

Luis Ávila¹, Y. Shakeel, A. Gedsun, M. Forti, S. Hunke, Y. Han, R. Aversa, J. Olbricht, T. Hammerschmidt, M. Chmielowski, R. Stotzka, E. Bitzek, T. Hickel, B. Skrotzki

¹ BAM (Federal Institute for Materials Research and Testing)



NATIONAL RESEARCH DATA
INFRASTRUCTURE FOR MATERIALS
SCIENCE & ENGINEERING

Framework for Curation and Distribution of Reference Datasets on the Example of Creep Data of Ni- Based Superalloys (IUC02)

International Materials Science and
Engineering Congress - MSE 2024

2024-09-26

Funded by

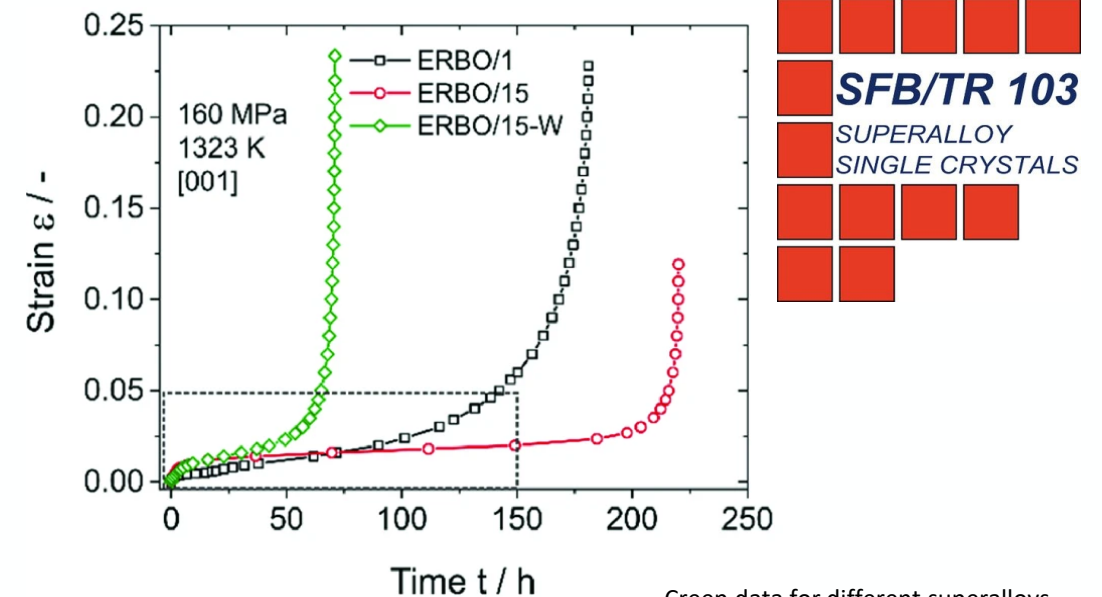
DFG Deutsche
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Introduction and Motivation

- Ni-based superalloys
 - High technical relevance
 - Optimization potential
- Possible usages of a *reference dataset*:
 - Re-use of data to generate new knowledge (e.g., as baseline for alloy design and optimization)
 - Reproduce experiments, e.g., to calibrate creep experiments in the own lab or computational procedures/algorithms
- Documentation/Metadata often incomplete or hardly accessible 😞 → FAIR
- Specially high requirements in terms of
 - **Documentation** (functionality) and
 - **Digital representation** (usability)



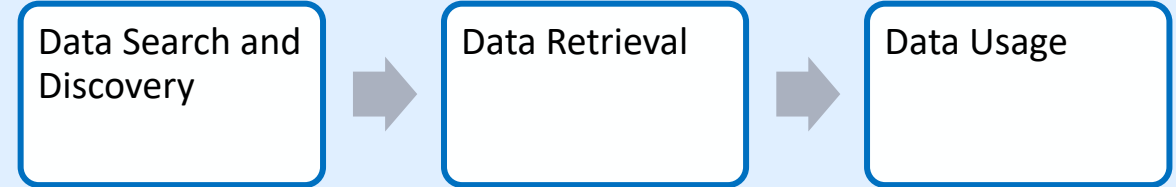
Creep data for different superalloys
(Horst et al, Superalloys 2020)

