



# Experimental investigation and thermodynamic assessment of Cr-Mo-Si ternary system

**Arun Ramasamy Chitra, Chongchong Tang, Carsten Schroer, Bronislava Gorr**

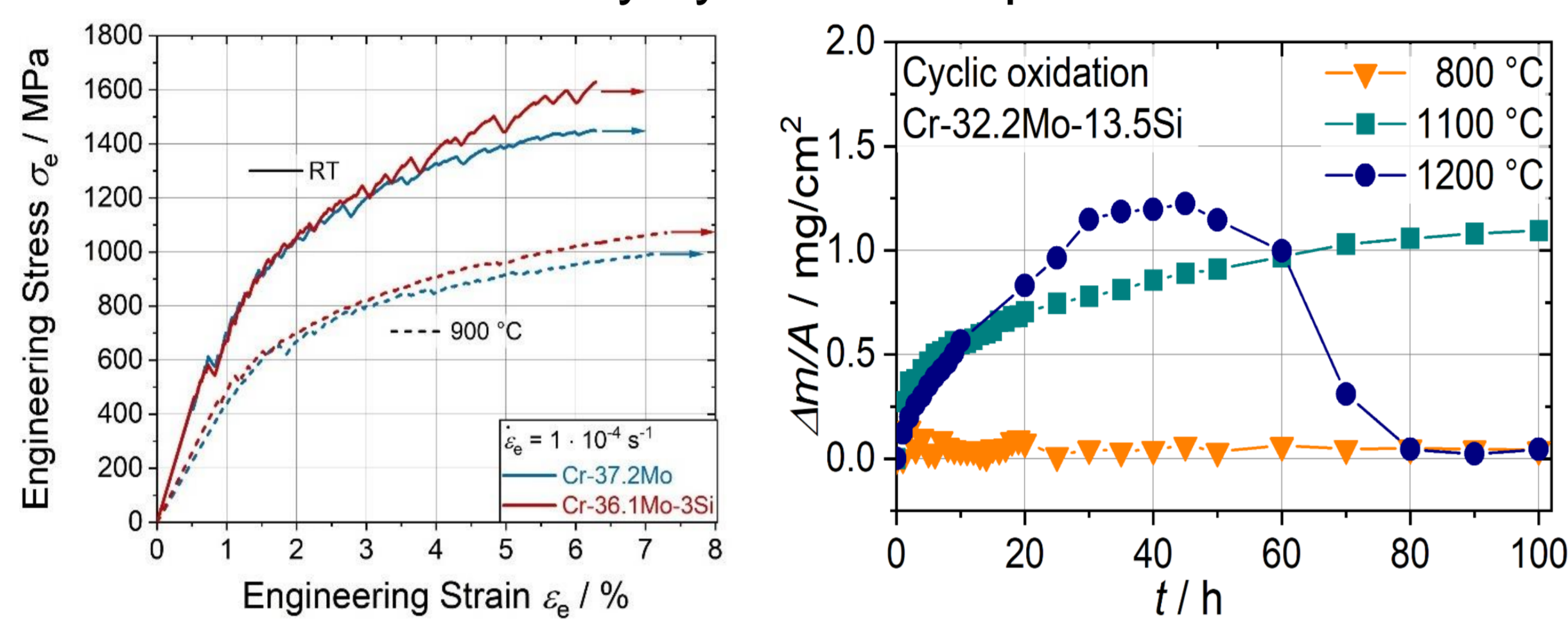
Karlsruhe Institute of Technology, Institute for Applied Materials – Applied Materials Physics (IAM-AWP)

Kaiserstraße 12, 76131 Karlsruhe, Germany

e-mail: arun.chitra@kit.edu

## Introduction and Motivation

- Alloys containing high concentrations of refractory metals demonstrate promising properties for high temperature applications [1].
- Unique property profile of newly developed alloy Cr-32.2Mo-13.5Si: plasticity at RT and oxidation resistance [2].
- Commercial thermodynamic database of the Cr-Mo-Si ternary system does not provide reliable results - thermodynamic assessment of this ternary system is required.



