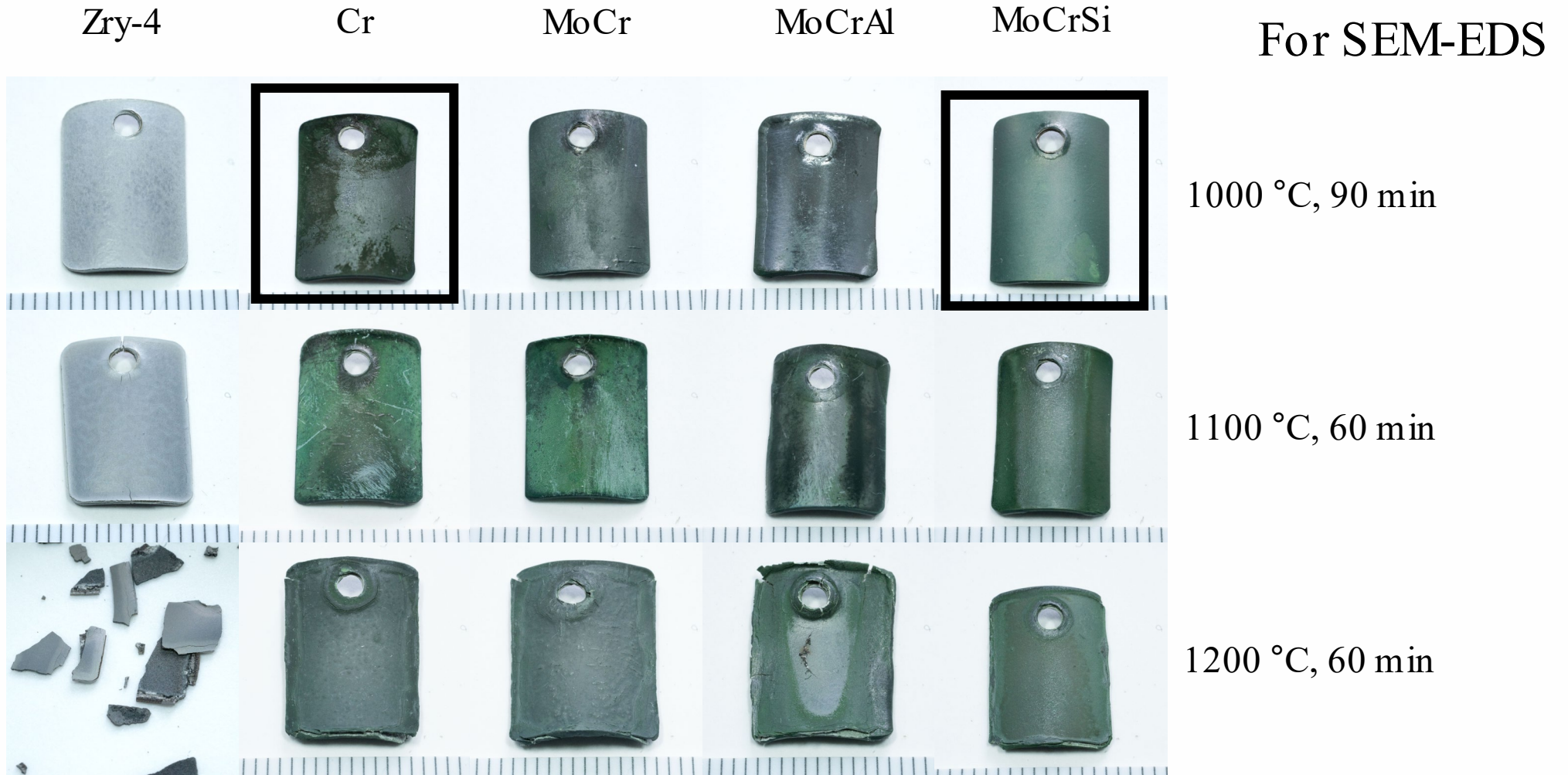
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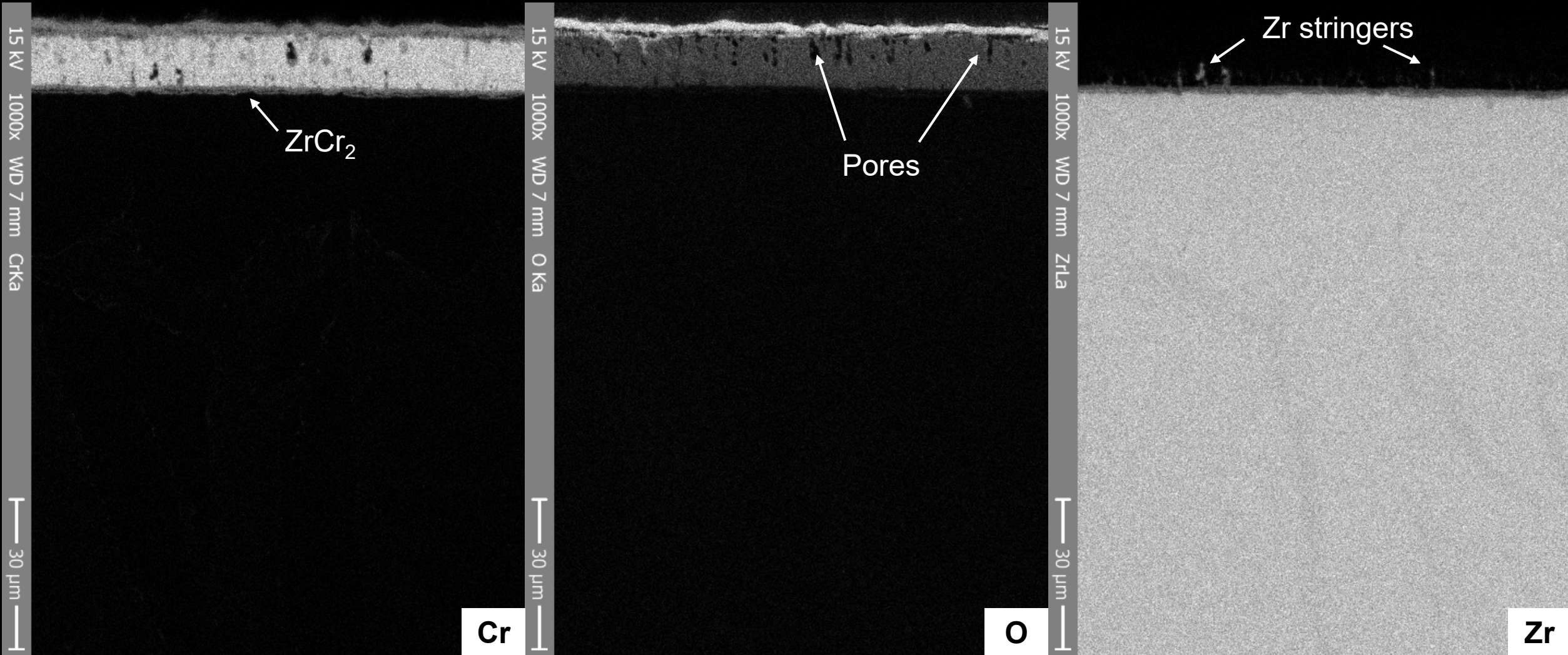


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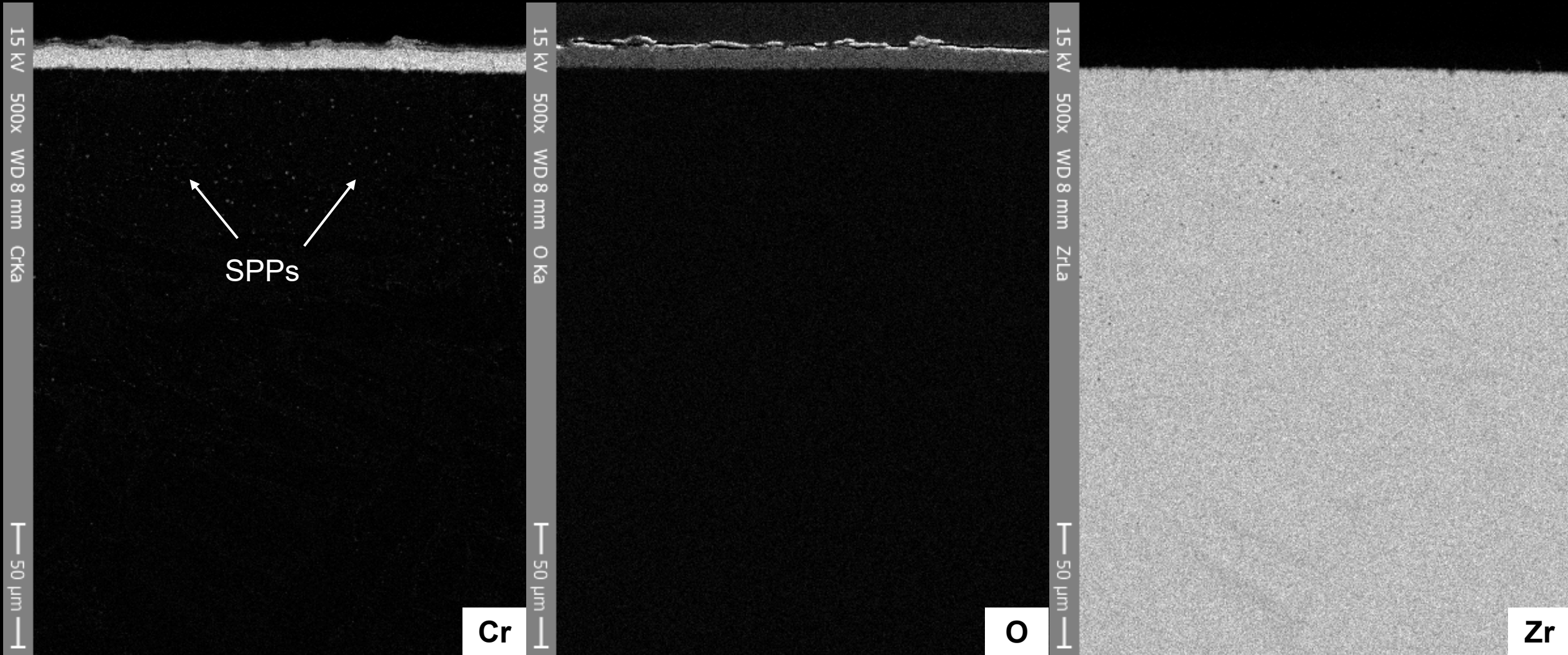