Overview of the Proposed Framework

Data Generation and Provision



Data Identification and Usage



➤ Definition for *Reference Data*



[Hickel et al.,
10.5281/zenodo.11667673]

- *Research data of exceptionally high quality*
- FAIR
- Functional (Documentation) and usable (Digital Representation)

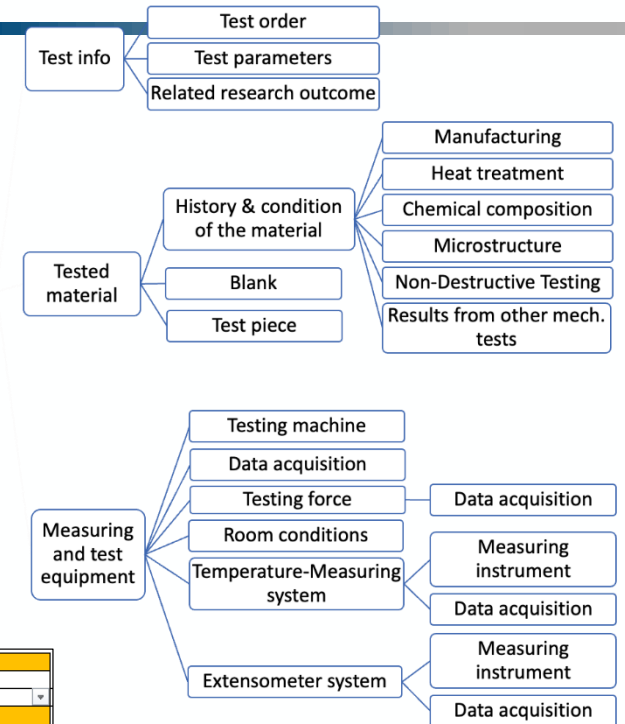
- Data schema
- Data provision and downstream usage possibilities
 - Data discovery and usage - FAIR digital object
 - Semantic structuring, ontology development

Data Schema



[Ávila C. et al.,
10.5281/zenodo.11668375]

- List of possible and use-case-related minimum requirements
- Defined **vocabulary**
- RDM Tool to enhance documentation practices
- Template for other methods
- Basis for shaping, sharing, and structuring the data



ENTRY	SYMBOL	UNIT	DATA TYPE	ICS 77.040.10	DIN EN ISO 204	Requirement	Code	JSON Schema
Date of test start			Date			Mandatory	65	<pre> "specifiedTestParameters": { "type": "object", "required": ["testingStandard", "specifiedTemperature", "initialStress", "testType", "endOfExperiment"], "properties": { "testingStandard": { "type": "string" }, "specifiedTemperature": { "description": "Symbol usually indicated as T", "\$ref": "#/\$defs/ComplexValue" }, "initialStress": { "description": "Symbol usually indicated as \$R_{f0}\$", "\$ref": "#/\$defs/ComplexValue" }, "testType": { "type": "string" }, "endOfExperiment": { "type": "string" }, "testForce": { "\$ref": "#/\$defs/ComplexValue" } } } </pre>
Date of test end			Date			Mandatory	66	
Test ID			Alphanumeric			Mandatory	67	
Project			Alphanumeric			Mandatory	68	
Test order			Alphanumeric			Optional	69	
Was the test performed according to a test standard?			Drop-down list			Mandatory	70	
Test standard			Alphanumeric			Mandatory	71	
Specified temperature	T	°C	Numeric			Mandatory	72	
Type of loading			Drop-down list			Mandatory	73	
Load control type			Drop-down list			Mandatory	74	
Initial stress	R _e	MPa	Numeric			Mandatory	75	
Test type			Drop-down list			Mandatory	76	
End of test criterium			Drop-down list			Mandatory	77	
End of test criterium - value (if not test piece break)			Numeric			Mandatory	78	
Test force		kN	Numeric			Optional	79	
Preload (Part of the test force)		kN	Numeric			Mandatory	80	
Other additional information (e.g. if constant stress)			Text			Optional	81	
Related article(s) available?			Drop-down list			Optional	82	
DOI Article 1			Alphanumeric / Link			Optional	83	
Short description of content article 1			Text			Optional	84	
DOI Article 2			Alphanumeric / Link			Optional	85	
Short description of content article 2			Text			Optional	86	
DOI Article n			Alphanumeric / Link			Optional	87	
						Optional	88	
						Optional	89	
						Optional	90	
						Optional	91	
						Optional	92	
						Optional	93	
						Optional	94	
						Optional	95	
						Optional	96	