Compression tests (left) and cyclic oxidation behavior (right) of Cr-32.2Mo-13.5Si alloys

## Experimental Section

- Modelling approach → CALPHAD (CALculation of PHase Diagrams)
- Alloys are manufactured by arc melting in argon atmosphere.
- Phase constitution is identified by powder XRD and SEM/BSE.
- Chemical composition of the phases is measured by Electron probe microanalysis (EPMA).
- Phase transition, solidus and liquidus temperatures are investigated by high-temperature differential thermal analysis (DTA) (ongoing studies).



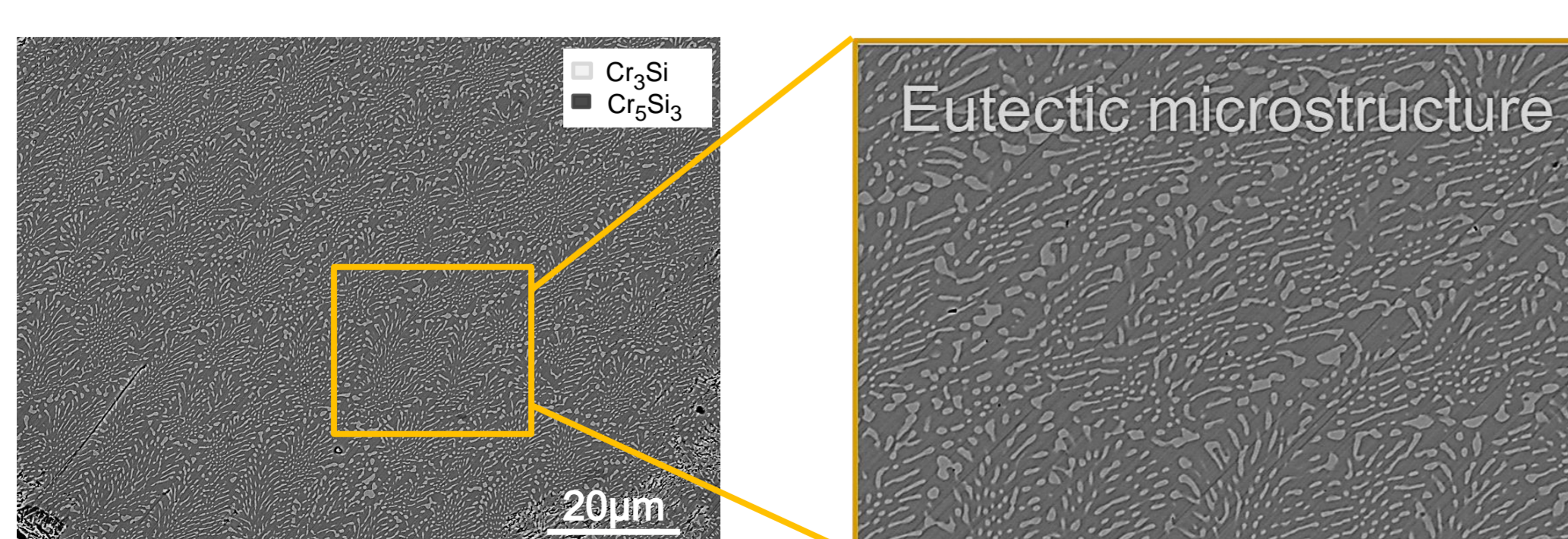
## Binary Subsystems

### Mo-Si and Cr-Mo systems:

- Mo-Si and Cr-Mo binary systems are well-assessed, and their thermodynamic description is adopted from [3] and [4], respectively.

### Cr-Si system:

- Available experimental and theoretical data on Cr-Si system do not allow to precisely determine the solidification behavior of the alloy 65Cr-35Si (at.%) and the phase transition (allotropic transformation) from  $\alpha$ -Cr<sub>5</sub>Si<sub>3</sub> to  $\beta$ -Cr<sub>5</sub>Si<sub>3</sub> above 1500°C.
- Our results on 65Cr-35Si confirms the eutectic solidification of Cr<sub>3</sub>Si and Cr<sub>5</sub>Si<sub>3</sub> phases.