Cr, 1000 °C, 90 min

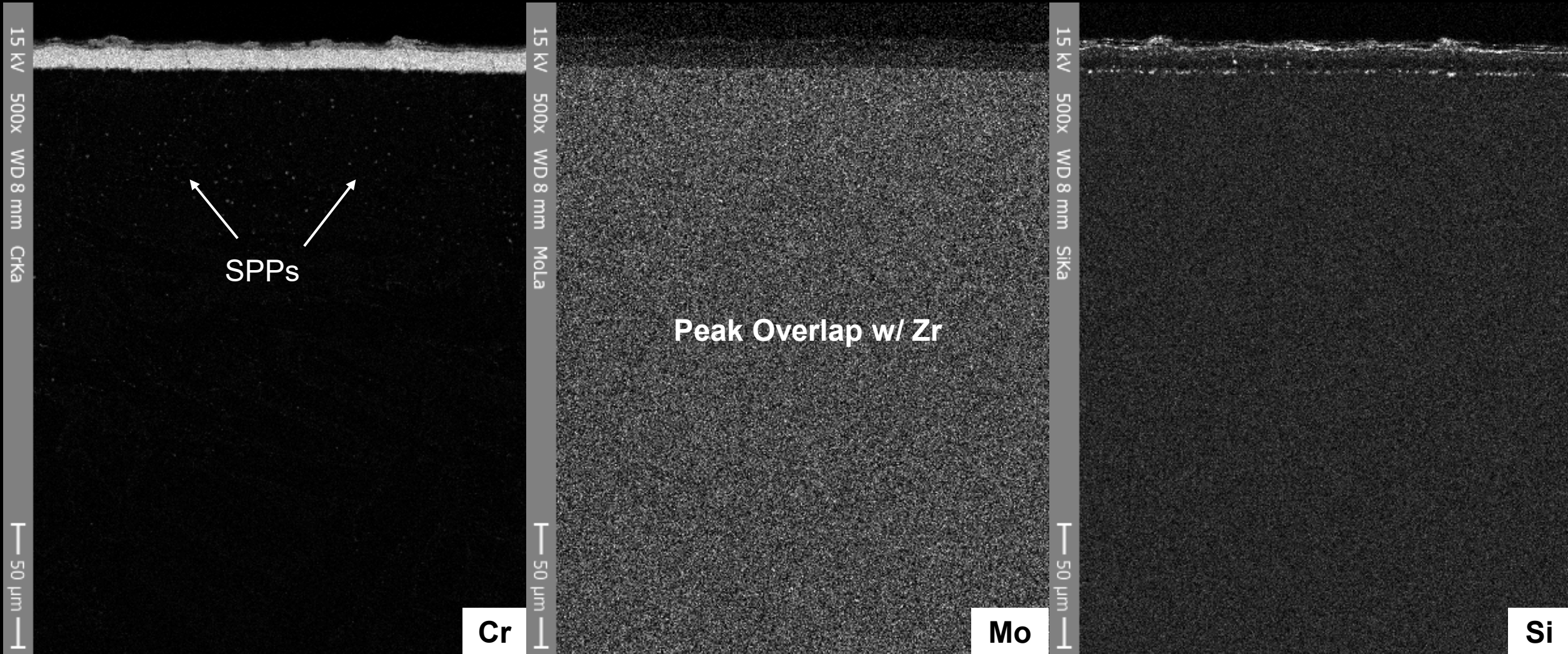




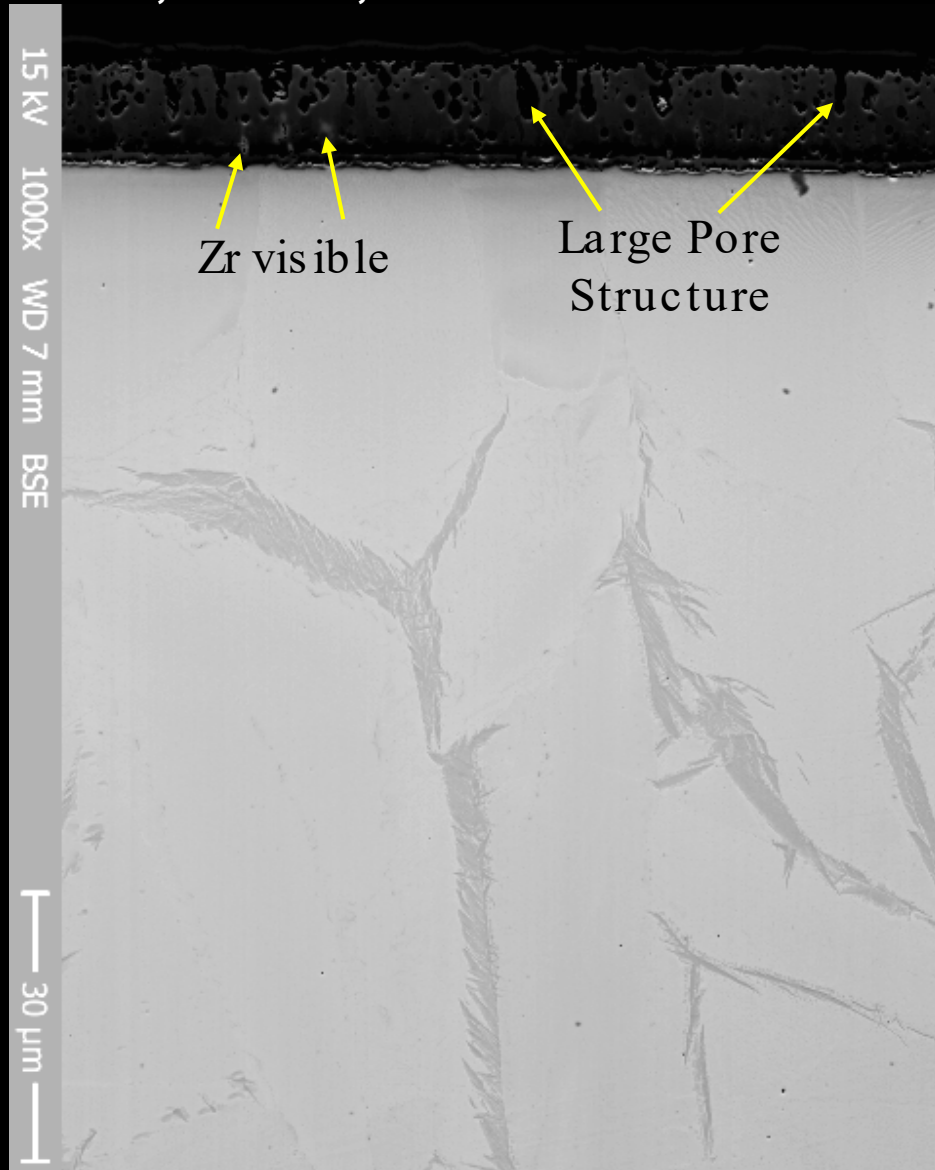
# MoCrSi, 1000 °C, 90 min



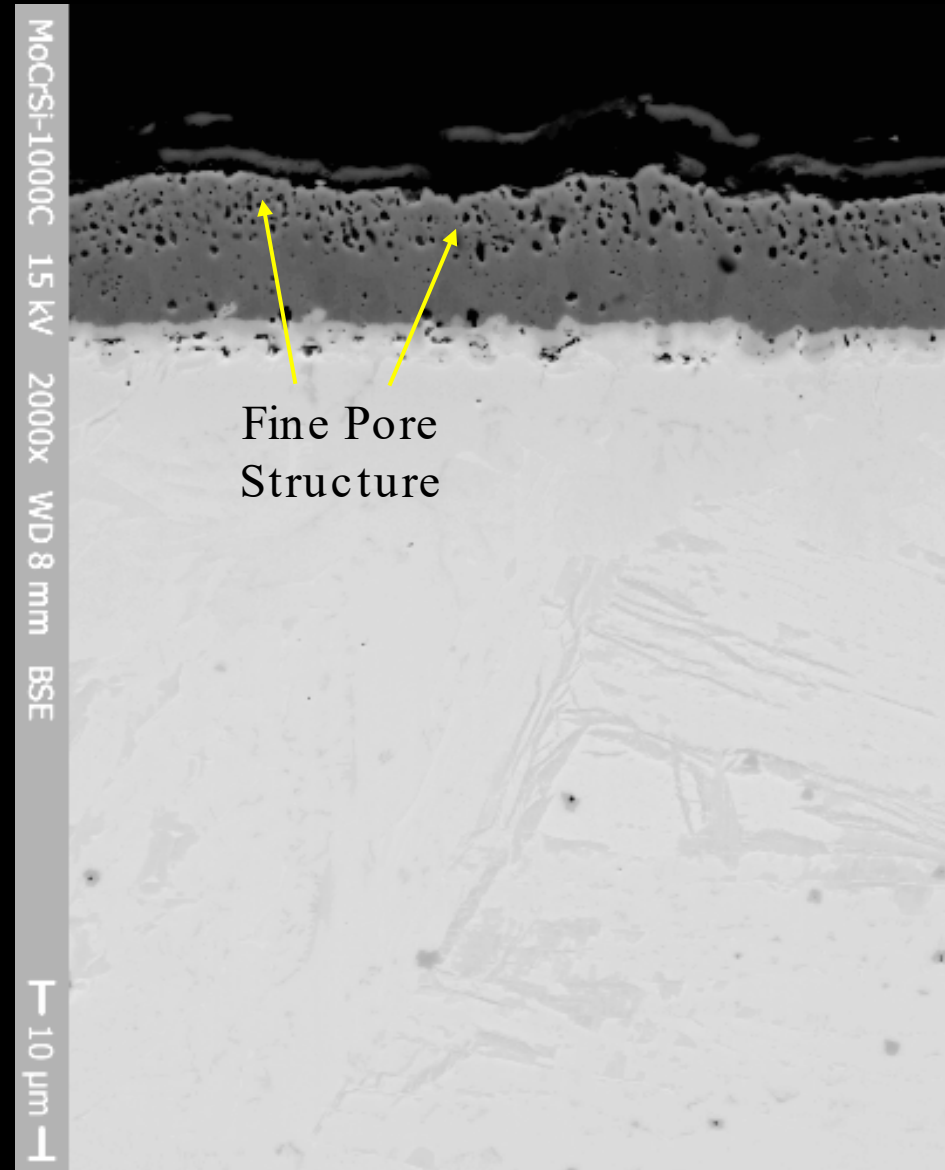
# MoCrSi, 1000 °C, 90 min



Cr, 1000 °C, 90 min



MoCrSi, 1000 °C, 90 min



Zry-4

1000 °C



Cr



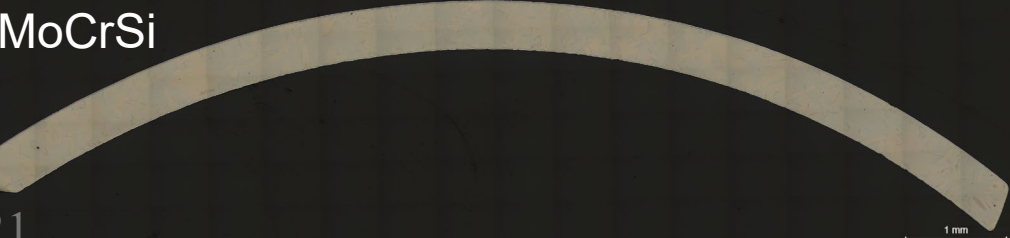
MoCr



MoCrAl



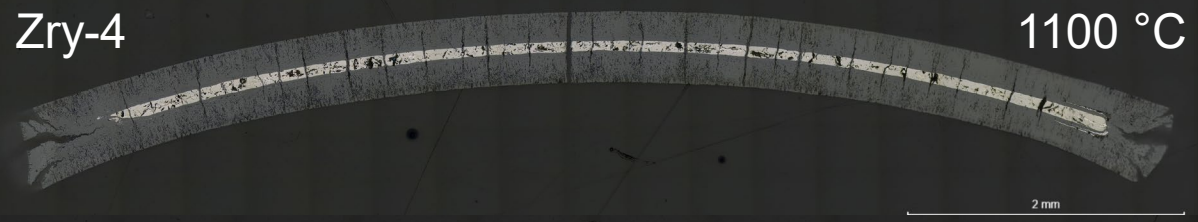
MoCrSi



21

Zry-4

1100 °C



Cr



MoCr

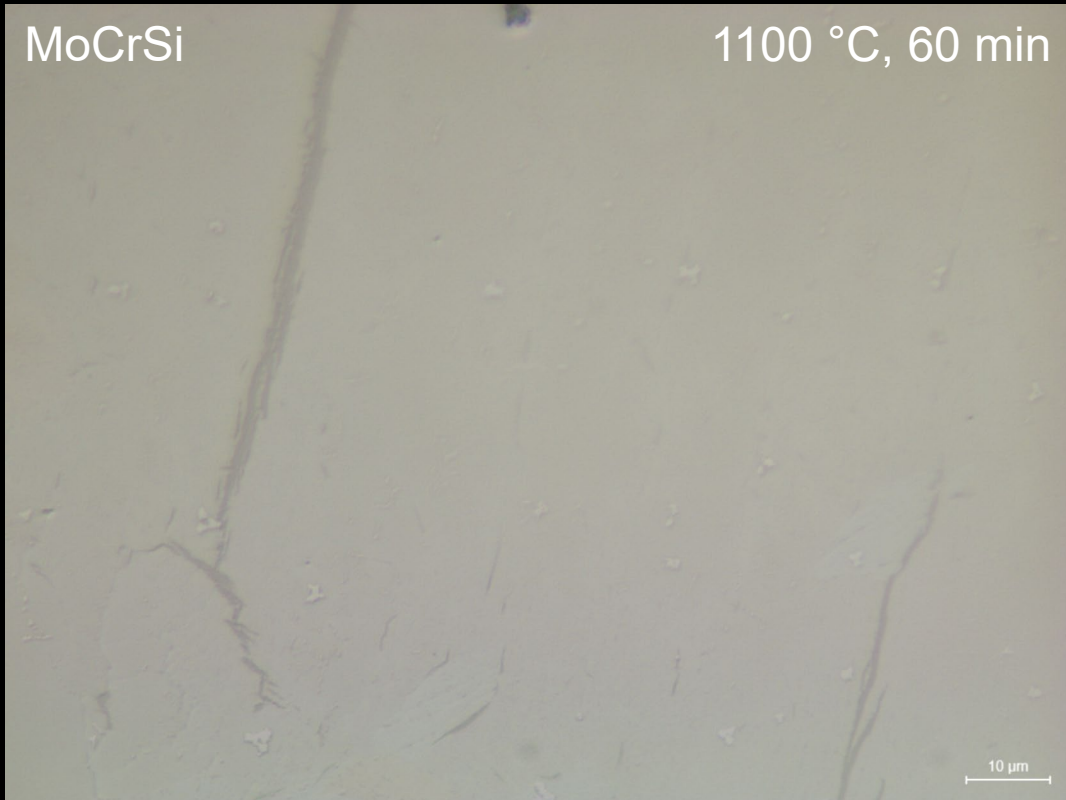


MoCrAl



MoCrSi

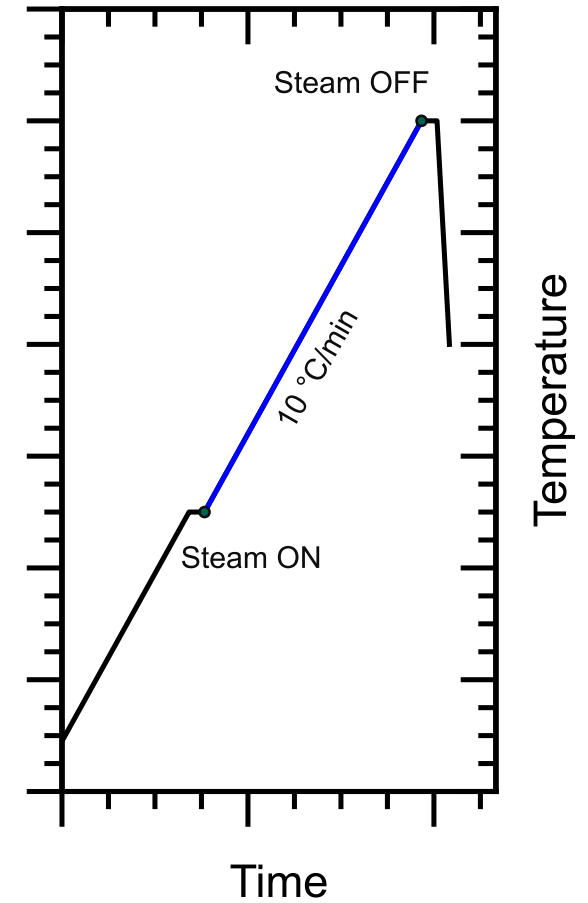
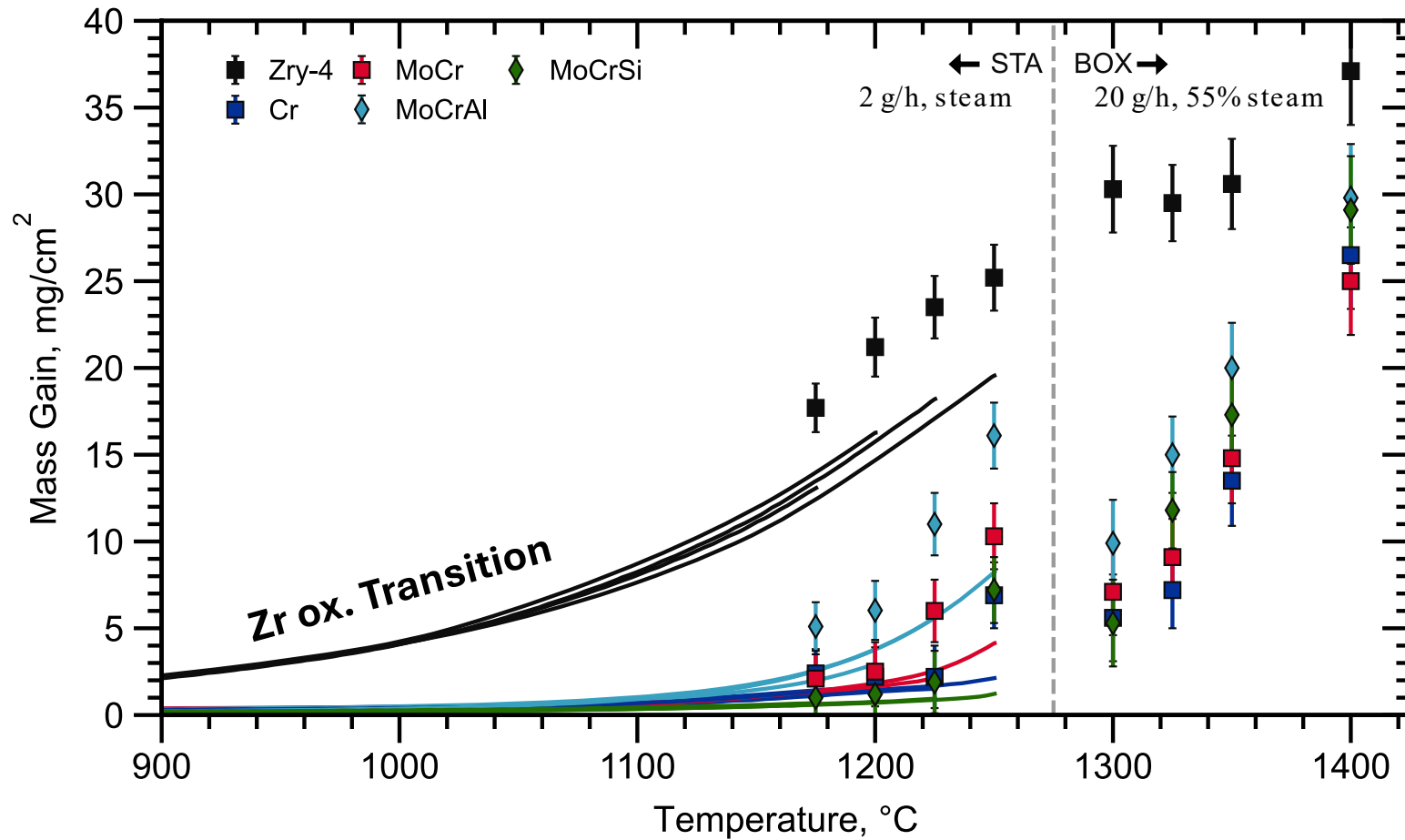




# CAT2 – Transient Steam Oxidation (STA/BOX)

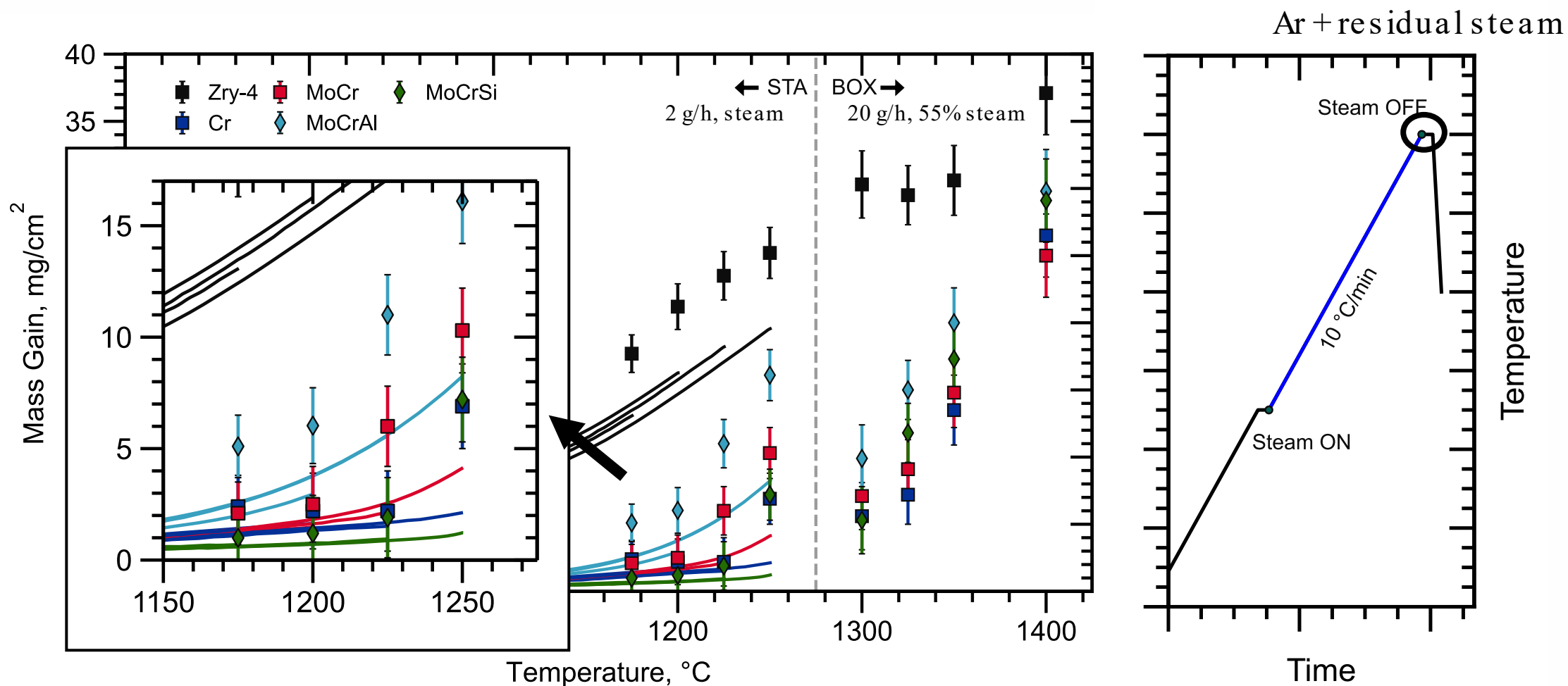
# Effect of Solute Additions and Interdiffusion Barrier

CAT2 – Transient Steam Oxidation (STA/BOX)



# Effect of Solute Additions and Interdiffusion Barrier

CAT2 – Transient Steam Oxidation (STA/BOX)

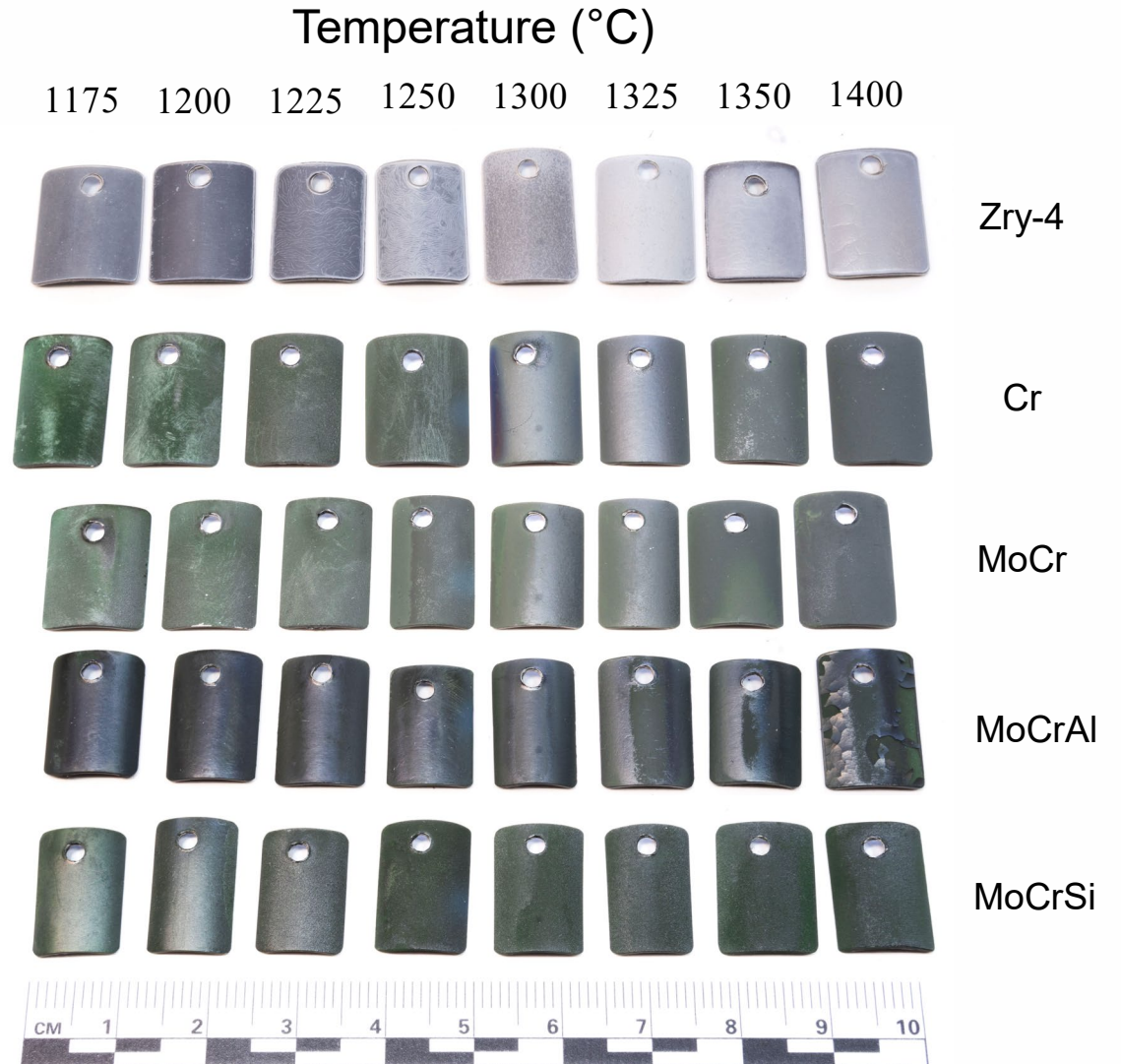




# Effect of Solute Additions and Interdiffusion Barrier

CAT2 – Transient Steam Oxidation (STA/BOX)

...further characterization at QU  
XRD, EDS/EBSD



# Early Takeaways

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1. Cr, MoCrSi coatings significantly reduce steam oxidation until 1225 °C – rapid transition
2. Al inclusions accelerate oxidation – faster permeation of oxygen into Zr
3. Cr and MoCrSi were compared following SEM-EDS after 1000 °C, 90 min:
  - Cr coating exhibits large pore structure & interfacial  $ZrCr_2$  intermetallic
  - MoCrSi has a fine pore structure & coarsened SPPs ( $ZrCr_2$ ) in Zr matrix

# Future Work

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- TGA steam exposures of thickness variant Cr coatings (previous study)
- TGA O<sub>2</sub> eutectic temperature ramps on chemistry variant coatings (current study)
- TGA steam oxidation of coated Zr-2.5Nb (future study) – CANDU®PT application
  - Markus Piro (McMaster University)
  - Supported by the NSERC CREATE-CORRECT Program

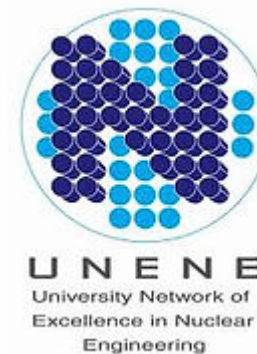
## Additional work:

- Autoclave exposure in CANDU® chemistry – Si dissolution
- Gaseous hydriding of coated Zry – heat treatment, c-ring tests
- Neutronics assessment of Cr coated CANDU bundles (DRAGON5/DONJON5)

# Acknowledgements

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- OECD-NEANEST TCOFF-II Fellowship for sponsorship of the work during this exchange
  - Daniel Shephard (administrative support)
- KIT High Temperature Materials Group
  - Martin Steinbrück, Diana Bachurina, Ulrike Stegmeier, and Mirco Große
  - And the rest of the QUENCH group for being pleasant hosts!