DIN EN ISO 204

ICS 77.040.10

Ersatz für
DIN EN IS

**Metallische Werkstoffe –
Einachsiger Zeitstandversuch unter Zugbeanspruchung –
Prüfverfahren (ISO 204:2023);
Deutsche Fassung EN ISO 204:2023**

Metallc materials –
Uniaxial creep testing in tension –
Method of test (ISO 204:2023);
German version EN ISO 204:2023

<https://doi.org/10.1080/09603409.2016.1186414>

Creep data as published

<https://doi.org/10.1002/adem.201400136>

Description of alloy composition, heat treatment and initial microstructure

Overview of the Proposed Framework

Data Generation and Provision

Data Generation and Documentation

Dataset Handling and Storage

Data Schema

Data Shaping, Sharing, and Publishing

Ontology

Data Identification and Usage

Data Search and Discovery

Data Retrieval

Data Usage

➤ Definition for Reference Data



[Hickel et al., 10.5281/zenodo.11667673]

Materials Data Infrastructure and Ontology Development for Exemplary Reference Dataset

Angelika Godesam, Yusra Shakel, Siroam Hunke, Lutz A. Avila C., Mariano Forti, Thomas Hammerschmidt, Jürgen Ollrich, Rainer Stotzka, Timann Hinkel, Birgit Szostaki

Introduction
Reference data (RD) is reliable data that are of utmost importance for sustainable materials development. Researchers rely on such RD especially for the validation of research results in domains or for materials where data is scarce. Within NFDI-MatWerk, we develop an infrastructure to distribute and validate reference datasets on the example of creep data. With our materials data infrastructure (MDI), we aim to understand and structure data along with its metadata to make it findable, accessible, interoperable, and reusable (FAIR).

In this poster, we present a so-called data journey (niche) depicting the processes and stages within a data lifecycle along with selected elements that are the basis to build our MDI for RD. A commonly-agreed data schema enables machine-actionable representation as FAIR Digital Object (FDO). The main concepts of the dataset are semantically described and represented in the form of the Reference Dataset Ontology for Creep data (RDOC), and integrated into the MSE Knowledge Graph.

Our Goal
Conceptualize & implement a digital infrastructure for:
 • Shaping, storing, sharing
 • Search, discovery, and usage of reference data

Key Takeaways
The infrastructure enables the researcher to:
 • Validate a dataset as a reference dataset → Metadata schema
 • Search/find data → FDO and instantiated ontology

Data Schema
 • List of possible and use-case-related minimum requirements
 • Usage of a defined vocabulary
 • FDOI tool to enhance documentation practices
 • Serves as a template for other methods
 • Basis for creating, sharing, and structuring the data

Schematic View of the Data Journey
 1. Data files are locally stored as CSV, XLS, PDF, etc.
 2. Data organized and prepared for publication
 3. Dataset and data schema are stored in a reference dataset
 4. FDOI tool to generate FDOI
 5. FDOI can be discovered through FDOI search and FDOI viewer

Ontology Development
 • Concepts for a universal Reference Dataset
 • Concepts for a Reference Dataset for Creep Testing

Data Discovery and Usage
 • FAIR Digital Object (FDOI)
 • FAIR DO Graph

Possible usages of reference data
 • Calibration/verification of measurement devices, procedures or algorithms
 • Comparison of data for interpretation of individual measurement results
 • Input for machine learning-based data analytics and for computational materials science (digital twin)
 • Best practice examples for measurement and documentation procedures