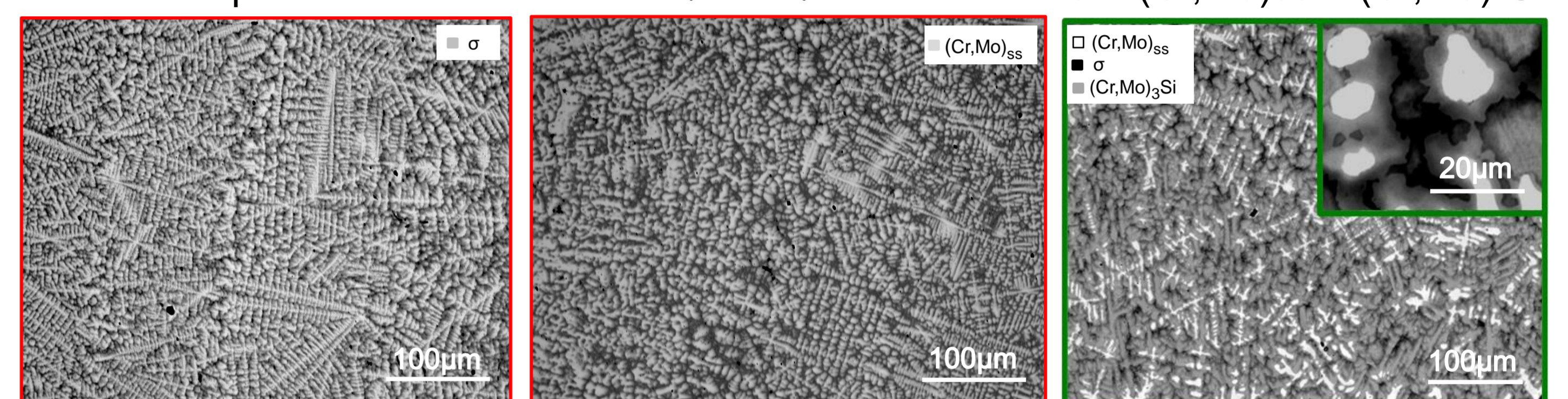
## Experimental Results of Cr-Mo-Si Alloys

### As-cast alloys (composition in at.%)

- To determine the solidification behavior, a series of Cr-Mo-Si alloys was produced and the results are reported below.