# Thank You!

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LinkedIn

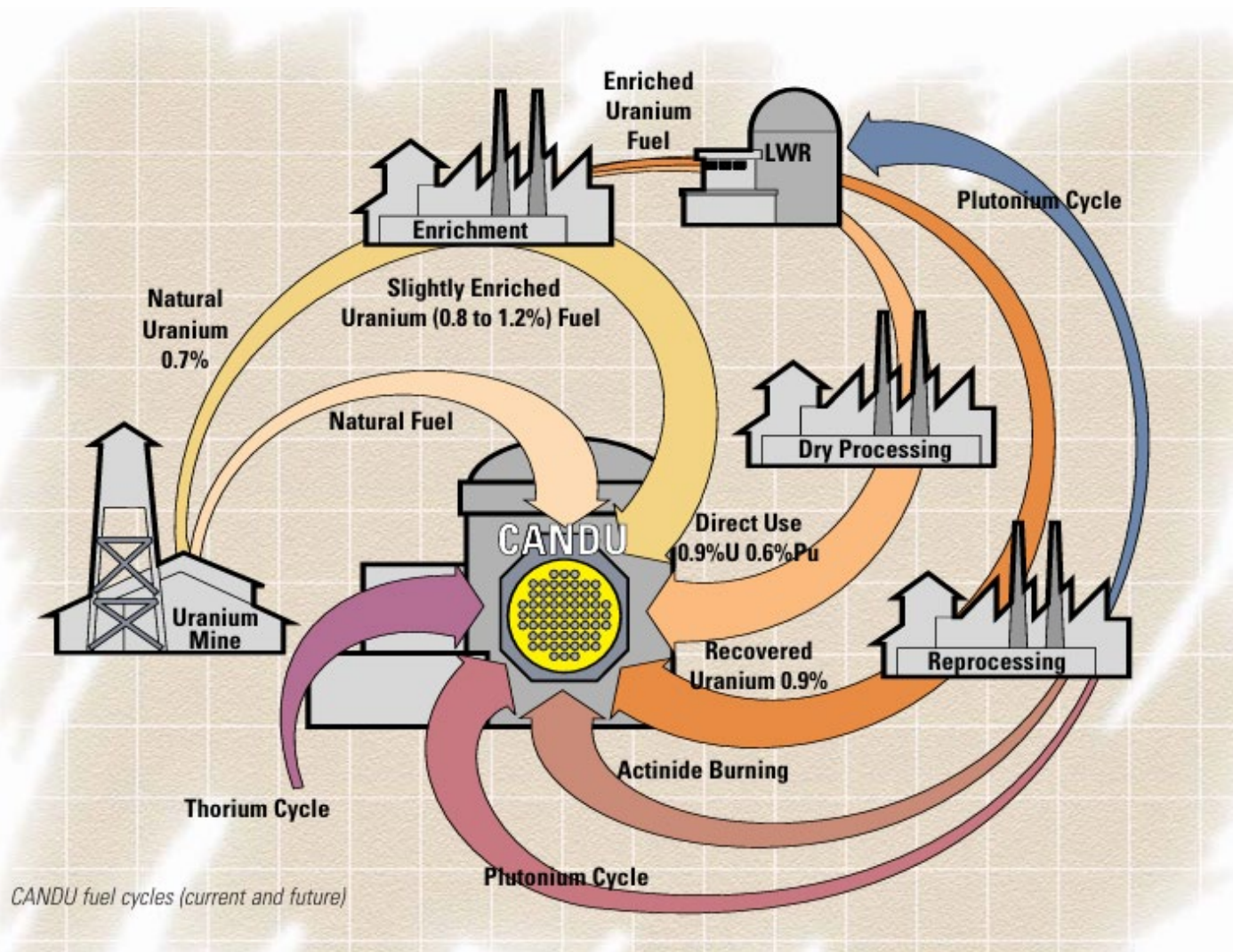


Hope to reconnect at NuMat2026 Halifax!

# Supplementary



# The CANDU® Future?



## CANDU® Fuel Cycles

1. Natural Uranium (NU)
2. Slightly-Enriched Uranium (SEU)
3. Direct Use PWR in CANDU (DUPIC)
4. Recovered Uranium (RU)
5. Thorium (Th)
6. Plutonium (Pu)
7. Actinides (reducing waste)
8. ...SMR fuels, CANDU ACR

## CANDU® Refurbishment (Retubing)

- Currently bringing several units back online after refurbishment
- Extends service life out to 60 years, further iterations out to 90+ years

*CANDU® CANFlex fuel cycles, from the CANDU® 6 Technical Summary*

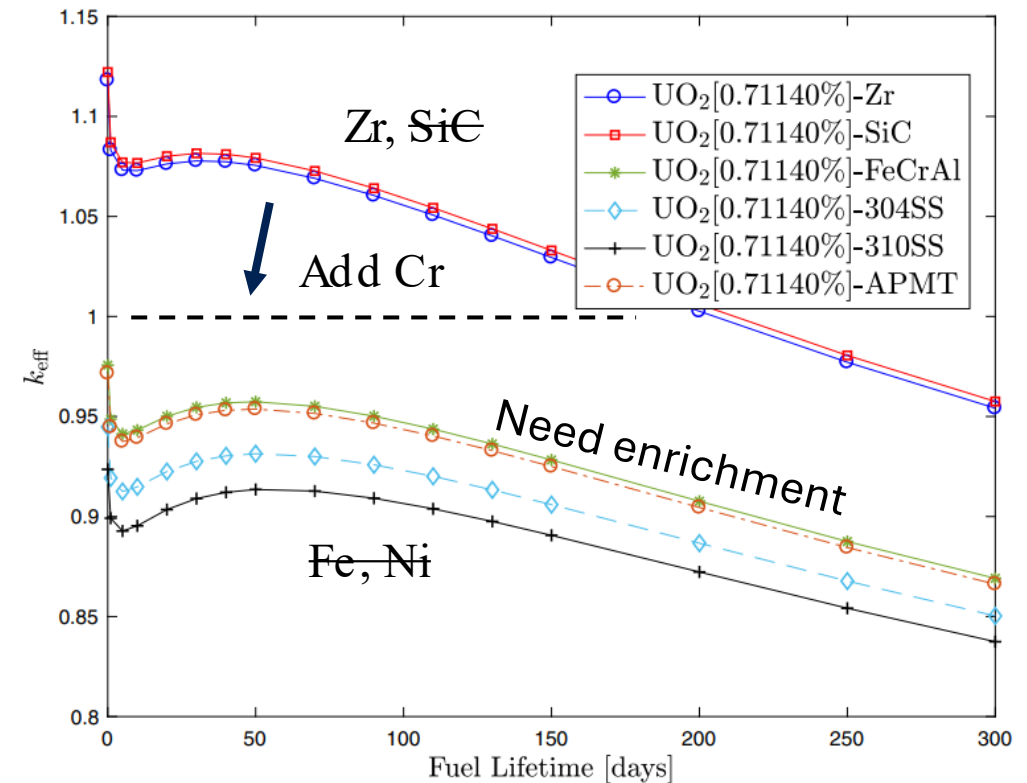


# Research Question

Can we optimize coating protectiveness vs. neutronics penalty?

## Methodology

- Prior work:
  - Minimum effective coating thickness (Cr, 5-20  $\mu\text{m}$ )
- Ongoing study:
  - Solute additions (Al, Si)
  - Mo interdiffusion barrier at Cr/Zry-4 interface



Effective multiplication factor vs. fuel residence time in a standard CANDU-6 natural cell lattice.

Naceur, A. & Marleau, G. Neutronic analysis for accident tolerant cladding candidates in CANDU-6 reactors. Annals of Nuclear Energy 113, 147–161 (2018).



**Nicolas Wefers**

KIT

## **Experimental Observations on the CHF Performance of Cr/ CrN-Coated Zircaloy-4 in Low-Pressure Flow Boiling**

Accident Tolerant Fuel (ATF) concepts based on chromium coatings are investigated with respect to their influence on critical heat flux (CHF) and boiling heat transfer behavior. The presented work builds on two preceding projects focusing on the onset of boiling crisis in Cr-based ATF claddings and extends the investigation towards post-CHF phenomena and their relevance for cladding integrity.

Experiments were conducted in both annular gap and small rod bundle geometries under pressurized water conditions. CHF was identified using a standardized procedure based on inlet enthalpy variation, while post-CHF tests employed an active power cut-off at a cladding temperature of 1000 °C. Test samples included Zr-4 reference cladding, Zr-4 coated with 8 µm CrN (with Ti interlayer), and Zr-4 coated with 16 µm Cr. Surface roughness remained comparable across samples, enabling a direct assessment of material effects.

Across all investigated flow conditions, CHF exhibits a robust linear dependence on inlet enthalpy (or boiling number), with correlation coefficients up to  $R \approx 0.99$ . The observed CHF differences between coated and uncoated samples are moderate, in the range of 8-9% with an accuracy of 3.5% and largely independent of mass flux, pressure and inlet subcooling. This indicates that CHF is primarily governed by flow conditions rather than by smooth Cr-based surface modifications below  $\sim 20$  µm thickness.

To gain mechanistic insight, high-speed visualizations were used to quantify nucleation site density (NSD) and bubble departure frequency (BDF). The results show that Cr-based coatings primarily affect NSD, while BDF remains comparatively unchanged. The tested pure Cr coatings delay NSD activation, whereas CrN coatings promote earlier bubble coalescence and transition to churn flow. Existing NSD correlations reproduce global trends but fail to distinguish material-specific effects.

Overall, the findings suggest limited CHF sensitivity to Cr-based ATF coatings, while subcooled boiling characteristics and post-CHF behavior remain key performance-limiting phenomena for future investigation.

# Experimental Observations on the CHF Performance of Cr/ CrN-Coated Zircaloy-4 in Low-Pressure Flow Boiling

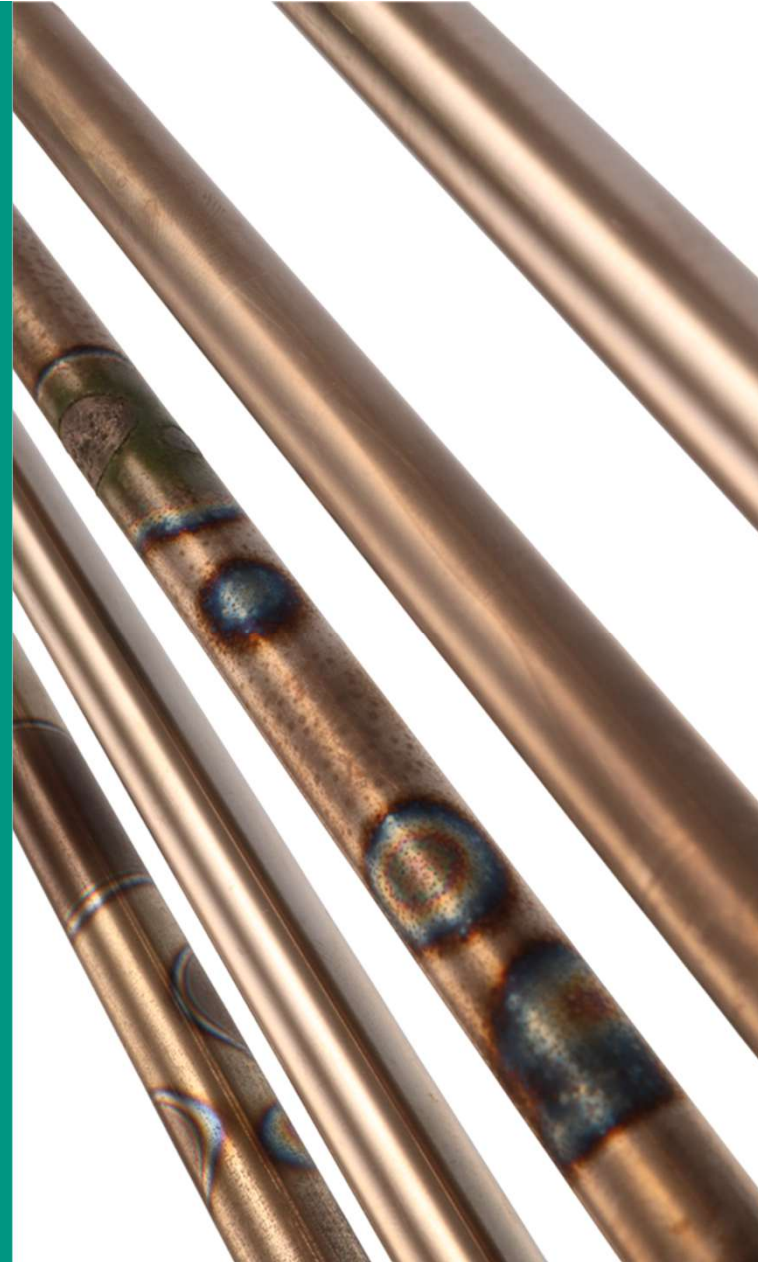
Nicolas Wefers<sup>1</sup>, Daniel Vlček<sup>2</sup>, Tereza Kinkorova<sup>2</sup>,  
Taron Petrosyan<sup>3</sup>, Stephan Gabriel<sup>1</sup>

<sup>1</sup>Karlsruhe Institute of Technology

<sup>2</sup>Czech Technical University in Prague

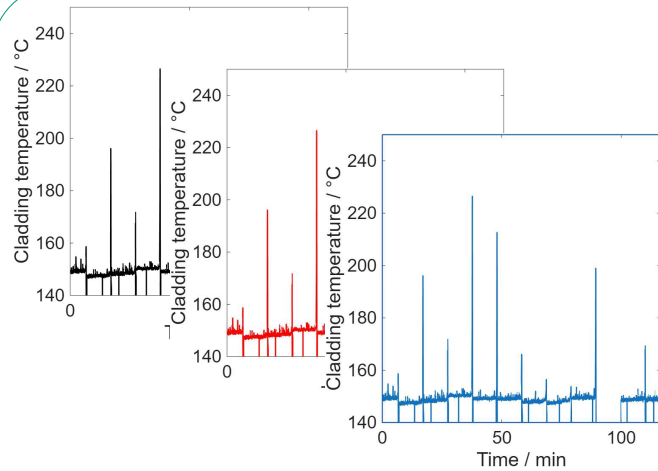
<sup>3</sup>Brno University of Technology

18. December 2025

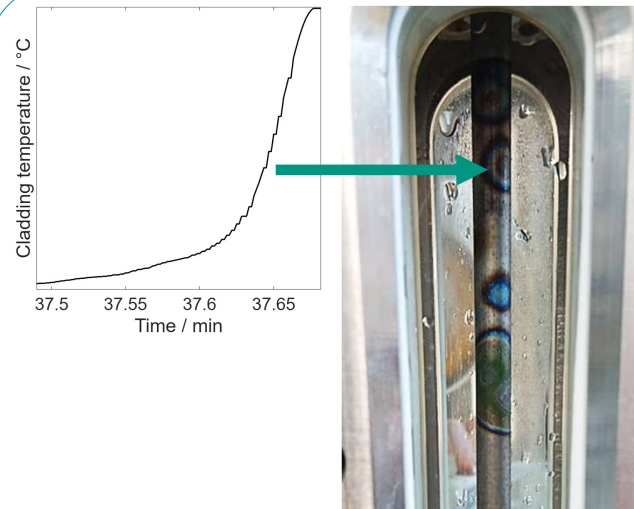


- 1. Outline & Motivation**
- 2. Experimental Set-Up**
- 3. CHF-Results**
- 4. Boiling Parameter**
- 5. Outlook & Future Work**

# Outline of ATF-Cladding Tube Activities



**GRS: KEK-MESA/ OFFEER: COATED**  
CHF-Benchmark of Cr-based ATF's  
at COSMOS lap



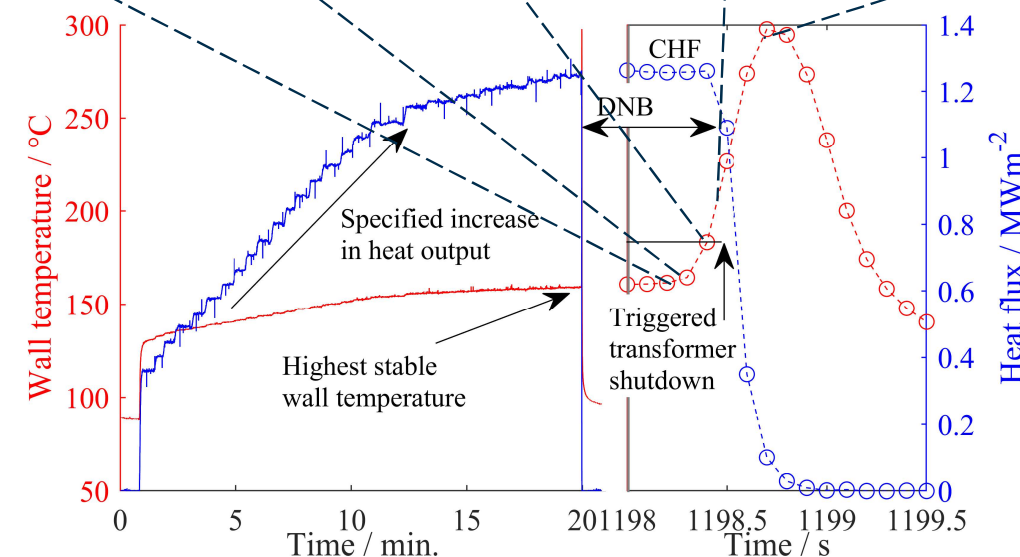
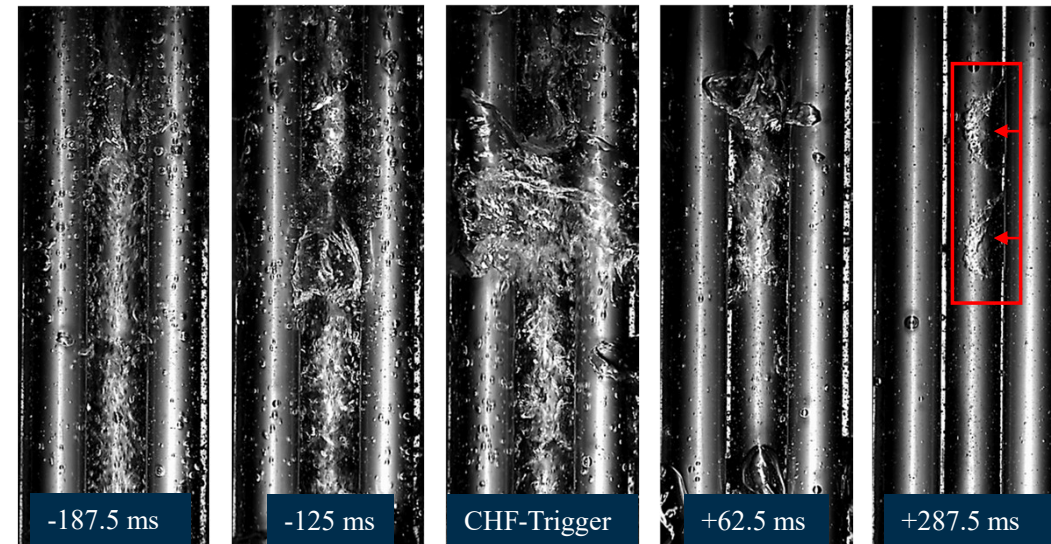
**OFFEERR: ChroTemp**  
Post-CHF behavior of Cr-based ATF's  
at COSMOS lap and post tests/  
simulation at CTU