➤ Data schema
 ➤ Data provision and downstream usage possibilities

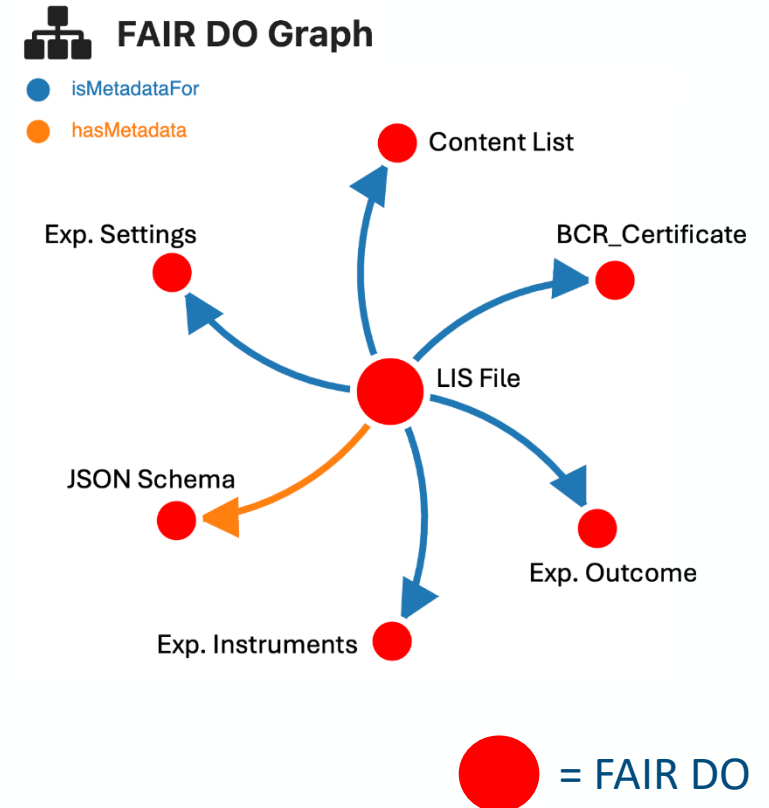
- Data Discovery and Usage - FAIR Digital Object
- Semantic Structuring, Ontology Development

Data Discovery and Usage - FAIR Digital Object

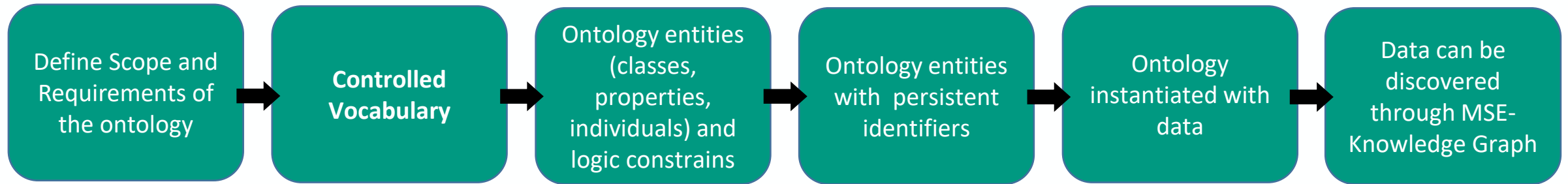
- Contact: Yusra Shakeel, KIT
- Globally accepted representation of research data as a sequence of bits (= a link)

PID	PID Profile	Type	Location URL	...
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- Contains all information towards FAIR
- Conception: technology agnostic
- Enhances data exchange by making FAIR data not only machine readable but also machine actionable across scientific disciplines
- Semantic structuring can complement this concept by incorporating domain-specific expert knowledge in the data discovery and retrieval and thus enhanced interoperability