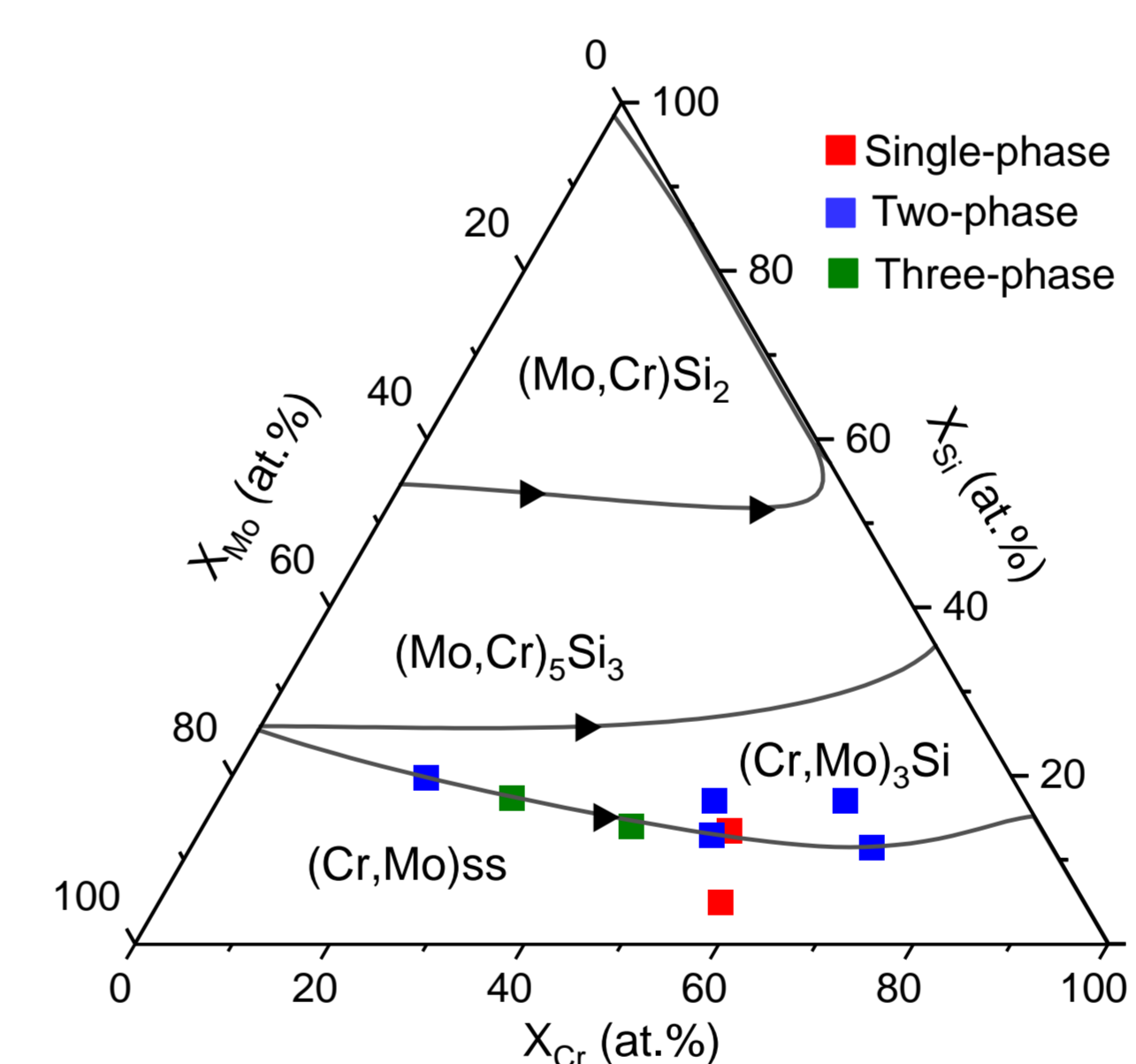
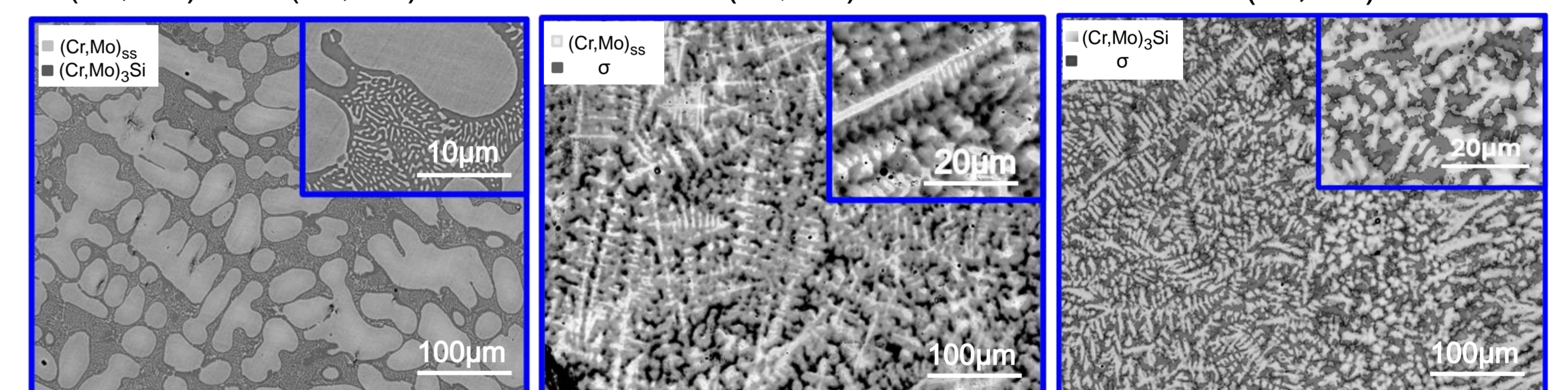
**Single-phase microstructure** **Three-phase microstructure**