**Further activities based on ChroTemp**  
Post-CHF impact on strength and  
fracture mechanics of cladding tubes

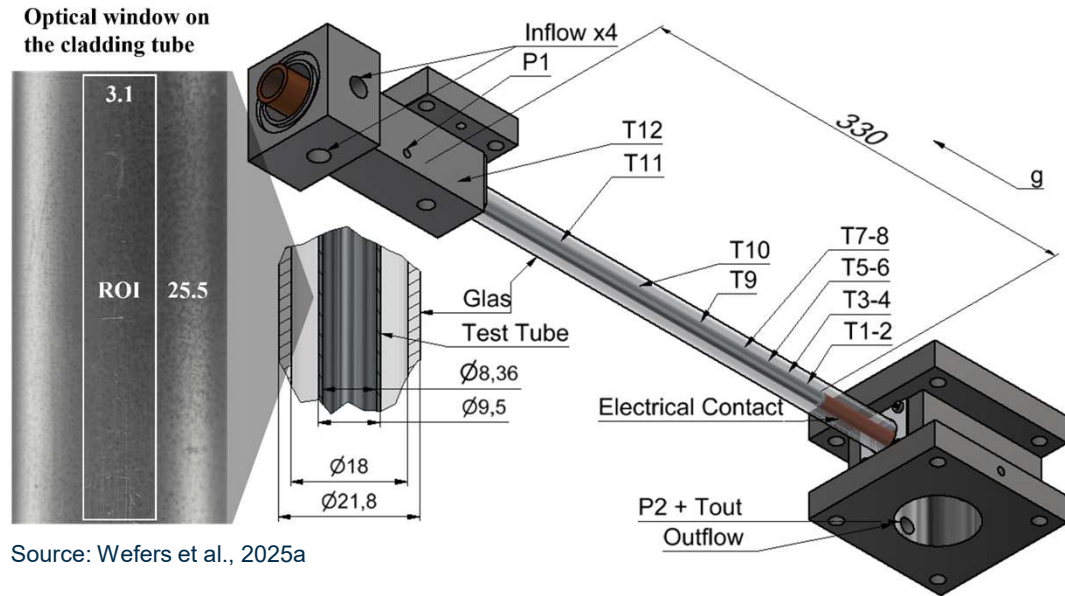
# Motivation & Background

- Critical Heat Flux (CHF): upper limit for safe heat removal in nuclear fuel—exceeding it triggers a boiling crisis, rapid temperature rise, and possible cladding damage
- Nucleation Site Density (NSD): quantifies the number of active bubble nucleation sites per unit area during boiling. Higher NSD usually enhances heat transfer, delaying CHF (good for safety)
- NSD is influenced by cladding material, surface roughness, wettability, and coatings
- Computational Fluid Dynamics (CFD): Predictive CFD models need accurate input data for boiling and CHF, including reliable NSD trends
- New ATF materials/coatings (like CrN, Cr) may shift NSD and CHF, boosting performance and safety
- Need to understand how these innovations impact boiling at the micro-scale and reactor-scale

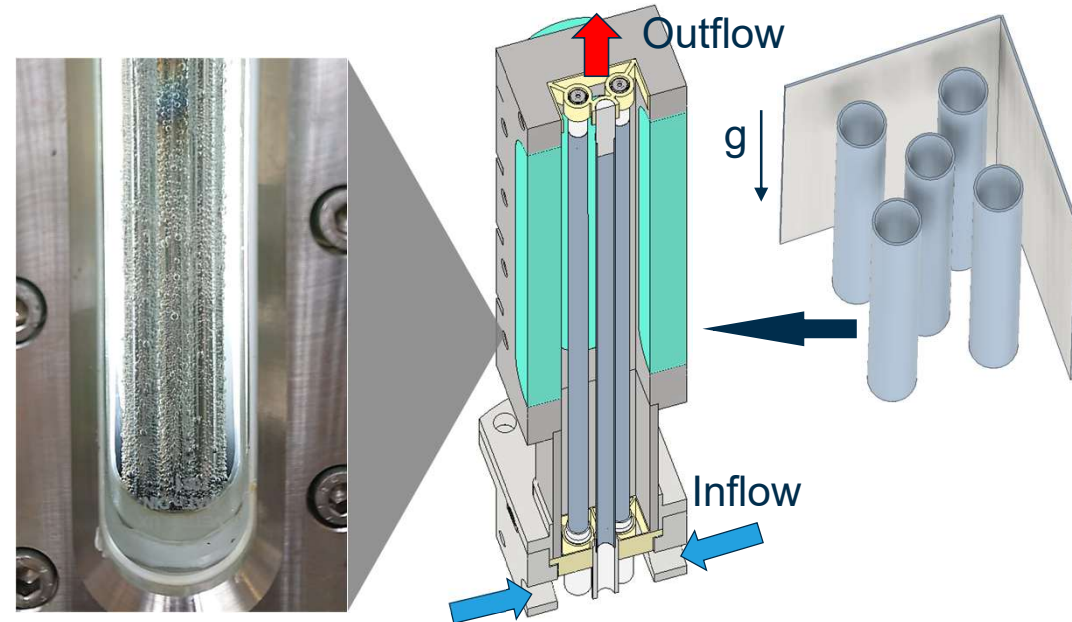


Source: Wefers et al., 2025b

# Experimental Set-Up



Source: Wefers et al., 2025a



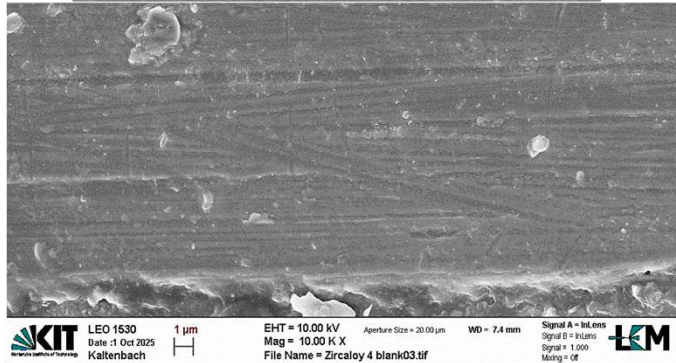
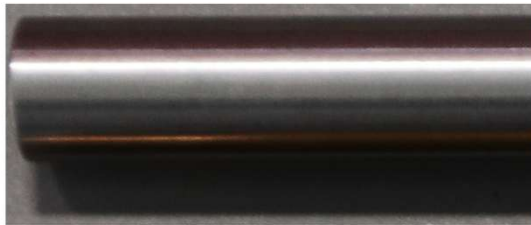
Adapted from Wefers et al., 2025b

## COSMOS-L: low-pressure flow boiling loop at KIT

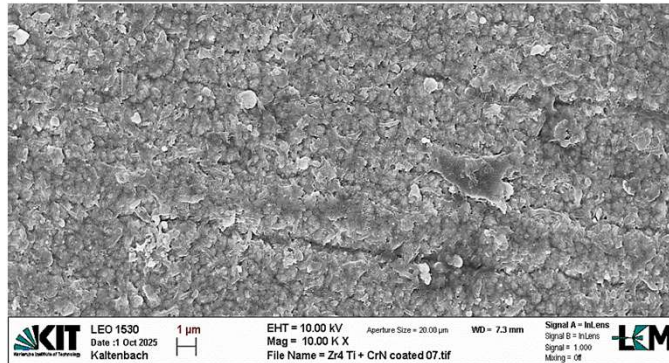
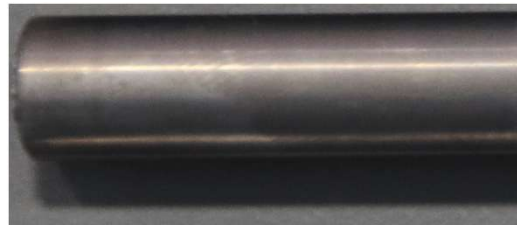
- Annular gap and assembly test section simulates rod bundle conditions
- Direct electrically heated (AC) claddings (heated length up to 400 mm)
- Glass outer tube/ sight glasses for optical access
- High-speed camera on a robot hand. Tracks bubbles, nucleation sites and DNB

# Cladding Samples

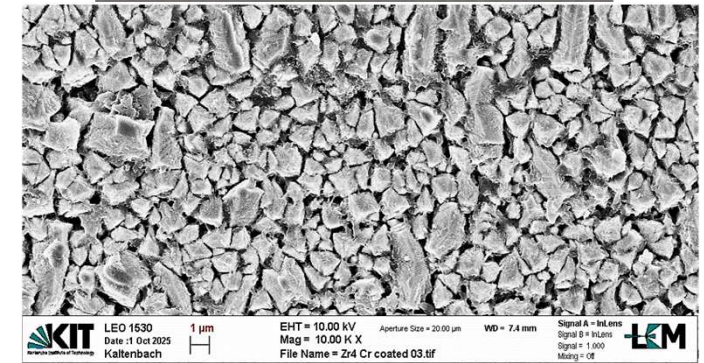
Bare Zircaloy-4



CrN coated Zircaloy-4 (8 μm)



Cr coated Zircaloy-4 (16 μm)



Mean Wetting Angle (°)

Specific Heat (J/kg·K) (300/400 K)

Thermal Cond. (W/m·K) (300/400 K)

84.5

281 / 302

13.4 / 14.2

73

460 / 480

2.0 / 1.8

78

449 / 500

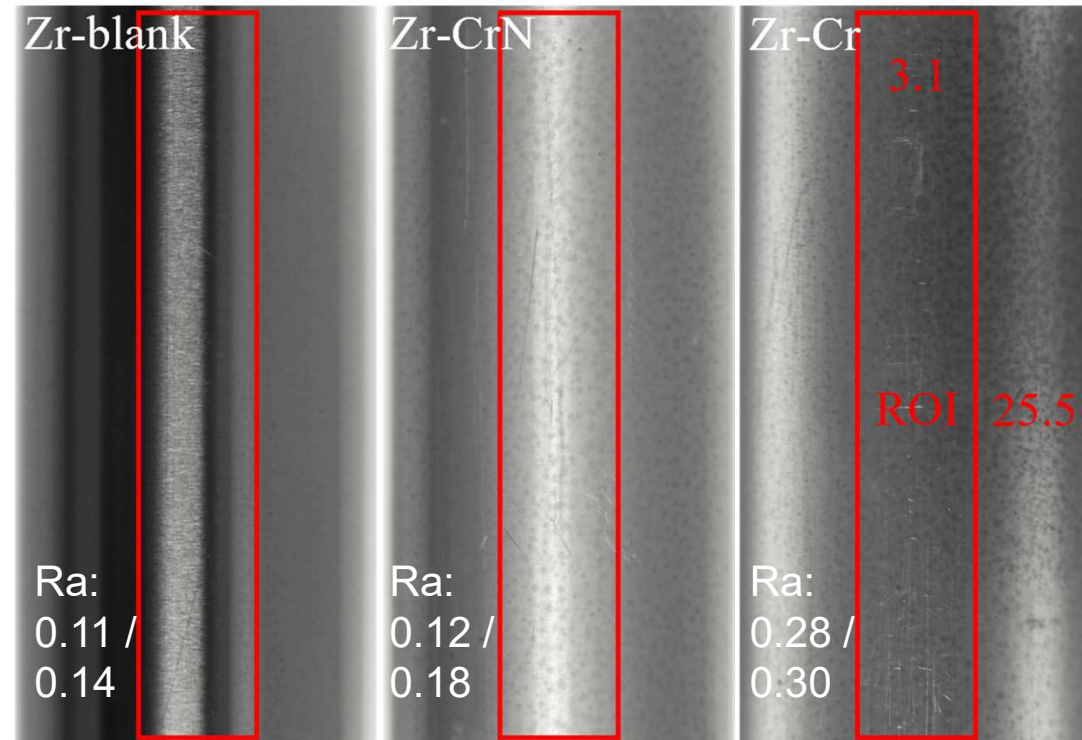
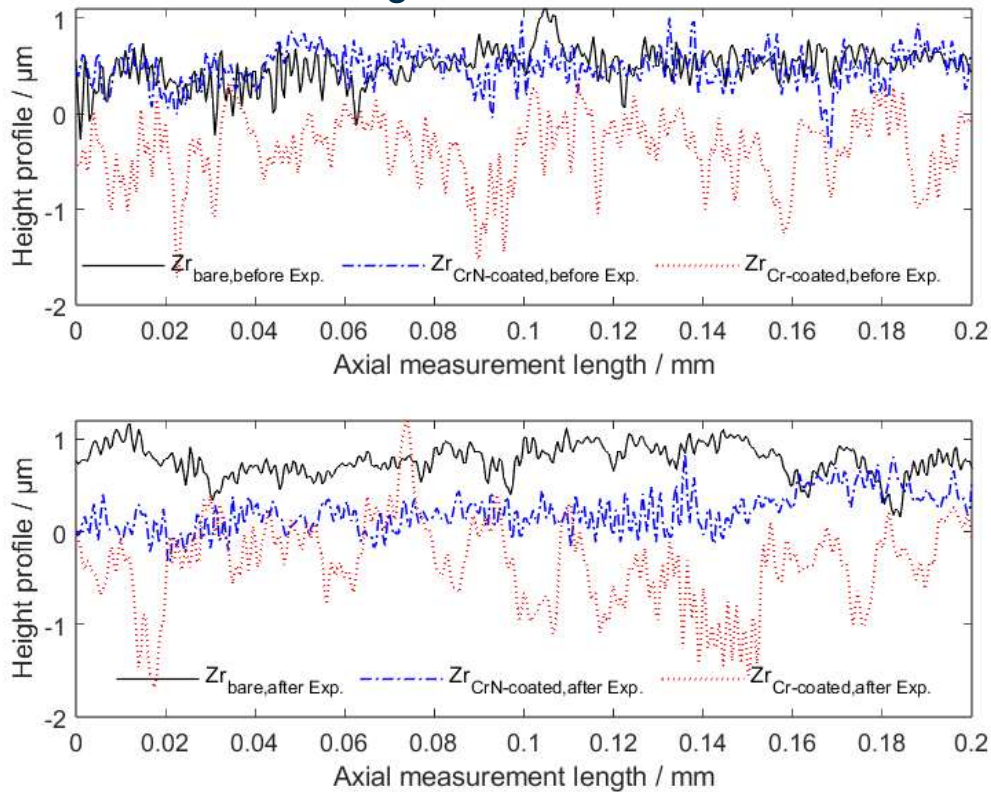
93.7 / 80

Adapted from Wefers et al., 2025a



# Surface Characterization and Area of Interest

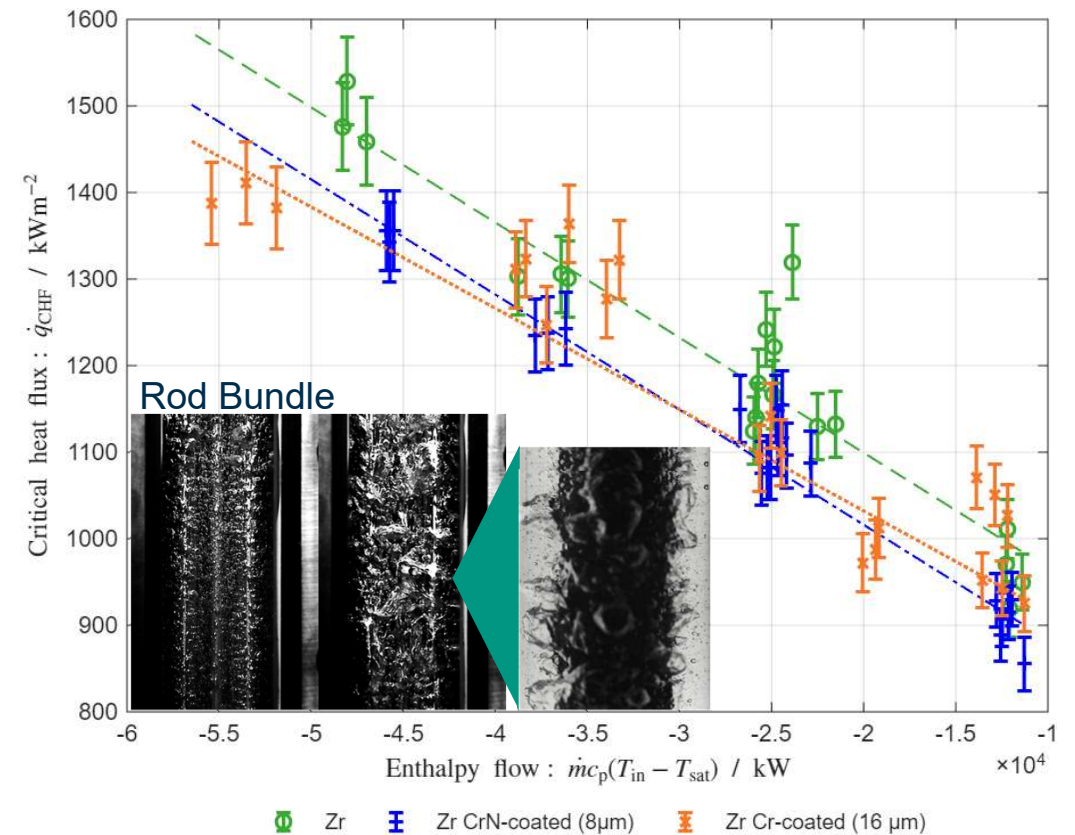
Surface Roughness - before/ after CHF



Source: Wefers et al., 2025a

# Key Observations

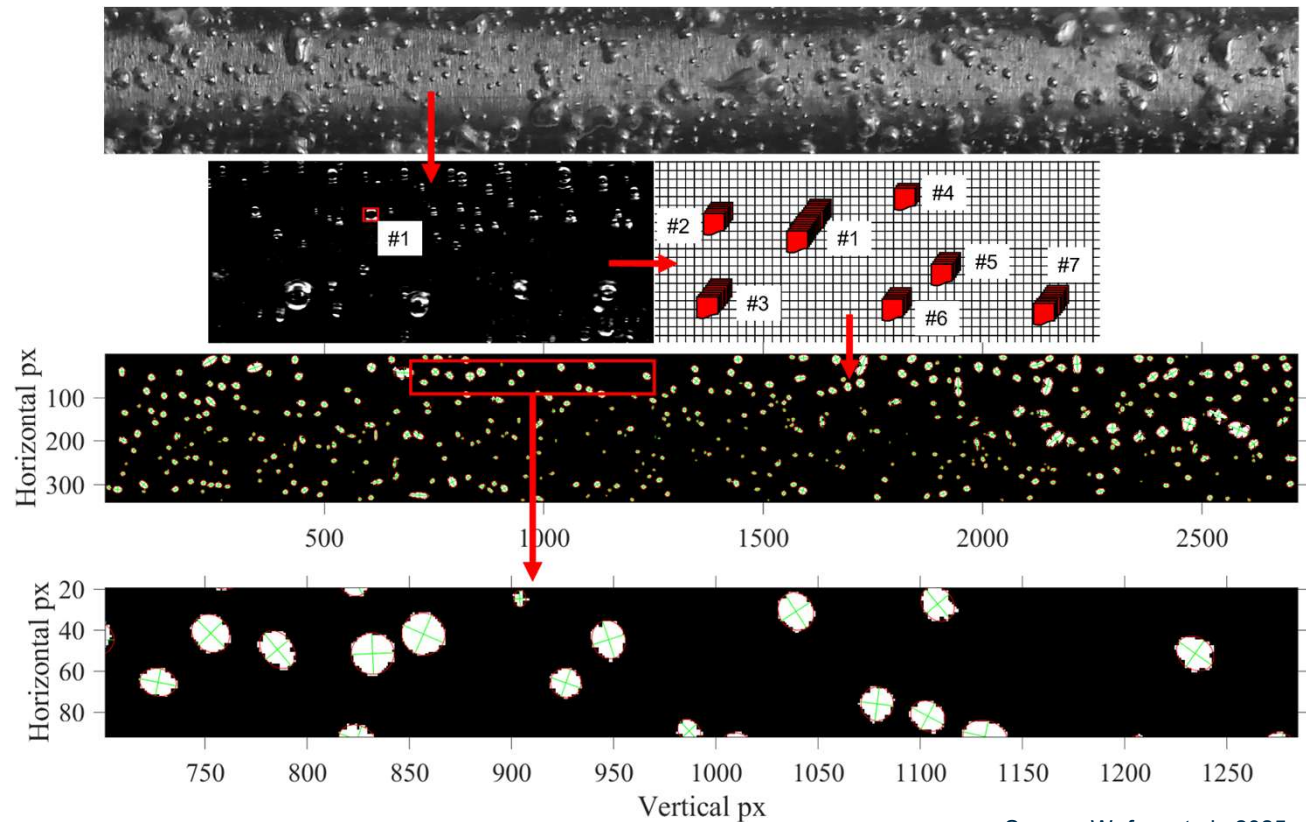
- All claddings: CHF increases linearly with boiling number or inlet enthalpy flow
- High correlation for all materials ( $R^2$  from 0.92 up to 0.99): trend is robust
- No significant difference in CHF trend between Zr-4, Cr, or CrN surfaces
- Offset between fits: only minor, coatings do not improve CHF significantly under these conditions (~8%)
- CHF also shows clear (inverse) correlation with excess enthalpy
- Again, surface coating effect is minimal: dominant parameters remain mass flux, pressure, subcooling