Semantic Structuring and Ontology development

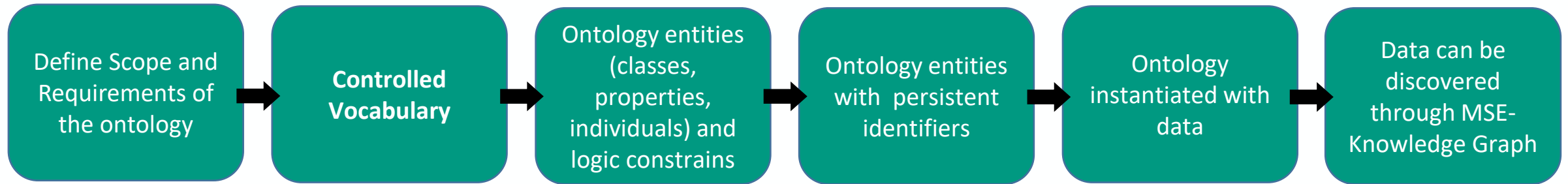


- Contact: Angelika Gedsun, Uni Freiburg
- Representation (semantically structured, annotated) of reference data and specifically creep testing in a conceptual way and aligned with the data schema
 - Concepts for an universal reference dataset
 - Reference Dataset Ontology – Creep (RDOC)



Miro-board for collaboration

Semantic Structuring and Ontology development



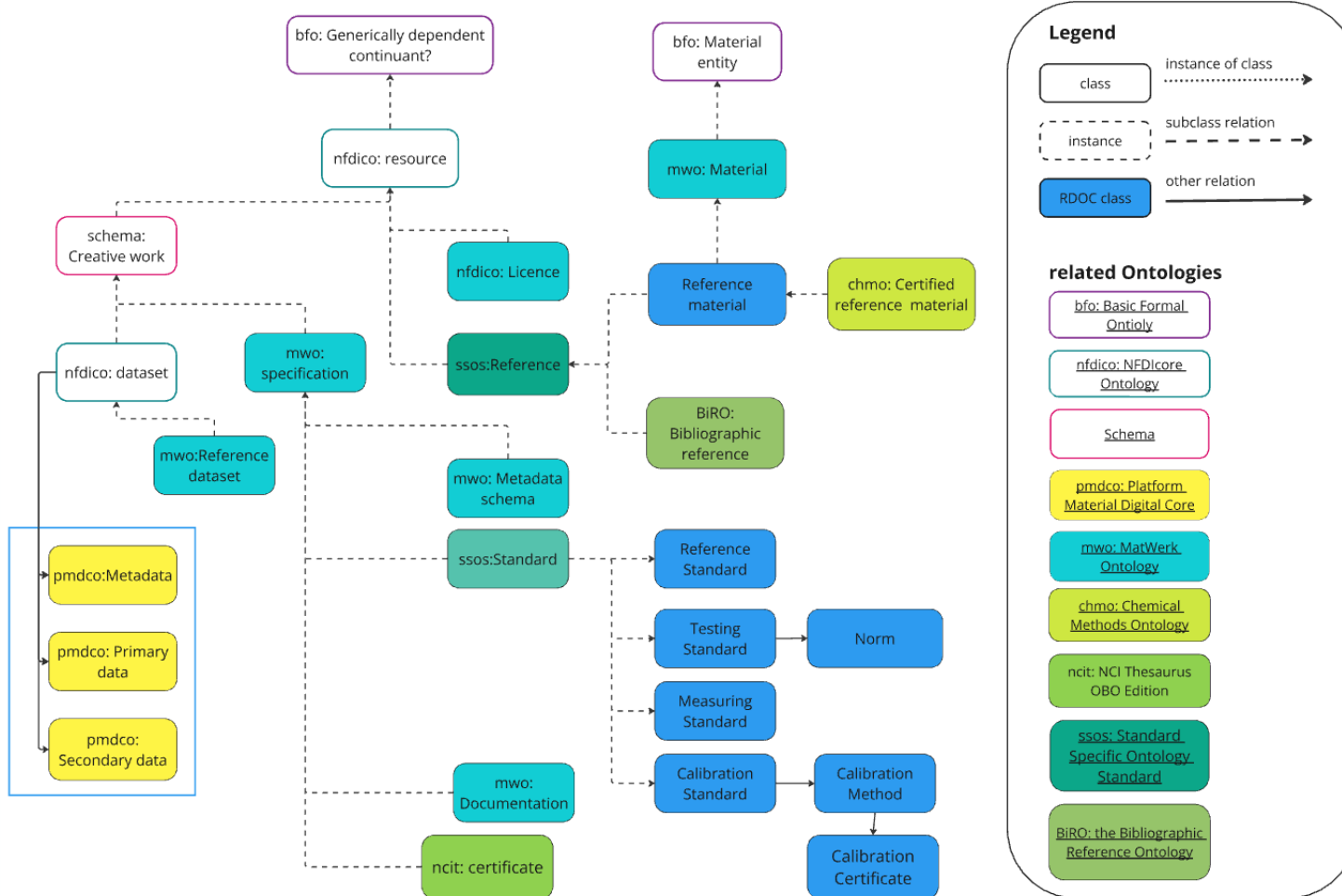
- Contact: Angelika Gedsun, Uni Freiburg
- Connect/Reuse existing ontologies:
 - SSOS: Standard Specific Ontology Standard, BFO: Basic Formal Ontology, NFDIcore Ontology, MWO: MatWerk Ontology
 - TTO (PMD) Tensile Test Ontology from PMD, HTO (PMD) Heat Treatment Ontology PMD, SSOS Standards-Specific Ontology Standard, Matadata4Ing, MWO MatWerk Ontology
- Align to higher-level ontologies: PMDco, NFDIcore, BFO