54.3Cr-32.2Mo-13.5Si  $\sigma$  phase  
57.7Cr-37.3Mo-5Si (Cr,Mo)ss  
30Cr-52.6Mo-17.4Si  $\sigma + (Cr,Mo)ss + (Cr,Mo)_3Si$



### Two-phase microstructure

70Cr-18.5Mo-11.5Si (Cr,Mo)ss + (Cr,Mo)<sub>3</sub>Si  
52.8Cr-34.2Mo-13Si  $\sigma + (Cr,Mo)ss$   
51Cr-32Mo-17Si  $\sigma + (Cr,Mo)_3Si$



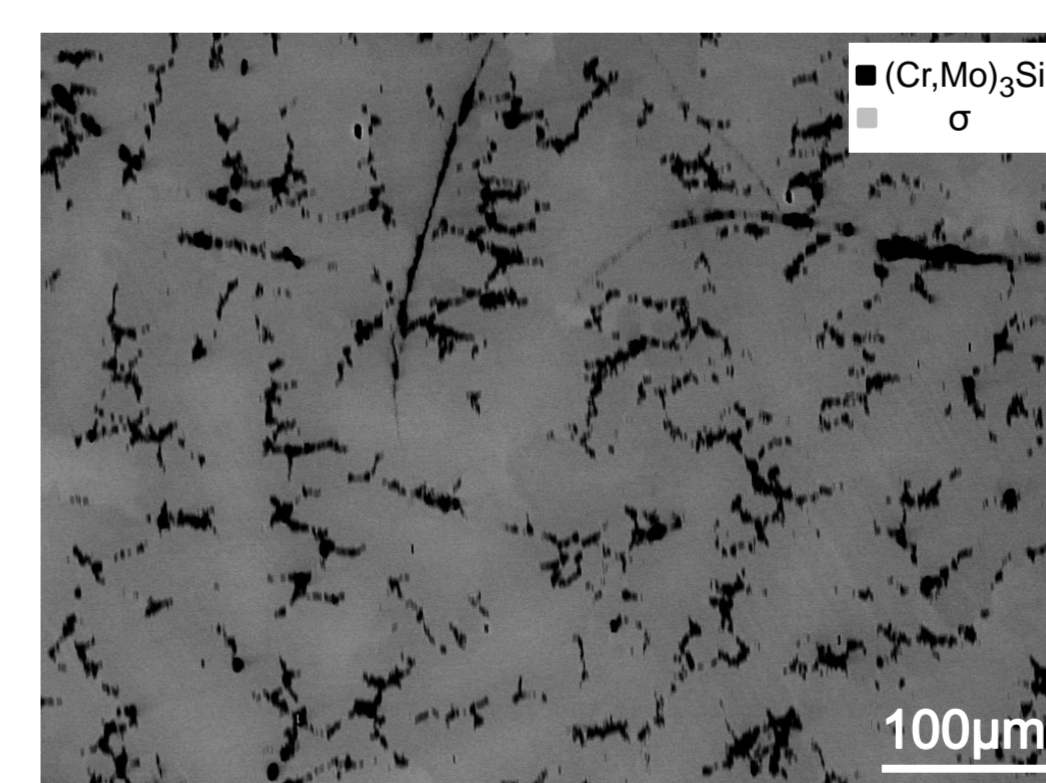
- As-cast alloys exhibit dendritic microstructure.
- Cr-rich (Alloy 70Cr-18.5Mo-11.5Si) and Si-poor (Alloy 57.7Cr-37.3Mo-5Si) regions does not contain  $\sigma$  phase.