Adapted from Wefers et al., 2025b

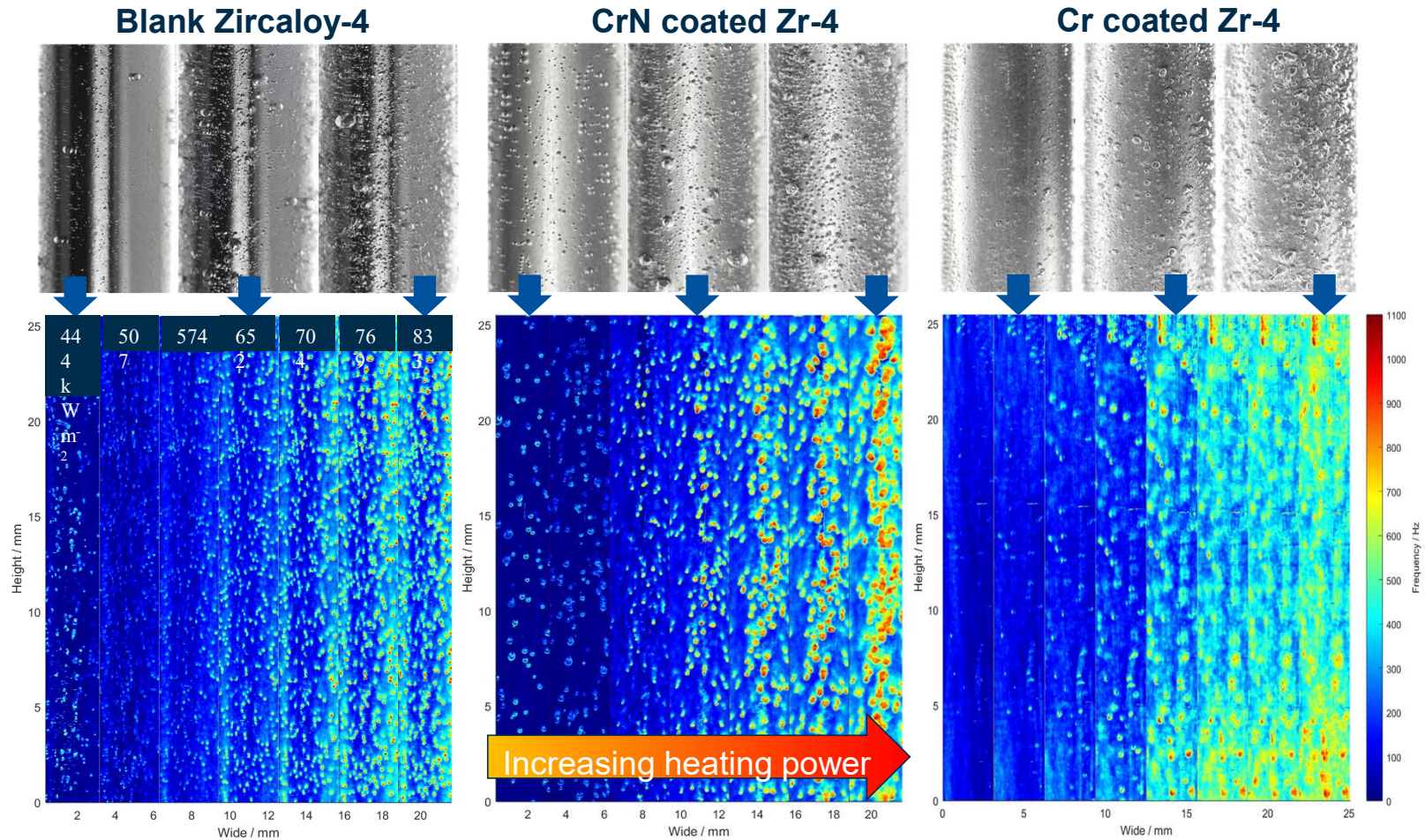
# Measurement & Image Analysis Method

- High-speed imaging: 5000 fps, region of interest near outlet
- Video: tracks bubble nucleation, growth, and departure
- Detection: custom code, tracks brightness changes (bubble flashes)
- Signal processing: adaptive filter (proper orthogonal decomposition, UNET) removes glare/noise
- Nucleation sites: counted by connected-pixel algorithm
- Frequency portraits: map bubble activity, visualize NSD and BDF
- All measurements synchronized with thermal-hydraulic data



Source: Wefers et al., 2025a

# Results NSD Images



Series of 2D histograms of boiling activity (Glaire point scores) at different heating rates

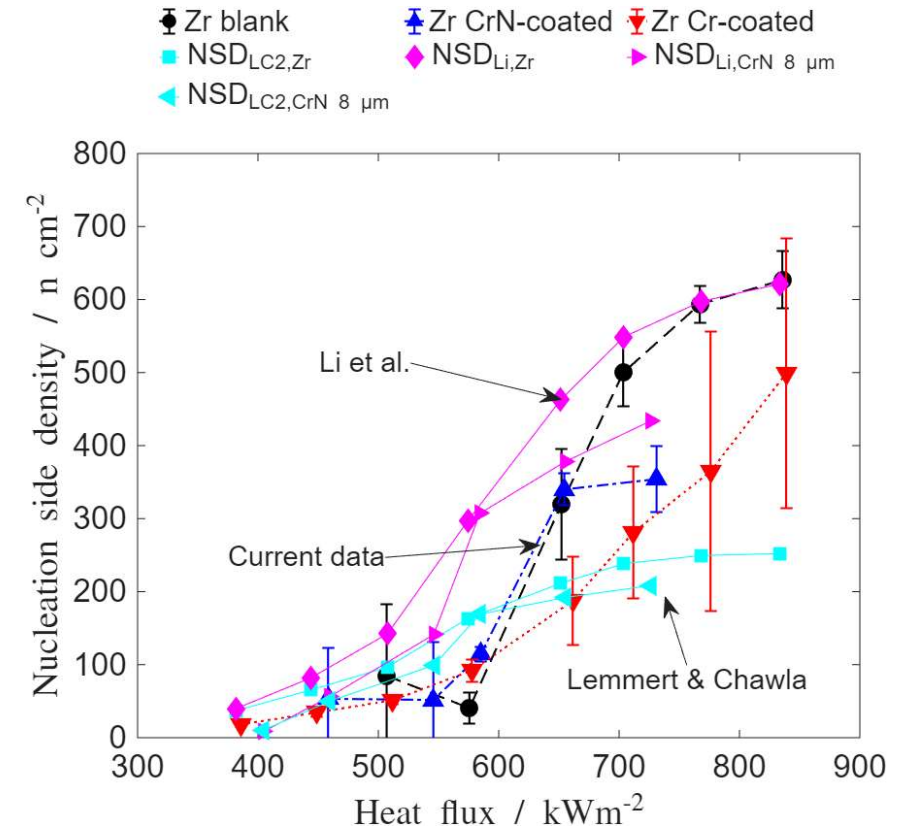
# Key Observations

## NSD:

- Zr-4: highest NSD overall
- Cr-coated: delayed NSD activation with heat flux
- CrN-coated: suppressed NSD at high flux (bubble merging)
- Lemmert & Chawla (1977) and Li et al. (2018) correlations capture overall trends but fail to separate material effects – issues with capturing the exact wall temperature

## BDF:

- Similar across materials
- Frequency distribution of the Cr-coating is smaller than in the smoother cases
- Cole's (1967) correlation with Tolubinski & Kostanchuk (1970) departure diameter matches average values but misses frequency increase at higher flux



Adapted from Wefers et al., 2025a

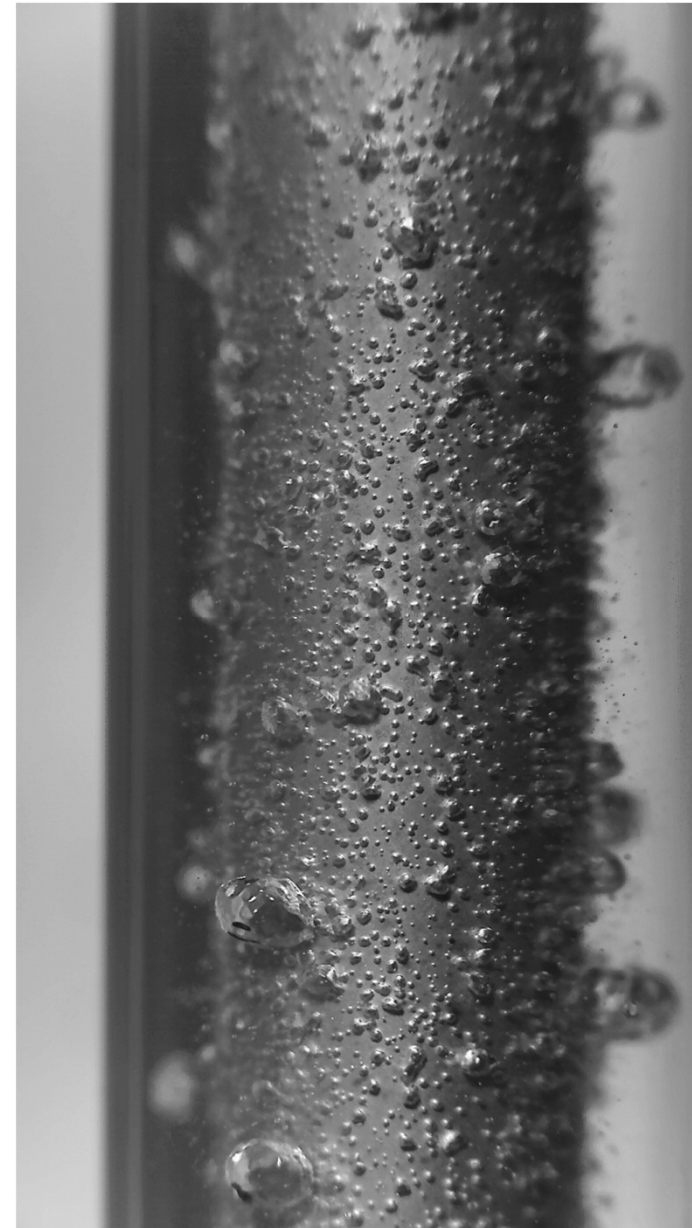
# Conclusion

## Coating/roughness effects:

- Clear influence on NSD, less on BDF
- Models capture general trends but miss coating- and defect-driven effects
- Small effect on CHF trend: CHF scaling governed by flow conditions

## Future & current work:

- Analyze bubble size and departure in more detail
- Advanced surface analysis (AFM, wettability vs. temperature)
- Wider range: pressure, mass flux, inlet temp, more coatings
- Integrate findings into CFD for better CHF prediction
- More materials and broader range for CHF experiments as well
- **ChroTemp – Post CHF Experiments:** oxidation and mechanical tests of the cladding tubes



# Acknowledgement

This work was supported by the OFFERR ChroTemp project as well as by the GRS as part of the KEK program (1501646). The author gratefully acknowledge the experimental and technical support provided by staff at the Karlsruhe Institute of Technology and the Czech Technical University in Prague and Brno.



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EUROPEAN USER FACILITY NETWORK



Funded by the  
European Union

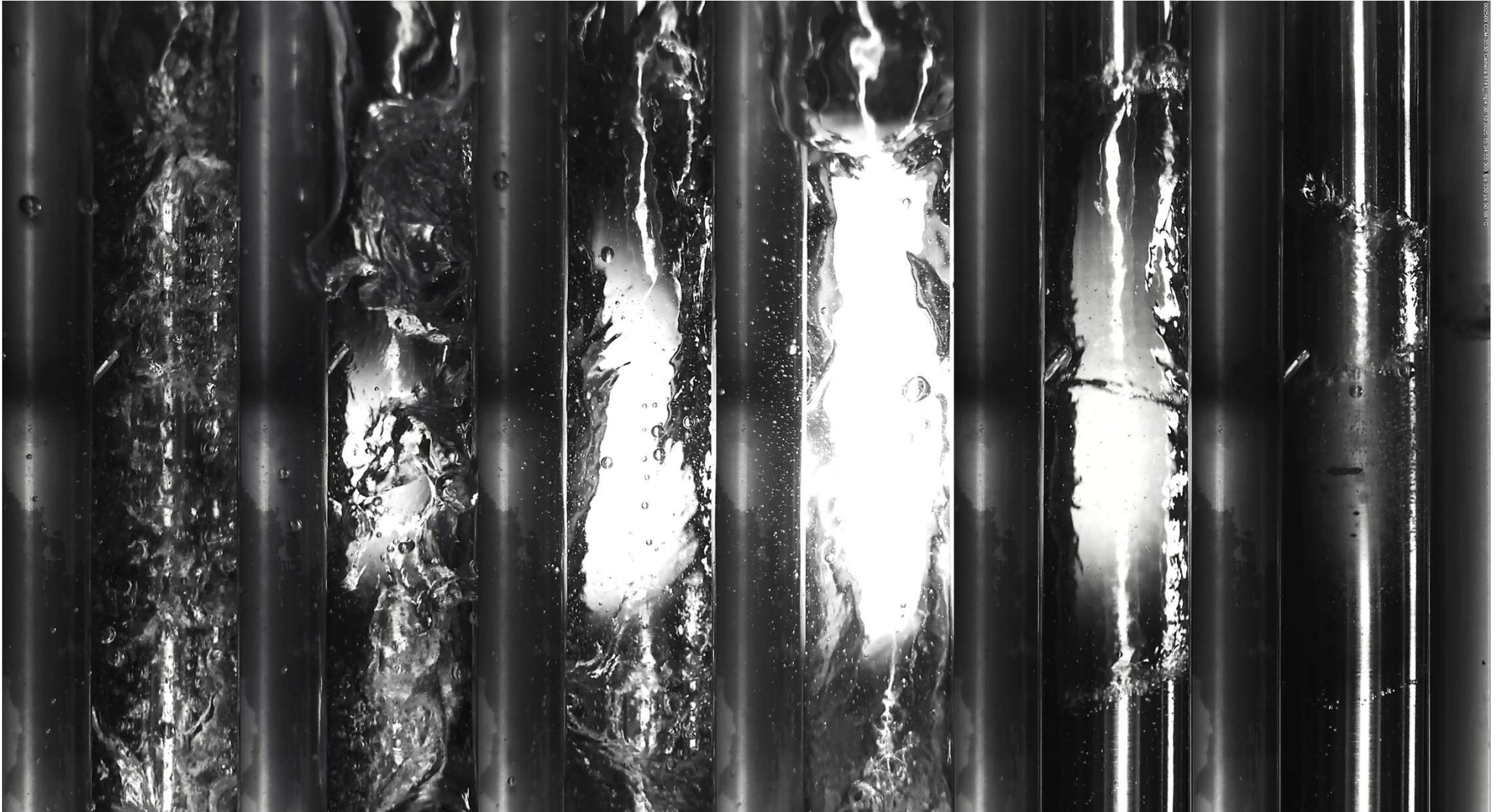


Supported by:



based on a decision of  
the German Bundestag

# Thank you for your attention!





# Image Sources

1. Wefers, N., Vlček, D., Heiler, W., & Gabriel, S. (2025). High-speed imaging and analysis of nucleation site density on nuclear fuel claddings. In Proceedings of NURETH-21 (Busan, South Korea, August 31–September 5).
2. Wefers, N., Vlček, D., Heiler, W., Gabriel, S., & Class, C. (2025). Influence of ATF cladding tube candidates on the critical heat flux in a vertical rod bundle during flow boiling of water at low pressure. Nuclear Technology, 1–18.



**Mirco Große**

KIT

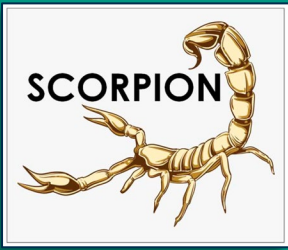
## **Update of the KIT contributions to the SCORPION project**

A certain porosity is needed in the fiber range of SiC<sub>f</sub>/SiC ceramic matrix compounds to ensure the pseudo-plastic deformation behavior. On the other hand, porosity increases the reacting surface and enhances chemical reactions. The formation of protective SiO<sub>2</sub> scales at SiC can close open porosity and with it neglect the negative effect on the chemical reaction kinetics.

High temperature oxidation tests (1600°C for 1 h) in different atmospheres were performed comparing compact and porous SiC. The tests were performed in steam, hydrogen + steam, oxygen and air atmospheres. The porous and compact samples had 37% and 97%, respectively, of the theoretical density of SiC. The pores had sizes between 0.5 and 5 µm.

The mass gain differs between the compact and the porous sample by up to three orders of magnitude. Hints for closing open porosity were only found for the reaction in oxygen. Surprising were the differences between the reaction in oxygen and in air. The reaction in air is stronger than the one in oxygen for both compact and the porous samples. Reasons for this effect can be a local reduction of the oxygen partial pressure in the pores and with it a change from passive to active oxidation and/or a chemical reaction of SiO<sub>2</sub> with nitrogen forming Si<sub>2</sub>N<sub>2</sub>O and consuming the protective SiO<sub>2</sub> scale.