Miro-board for collaboration

Semantic Structuring and Ontology development

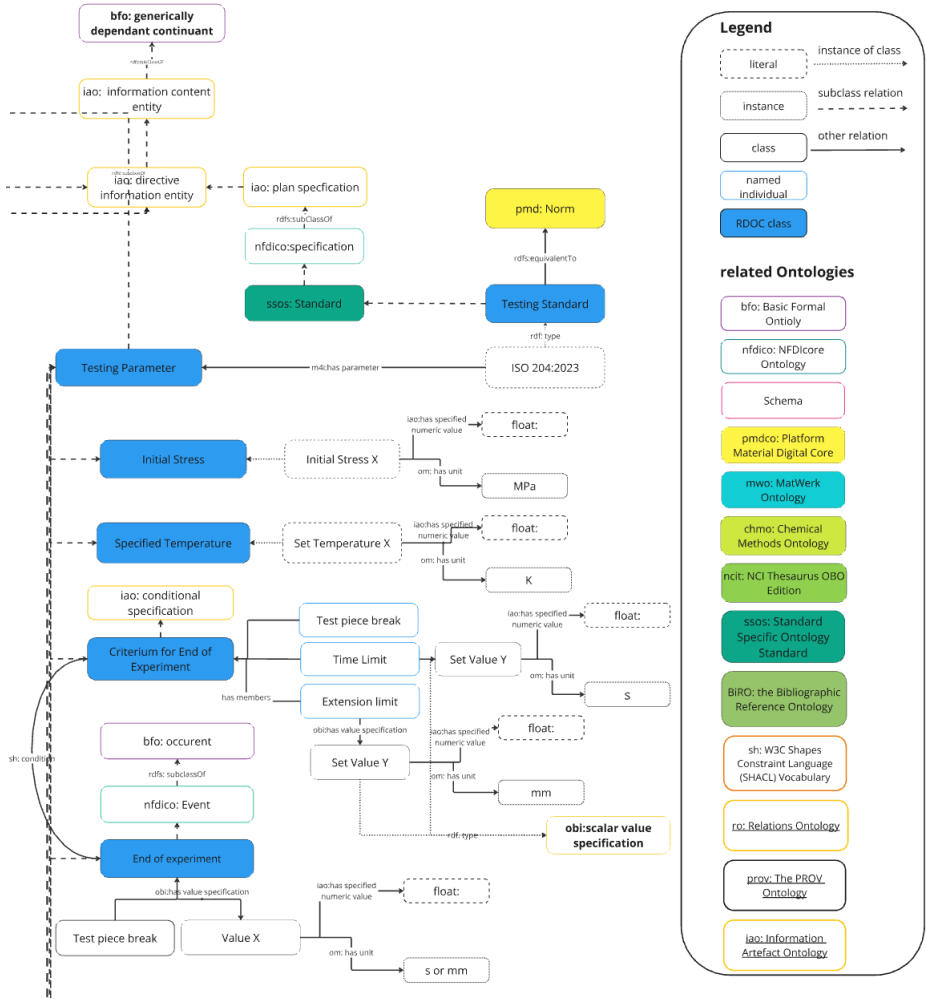
- Concepts for an universal reference dataset