Calculated liquidus projection using commercial Cr-Mo-Si database

### Thermally-treated alloys

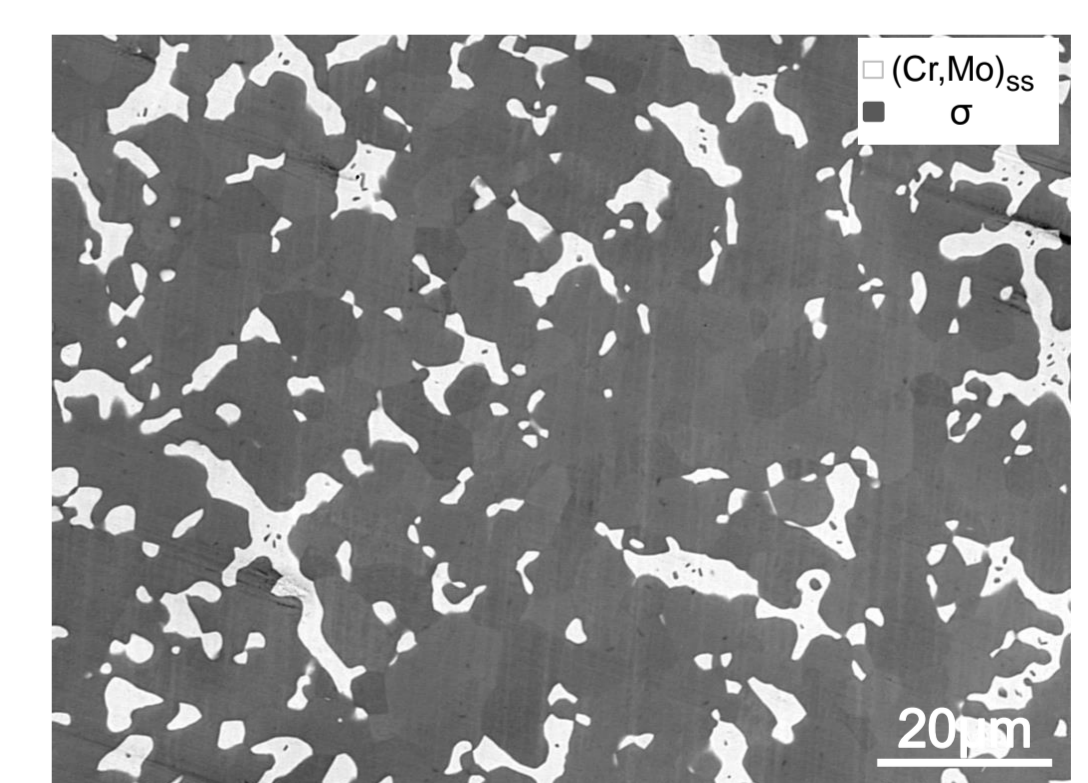
- To investigate phase equilibria (1500°C, 70h, Ar).

54.3Cr-32.2Mo-13.5Si



$\sigma \rightarrow \sigma + (Cr,Mo)_3Si$

30Cr-52.6Mo-17.4Si



$\sigma + (Cr,Mo)_3Si + (Cr,Mo)ss \rightarrow \sigma + (Cr,Mo)ss$

## Conclusions and Outlook

- Eutectic solidification path of the alloy 65Cr-35Si is established.
- One-, two- and three-phase microstructure in Cr-Mo-Si alloys (as-cast state) are investigated.
- First experimental evidence of  $\sigma$  phase formation at high Si content in Cr-Mo-Si alloys.
- Thermodynamic reassessment of Cr-Si system and further development of the database for Cr-Mo-Si system are pending.

[1] J.H. Perepezko, Science 326, 1068 (2009)

[2] F. Hinrichs et al., Corrosion Science 207, (2022), 110566

[3] A. Czerny et al., AEM (2024), 2302085

[4] K. Frisk et al., Calphad 12, 247-254 (1988)