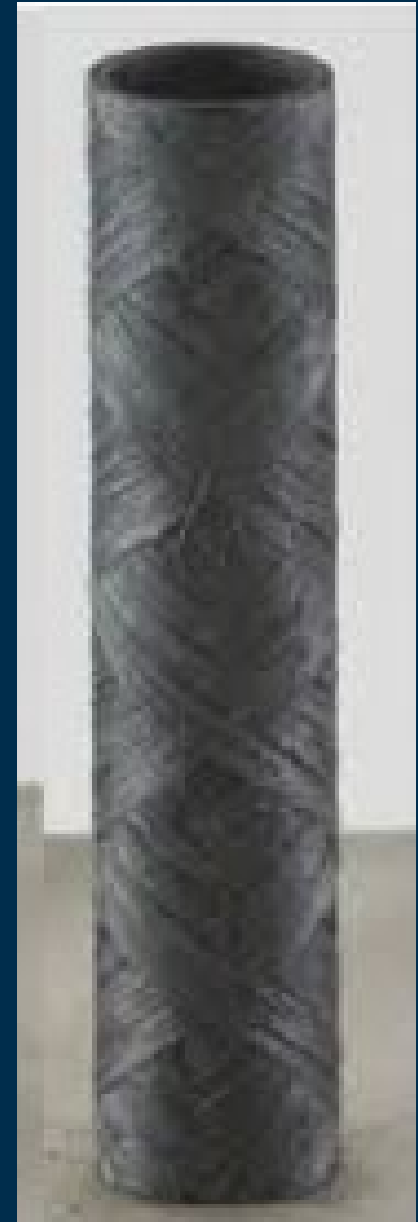
It can be concluded from these results that no closing of pores with sizes in the order of magnitude of few micrometres would occur during severe nuclear accidents. Open porosity must be prevented for cladding tubes made of SiC<sub>f</sub>/SiC ceramic matrix compounds.



# Update of the KIT contributions to the SCORPION project

Mirco Grosse, Martin Steinbrück, Tobias Fey, Konstantina  
Lambrinou

30. Intern. QUENCH Workshop,  
KIT Campus North, 2025/12/18

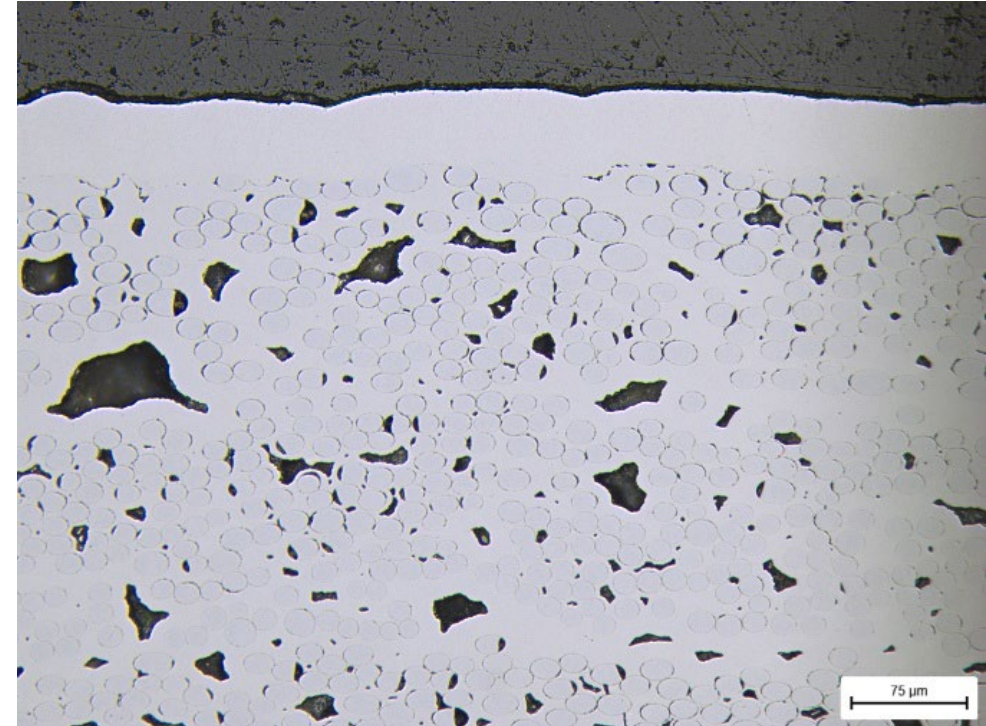


# Introduction

Porosity in the fiber range is needed for the quasi ductility.

Open porosity results in an increase of the reacting surface.

Does the formation of  $\text{SiO}_2$  close the open porosity?

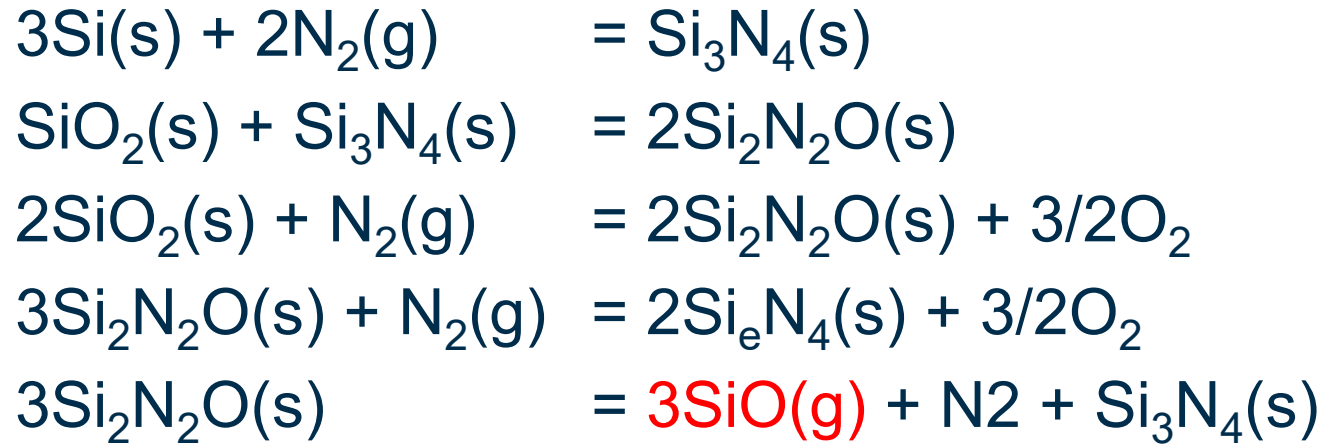


# Introduction

- $\text{SiC(s)} + 2\text{H}_2\text{O(aq,g)} = \text{SiO}_2\text{(s)} + \text{CH}_4\text{(g)}$
- $\text{SiC(s)} + 2\text{H}_2\text{O(aq,g)} = \text{SiO}_2\text{(s)} + 2\text{H}_2\text{(g)} + \text{C(s)}$
- $\text{SiC(s)} + 3\text{H}_2\text{O(aq,g)} = \text{SiO}_2\text{(s)} + 3\text{H}_2\text{(g)} + \text{CO(g)}$  **passive oxidation**
- **$\text{SiC(s)} + 4\text{H}_2\text{O(aq,g)} = \text{SiO}_2\text{(s)} + 4\text{H}_2\text{(g)} + \text{CO}_2\text{(g)}$**
- **$\text{SiO}_2\text{(s)} + 2\text{H}_2\text{O(aq)} = \text{Si(OH)}_4\text{(aq)}$**
- $\text{SiC(s)} + \text{H}_2\text{O(g)} = \text{SiO(g)} + \text{CO(g)}$  (for low  $p_{\text{O}_2}$ ) **active oxidation**
- **$2\text{SiO}_2\text{(s,l)} + \text{SiC(s)} = 3\text{SiO(g)} + \text{CO(g)}$  (at VHT)**



# Introduction



consumption of the protective  
SiO<sub>2</sub> scale

relevant at T > 1700°C

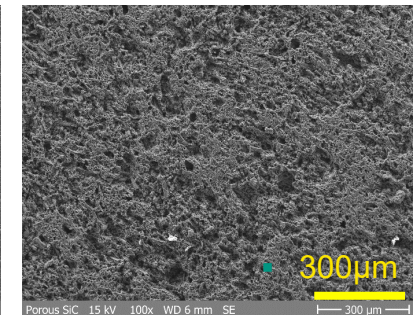
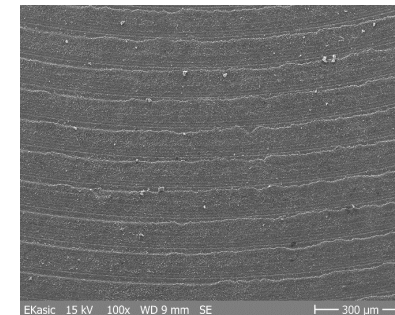
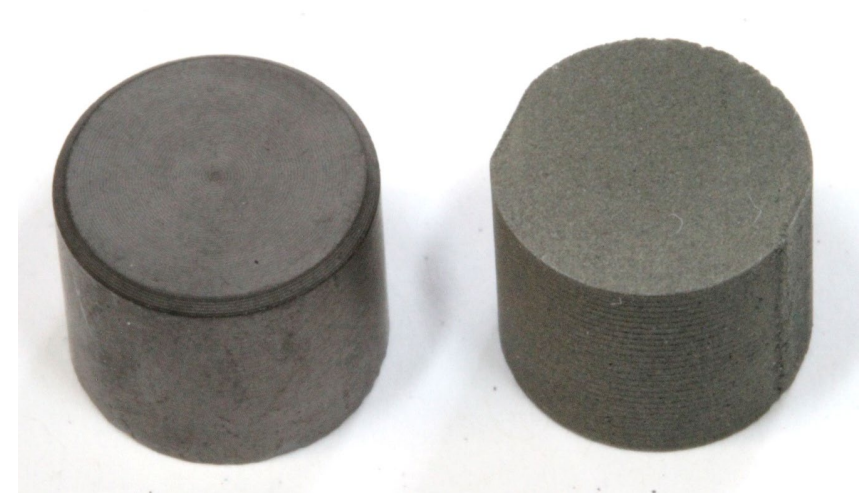


# Materials and test conditions

	compact SiC	Porous SiC
Origin	EKasic®	FAU Erlangen
Density [g/cm <sup>3</sup> ]	3.17 ± 0.050	1.19 ± 0.055
Percentage of theoretical density	98.6 ± 1.6 %	37.1 ± 1.7 %

## Atmospheres:

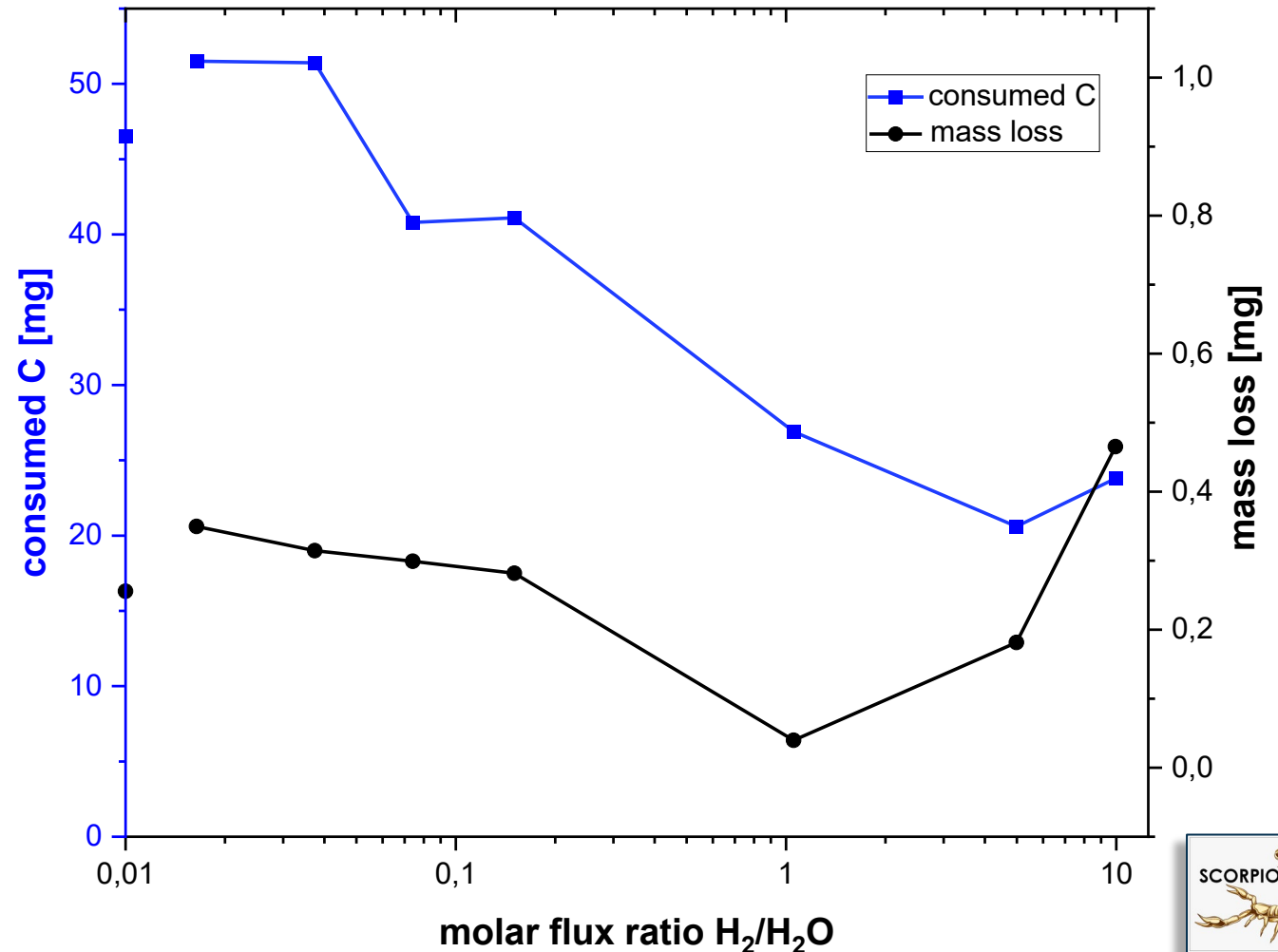
- Steam (passive oxidation)
- H<sub>2</sub> + steam (active oxidation)
- Air (passive oxidation?)
- Oxygen (passive oxidation)



# Materials and test conditions

Transition of passive to active oxidation in the range of the molar flux ratio  $H_2/H_2O$  of 1 .. 5.

High hydrogen concentrations can occur locally in cracks or pores.

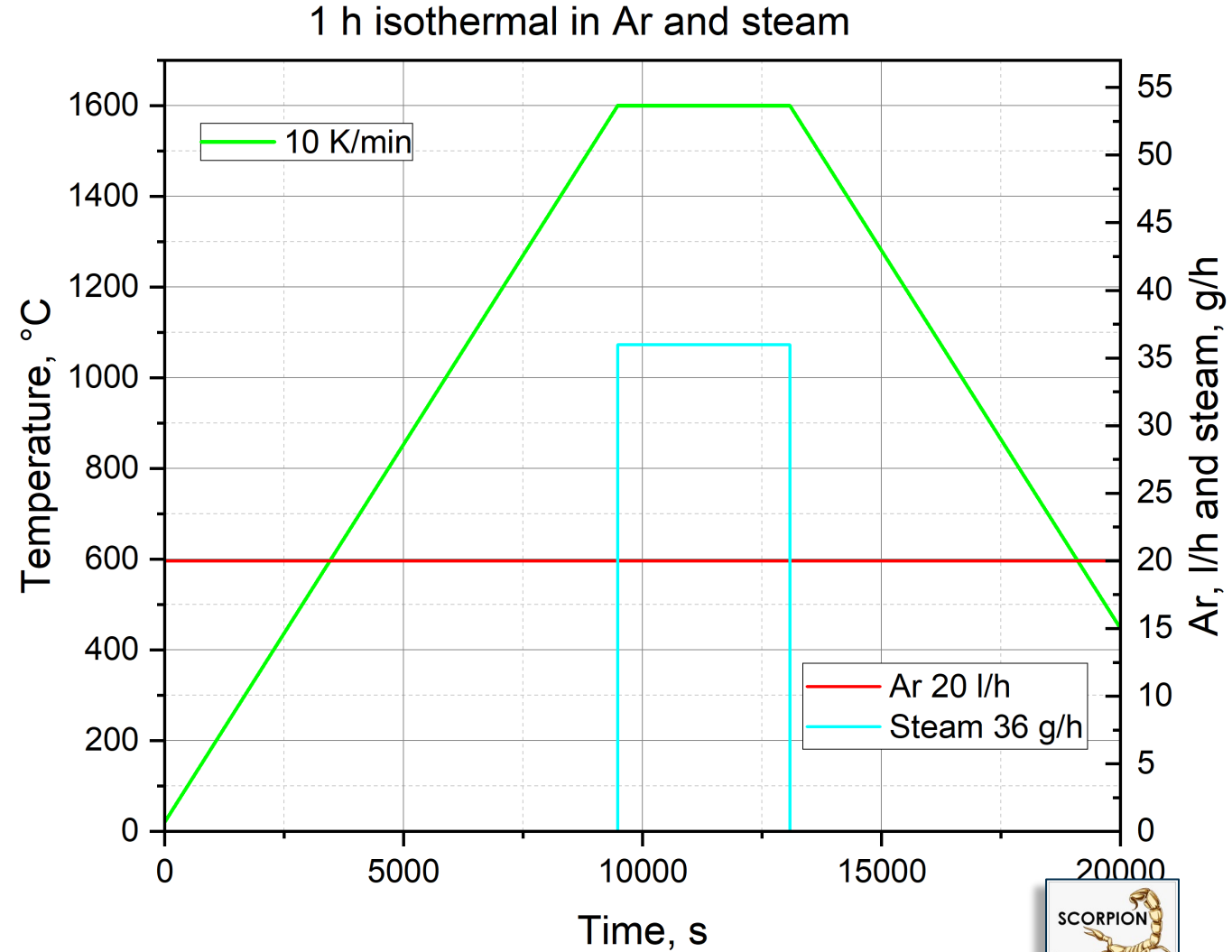




# Materials and test conditions

**Total gas flows were kept constant (65 l/h)**

- 20 l/h Ar + 36 g/h ( ~45 l/h) steam
- 20 l/h Ar + 38 g/h H<sub>2</sub> + 6 g/h (~7 l/h) steam
- 20 l/h Ar + 45 l/h air
- 20 l/h Ar + 45 l/h O<sub>2</sub>