Miro-board for collaboration

Semantic Structuring and Ontology development

- Reference Dataset Ontology – Creep (RDOC)



Miro-board for collaboration

- Framework for RD covering the data generation, provision, identification and usage
- The proposed framework considers from the very beginning the intended use of the data
- Community-agreed definition for reference data (RD) in the MSE domain and a (extendable) data schema (template) for creep (of SX-Ni-based superalloys)
- Community involvement (domain-expert knowledge) is crucial
- Ongoing work / Next steps: Implementation including the publication and (re-)use of a BAM reference dataset (Creep data of CMSX-6 Alloy)

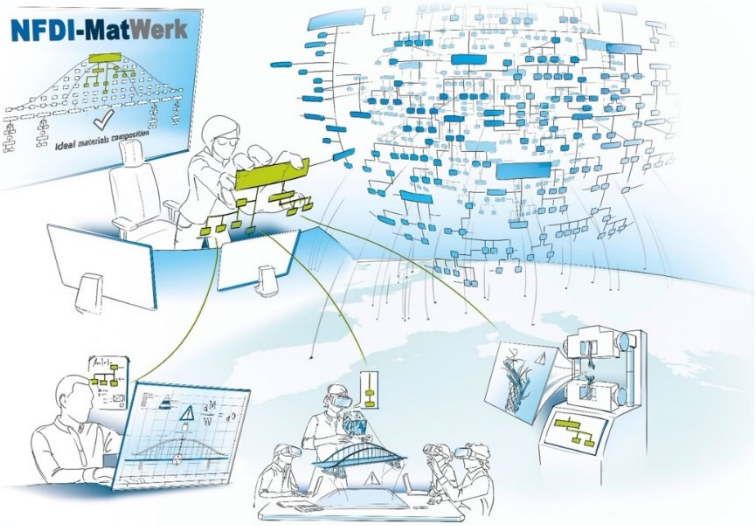
Research Data Management for Reference Data in Materials Science and Engineering Exemplified for Creep Data of Ni-Based Superalloys: Reference Data Concept and Framework for Data Generation, Distribution, and Utilization

L. A. Ávila C.^{1*}, Y. Shakeel², A. Gedsun³, M. Forti⁴, S. Hunke⁵, J. Olbricht¹, M. Chmielowski⁶, R. Stötzka², E. Bitzek⁶, Hammerschmidt⁴, R. Aversa²

¹ Bundesanstalt für Materialforschung und -prüfung, ² Karlsruhe Institute of Technology, ³ Albert-Ludwigs-Universität Freiburg, ⁴ Ruhr-Universität Bochum, ⁵ RWTH Aachen, ⁶ Friedrich-Alexander-Universität Erlangen-Nürnberg

*luis.avila@bam.de

In Revision



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Thank you for your Attention!!

Contact:

Dr. Luis Ávila: luis.avila@bam.de

M. Sc. Yusra Shakeel: yusra.shakeel@kit.edu

Dr. Angelika Gedsun: angelika.gedsun@imtek.uni-freiburg.de

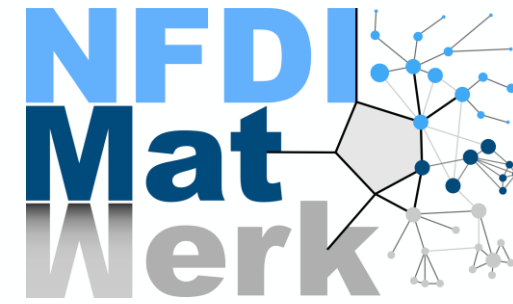
Dr. Jürgen Olbricht: juergen.olbricht@bam.de

Dr. Thomas Hammerschmidt: thomas.hammerschmidt@rub.de

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www.nfdi-matwerk.de