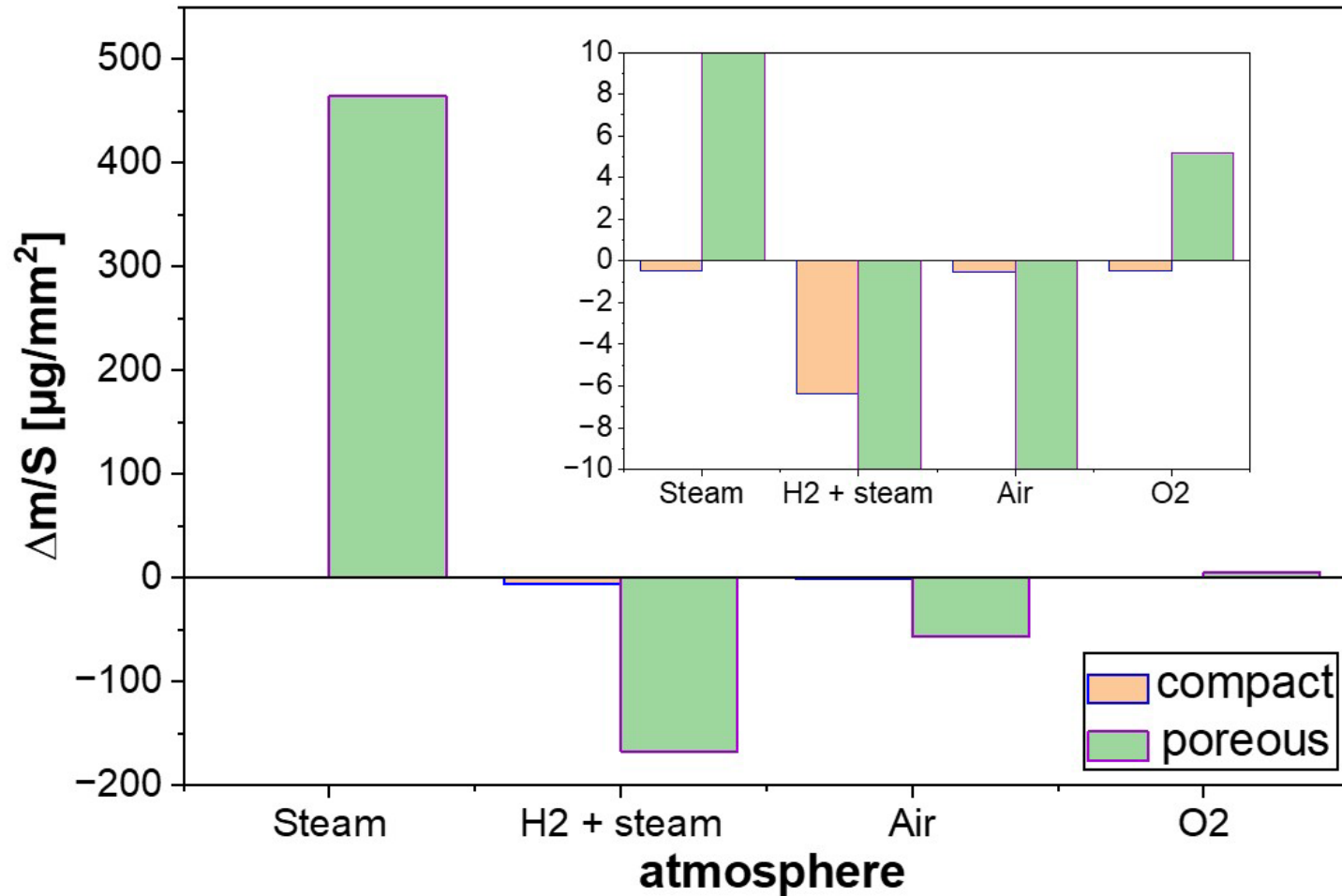


# Results

Sample	steam	H <sub>2</sub> + steam	air	oxygen
compact				
porous				



# Results



Orders of magnitude higher mass changes in the porous material

Only mass lost of the compact material

Mass gain of the porous material in steam and oxygen

Mass change is higher in steam than in hydrogen steam for the compact material

Effect of nitrogen:

- chemical reaction
- blockage of the oxygen transport into the pores



# Results

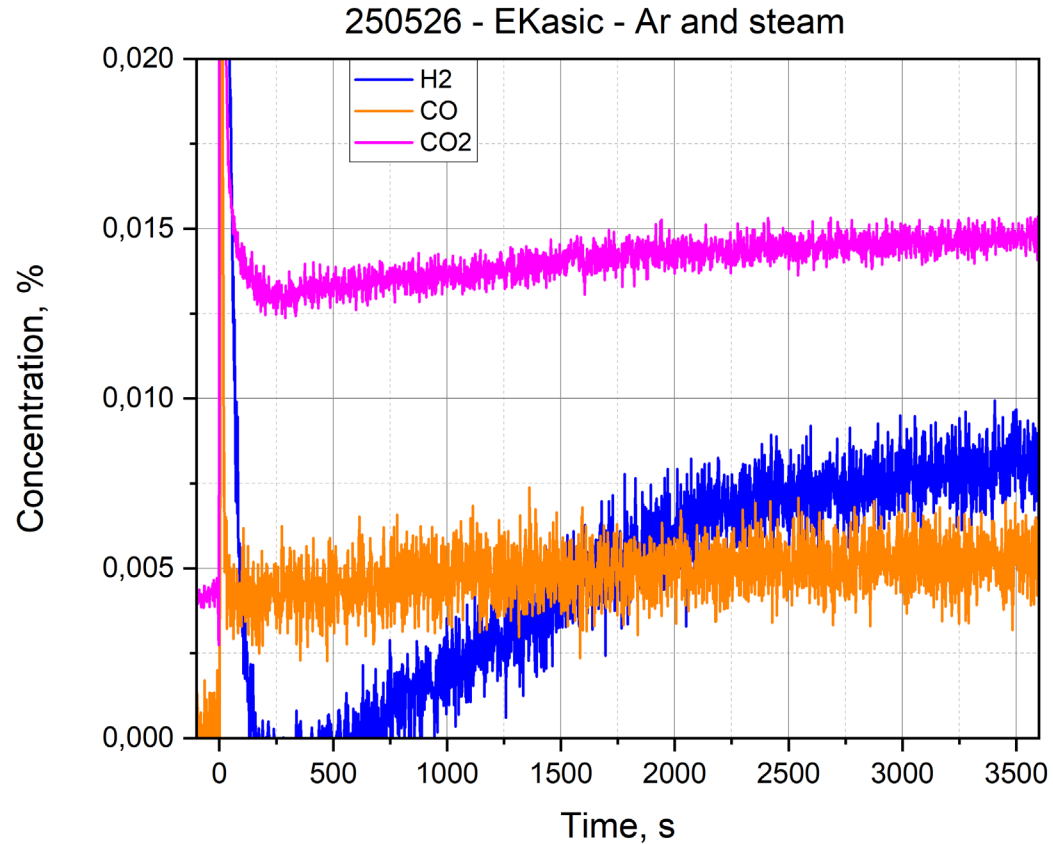
	Compact SiC	Porous SiC
steam	-0.49 g/m <sup>2</sup>	464.3 g/m <sup>2</sup>
H <sub>2</sub> + steam	-6.36 g/m <sup>2</sup>	-157.3 g/m <sup>2</sup>
air	-0.54 g/m <sup>2</sup>	-57.2 g/m <sup>2</sup>
oxygen	-0.49 g/m <sup>2</sup>	6.2 g/m <sup>2</sup>

- Nearly the same mass change of the compact samples but strong differences in the mass changes of the porous samples in steam, air and oxygen.
- Higher mass loss in air than in steam or oxygen
  - Reduction of the oxygen partial pressure by the nitrogen resulting in active oxidation?
  - Chemical interactions with nitrogen? Formation of Si<sub>3</sub>N<sub>4</sub> or Si<sub>2</sub>N<sub>2</sub>O?
- Closing of open porosity in oxygen but not in steam.

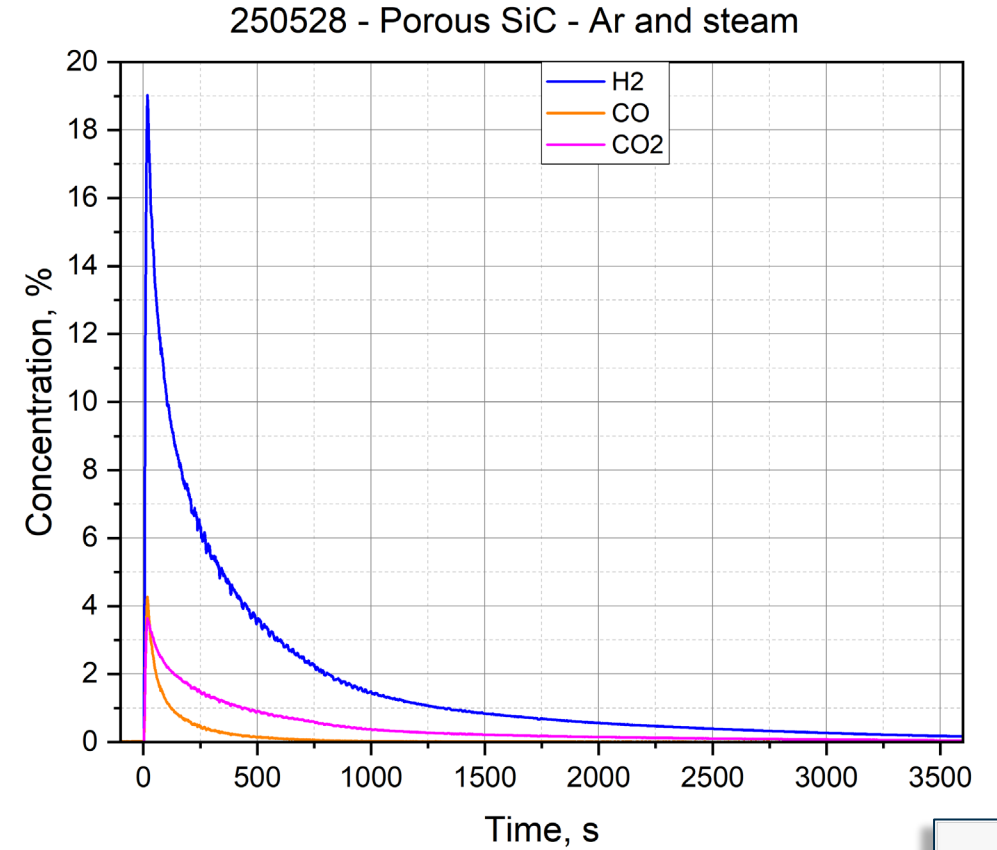


# Results

## Gas release during reaction in steam



**Compact material**

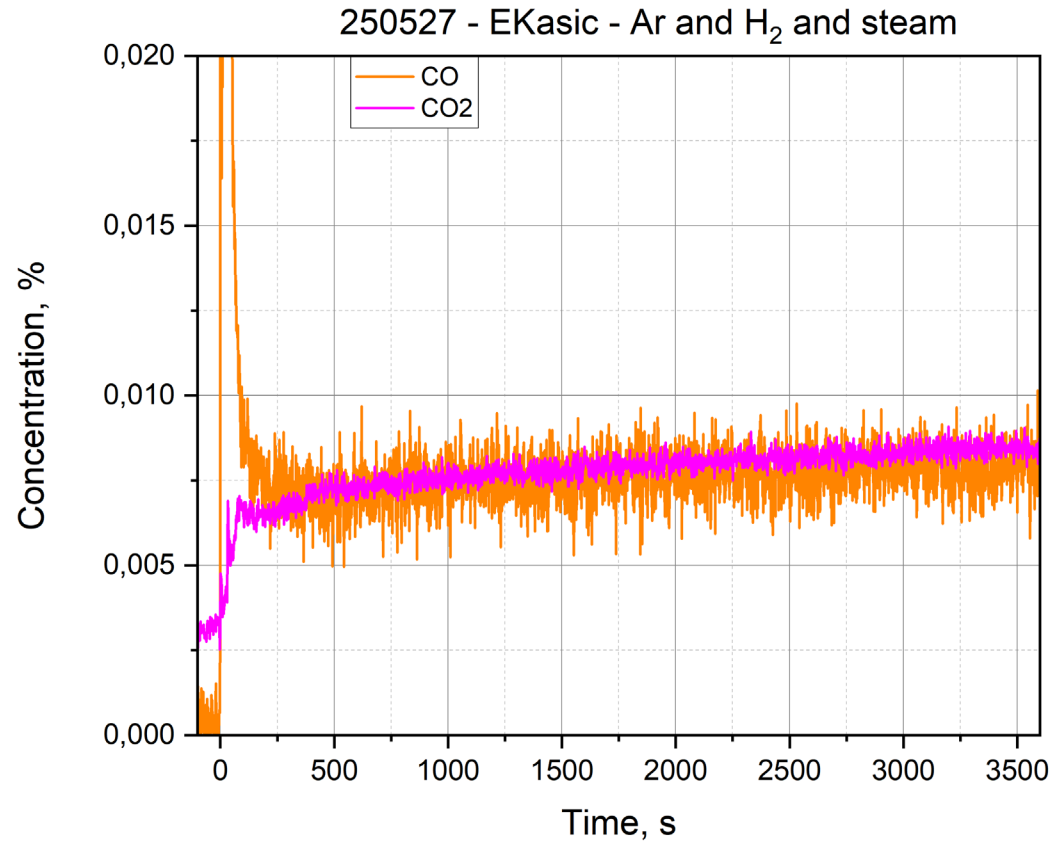


**porous material**

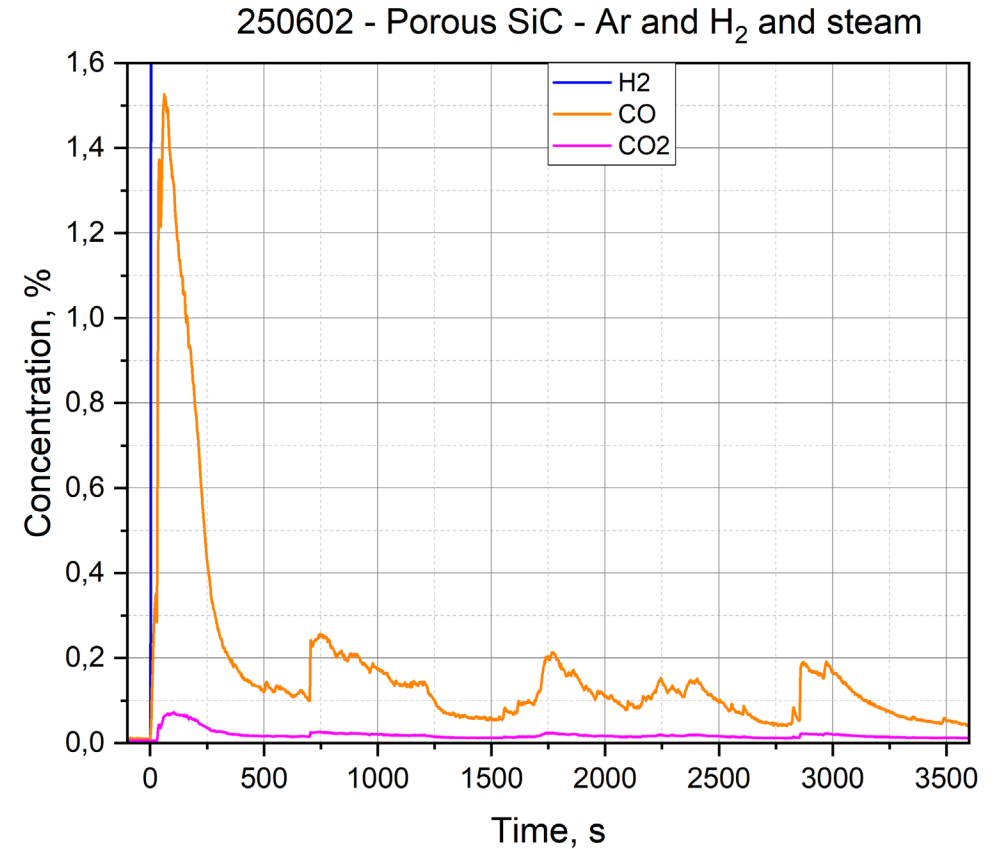


# Results

## Gas release during reaction in hydrogen + steam



**Compact material**

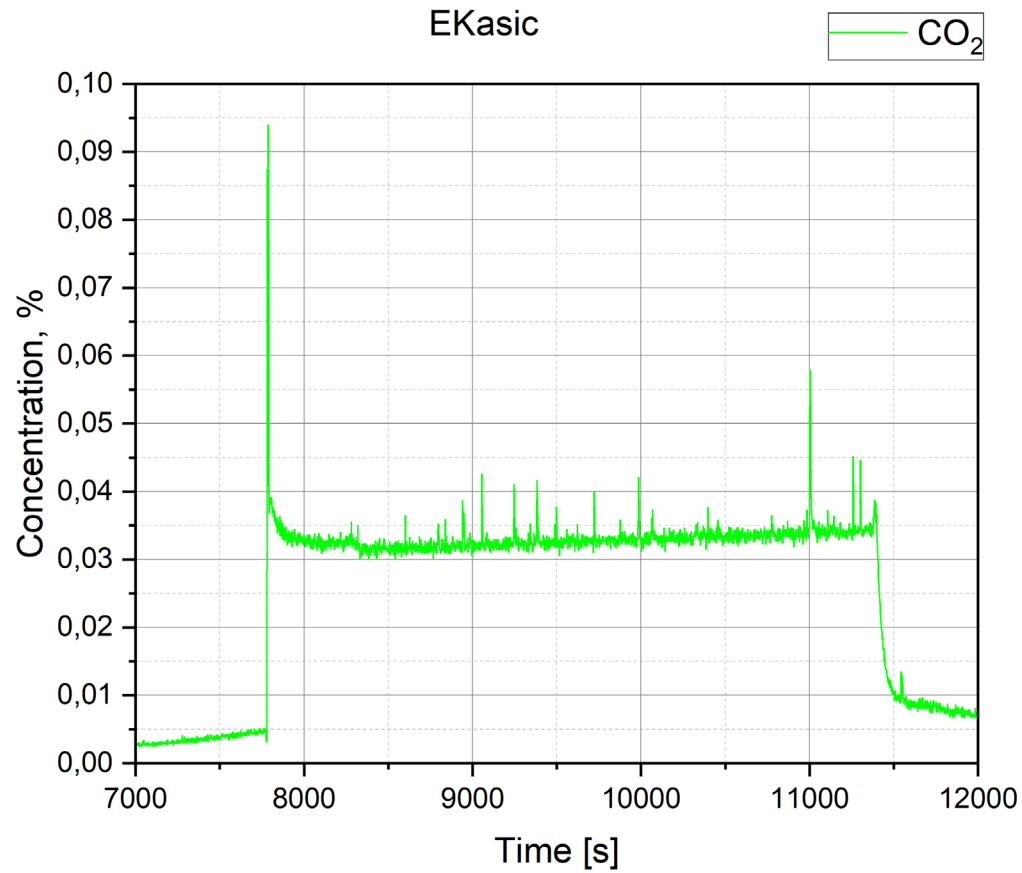


**porous material**

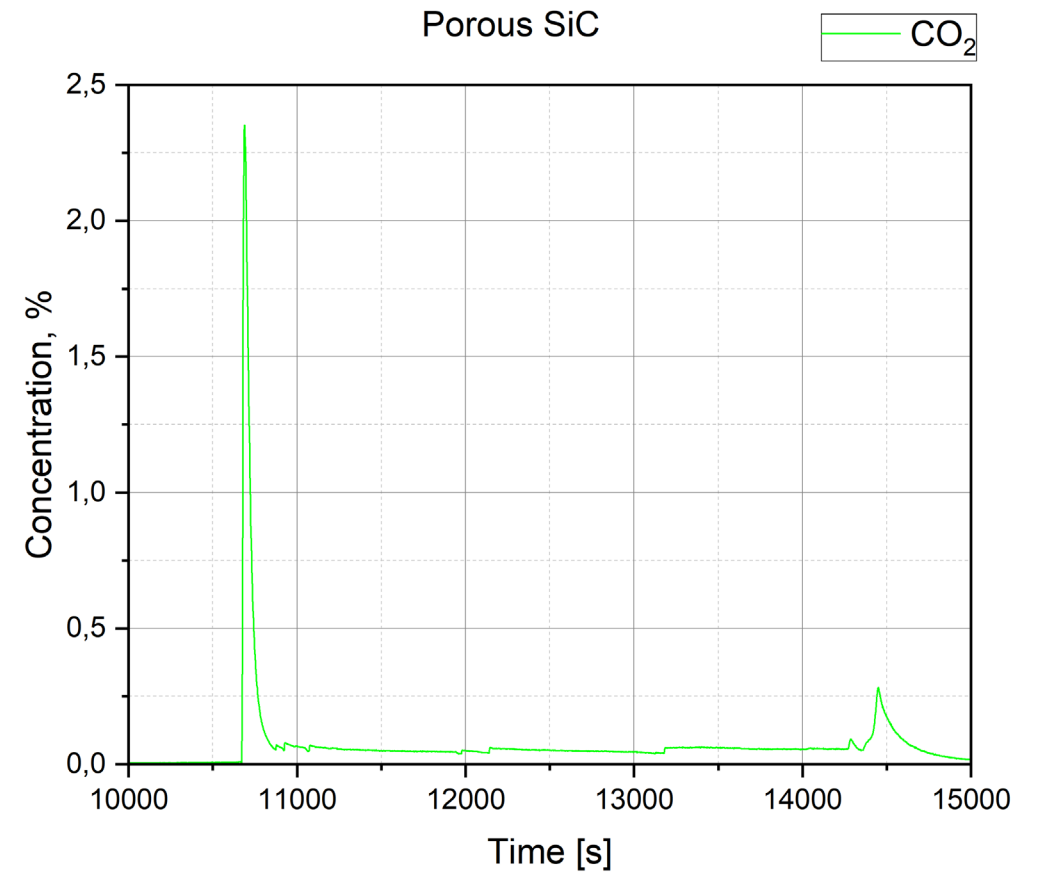


# Results

## Gas release during reaction in air



**Compact material**

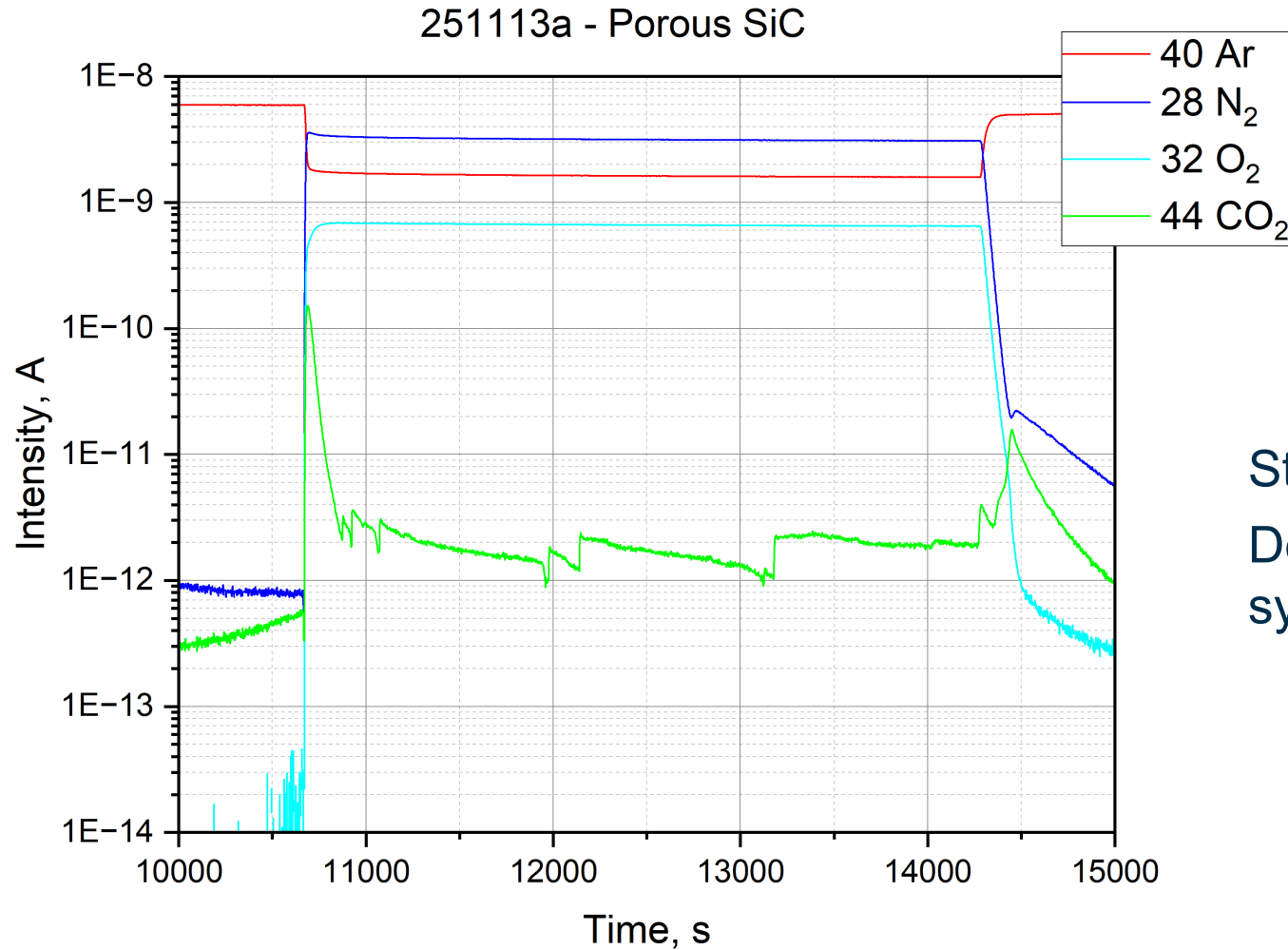


**porous material**



# Results

## Gas release during reaction in air



Steps in the CO<sub>2</sub> release

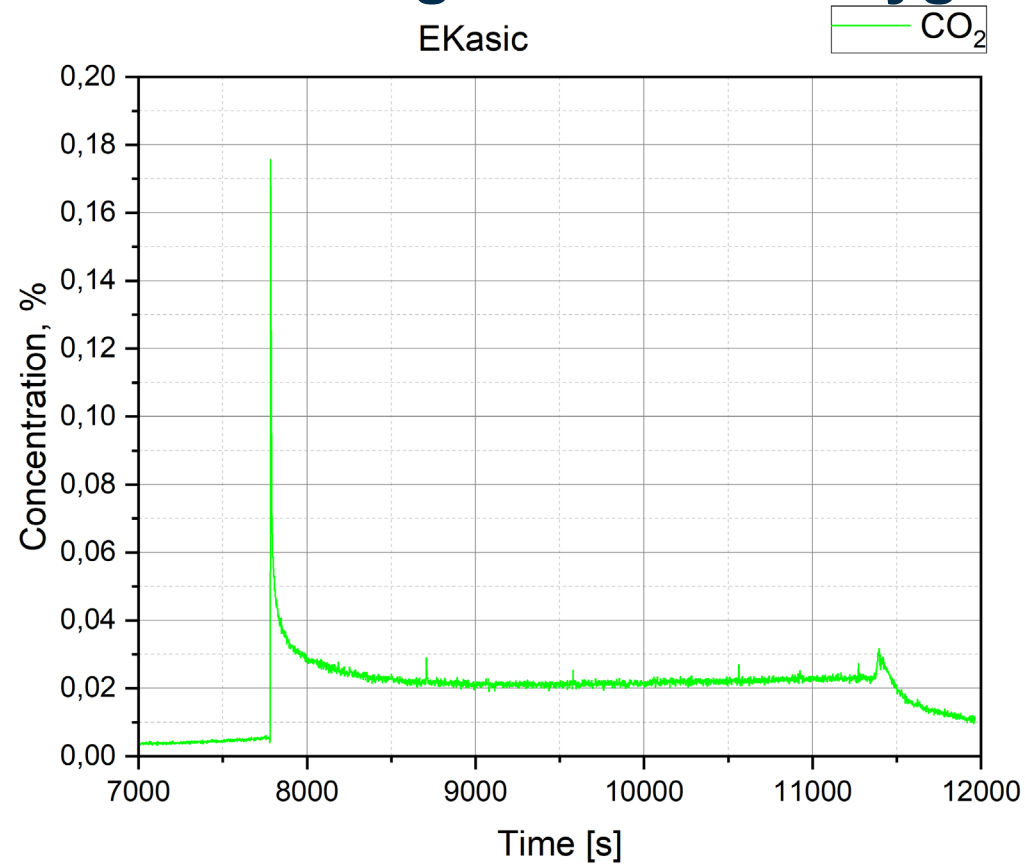
Does the oxidation opens new pore systems below the surface?



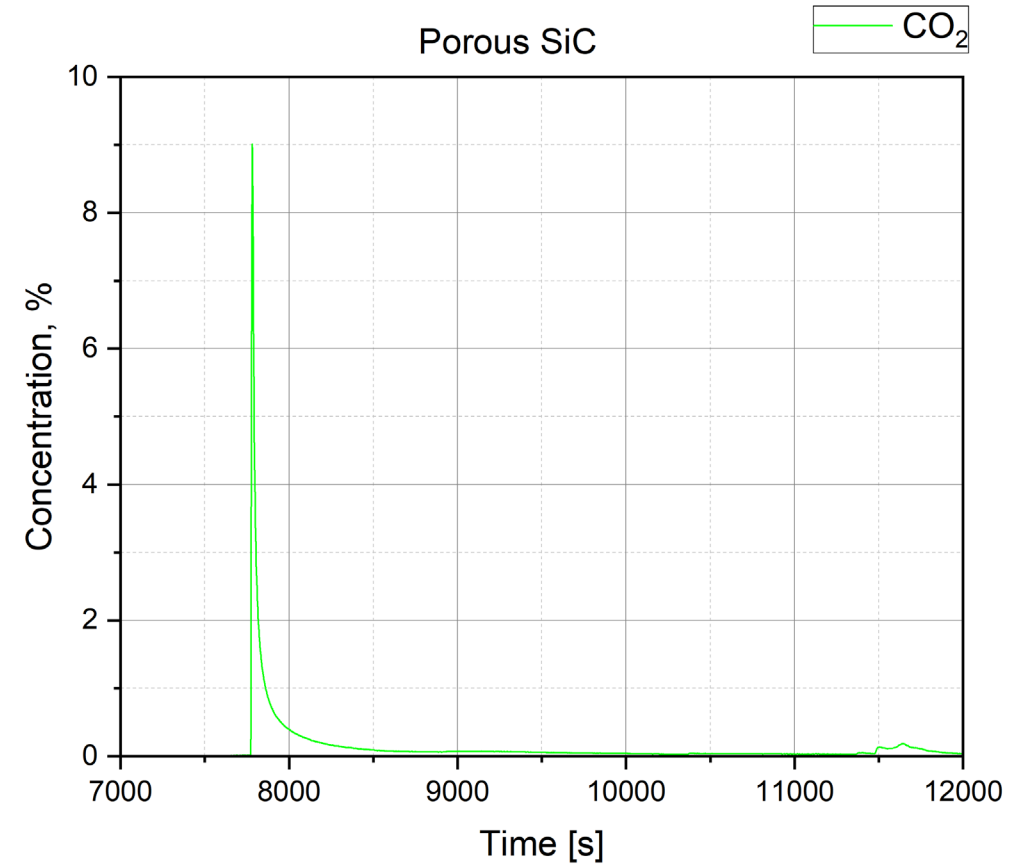


# Results

## Gas release during reaction in oxygen



**Compact material**



**porous material**

# Conclusions and Next Steps

- Open porosity results in a much higher reaction rate because of the larger reacting surface.
- The open porosity is not closed in steam but in oxygen. The reason is the formation of volatile  $\text{Si(OH)}_4$  in steam.
- The mass loss is in air higher than in steam and oxygen. Reasons can be the reduction of the oxygen partial pressure in air and/or the formation of  $\text{Si}_3\text{N}_4$  or  $\text{Si}_2\text{N}_2\text{O}$ .

**Prevent contact of porous part of the CMC with steam, oxygen or air!**

**Next step:** Corrosion and high temperature oxidation tests with coated SiC CMC tube segments.



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Many thanks to Ulrike Stegmaier for performing the tests and the post-test analyses.

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# Thank you for your attention!

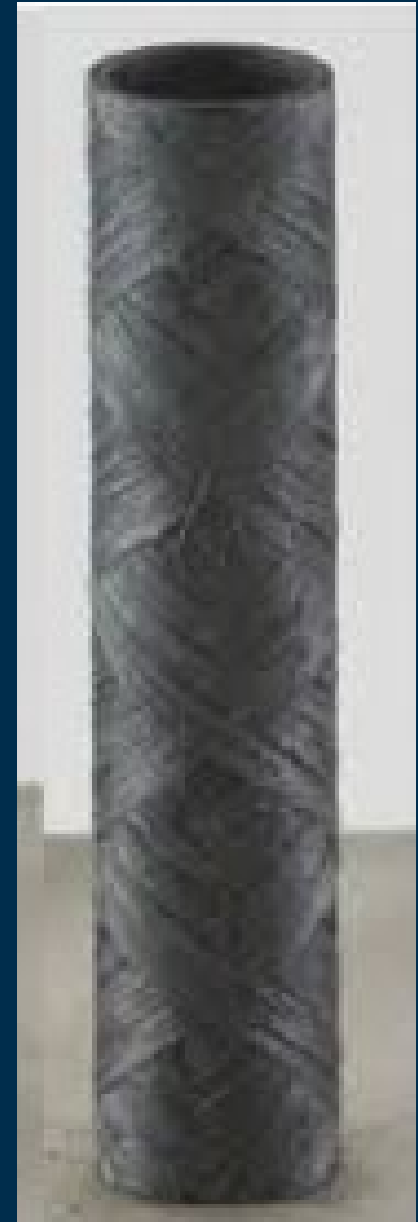




# Update of the KIT contributions to the SCORPION project

Ulrike Stegmaier, Mirco Grosse, Martin Steinbrück, Tobias Fey,  
Konstentza Lambrinou

30. Intern. QUENCH Workshop,  
KIT Campus North, 2025/12/18



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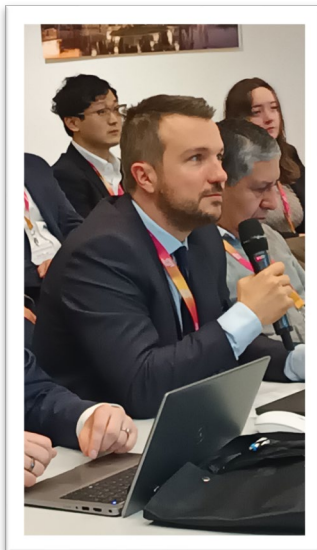
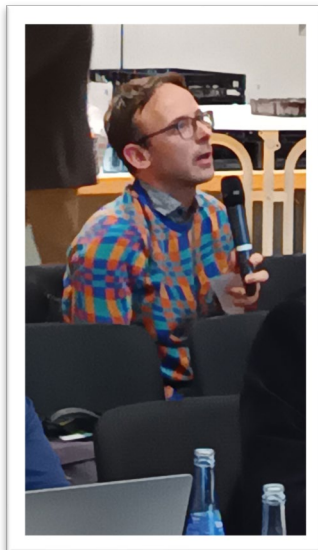
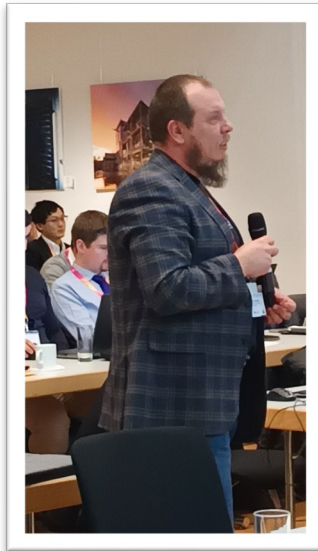
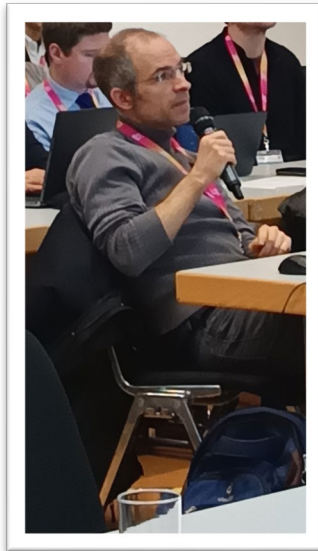
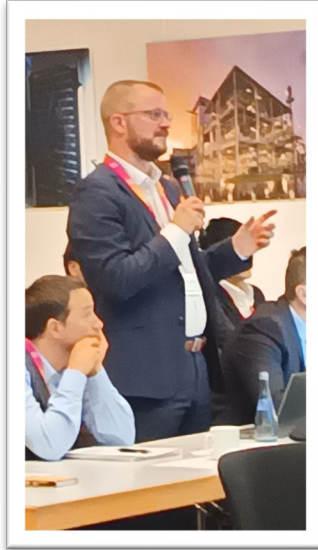
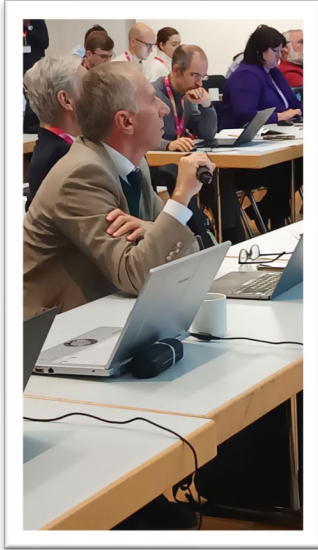
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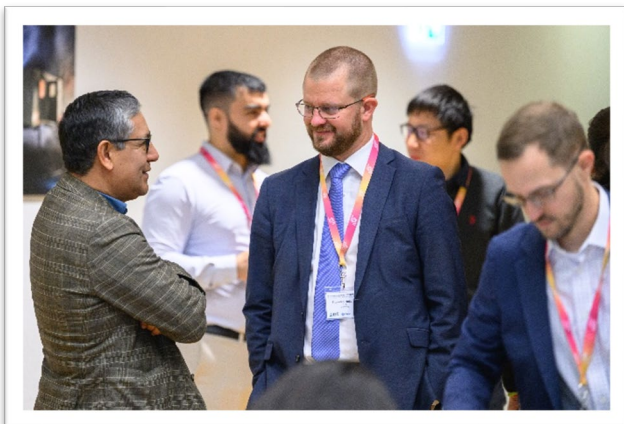
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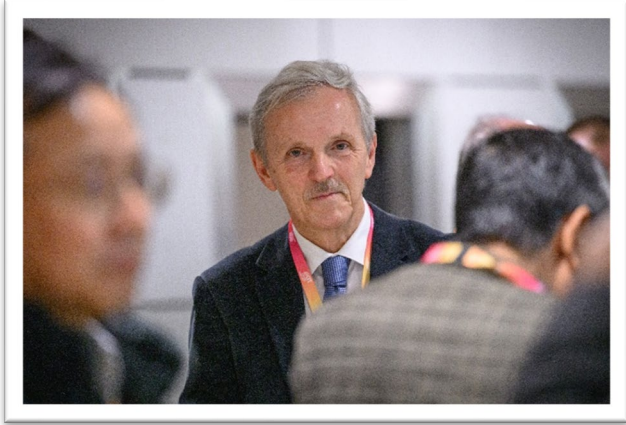
















Any comments, corrections,  
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