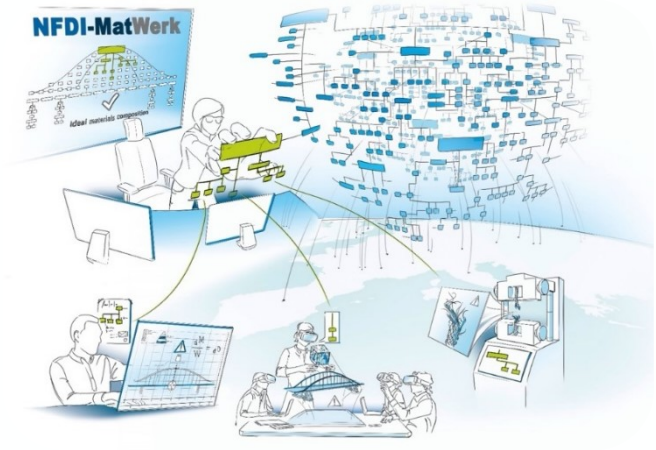


NFDI MatWerk

NATIONAL RESEARCH DATA INFRASTRUCTURE FOR MATERIALS SCIENCE & ENGINEERING

Luis Ávila[1], 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)

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 Forschungsgemeinschaft German Research Foundation

Project number 460247524

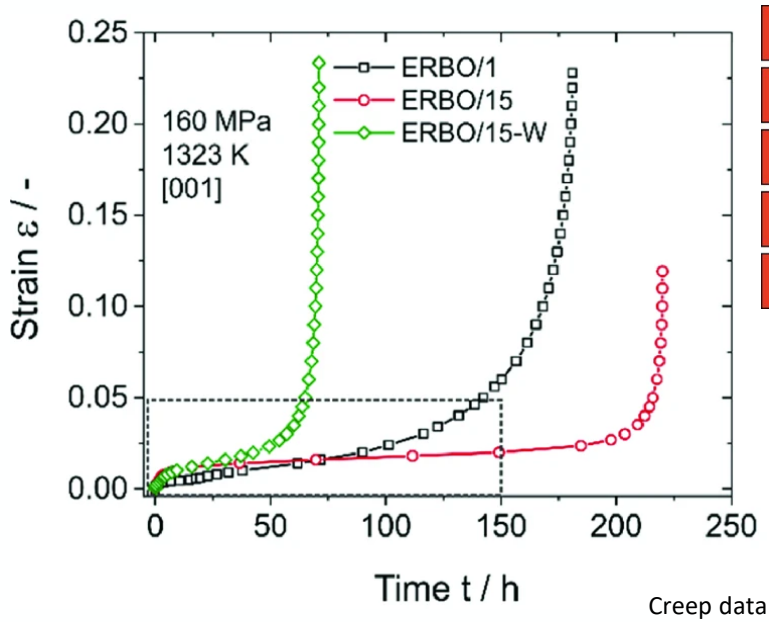
Introduction and Motivation

- Ni-based superalloys
  - High technical relevance
  - Optimization potential

- Possible usages of a ***reference dataset***:
  - **R**e-use of data to generate new knowledge (e.g., as baseline for alloy design and optimization)
  - **R**eproduce experiments, e.g., to calibrate creep experiments in the own lab or computational procedures/algorithms

- Documentation/Metadata often incomplete or hardly accessible 😕 → FAI**R**

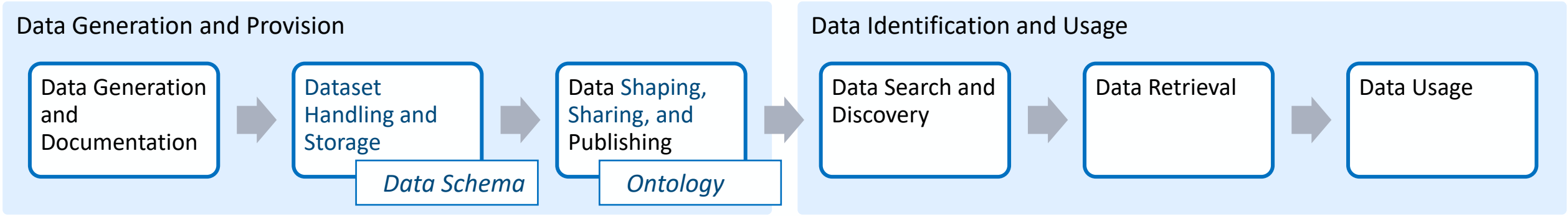
- Specially high requirements in terms of
  - **Documentation** (functionality) and
  - **Digital representation** (usability)



SFB/TR 103
SUPERALLOY SINGLE CRYSTALS

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

Overview of the Proposed Framework



- Definition for ***Reference Data***

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

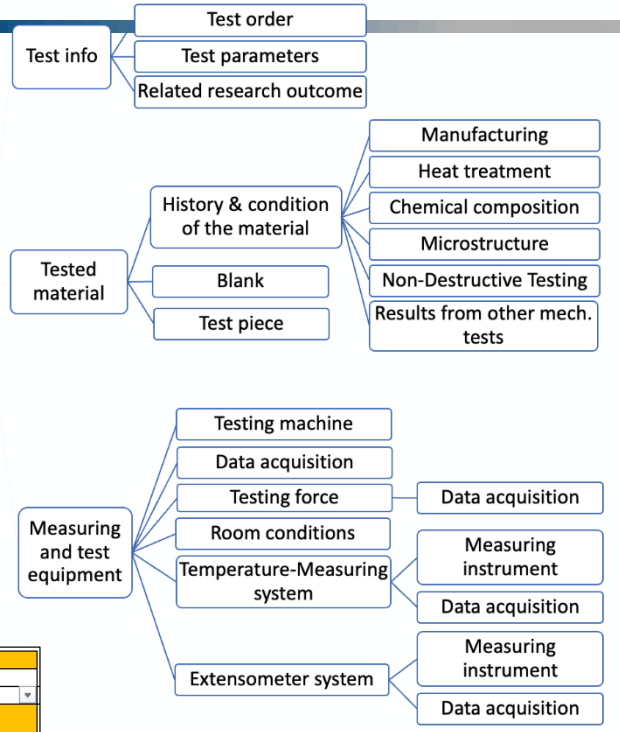
- *Research data* of exceptionally high quality
- FAIR
- Functional (Documentation) and usable (Digital Representation)

- 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	Requirement
Date of test start			Date	Mandatory
Data of test end			Date	Mandatory
Test ID			Alphanumeric	Mandatory
Project			Alphanumeric	Optional
Test order			Alphanumeric	Optional
Was the test performed according to a test standard?			Drop-down list	Mandatory
Test standard			Alphanumeric	Mandatory
Specified temperature	T	°C	Numeric	Mandatory
Type of loading			Drop-down list	Mandatory
Load control type			Drop-down list	Mandatory
Initial stress	R_o	MPa	Numeric	Mandatory
Test type			Drop-down list	Mandatory
End of test criterium			Drop-down list	Mandatory
End of test criterium - value (if not test piece break)			Numeric	Mandatory
Test force		kN	Numeric	Optional
Preload (Part of the test force)		kN	Numeric	Mandatory
Other additional information (e.g. if constant stress)			Text	Optional
Related article(s) available?			Drop-down list	Optional
DOI Article 1			Alphanumeric / Link	Optional
Short description of content article 1			Text	Optional
DOI Article 2			Alphanumeric / Link	Optional
Short description of content article 2			Text	Optional
DOI Article n			Alphanumeric / Link	Optional

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

Metallic 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


```
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  }
}
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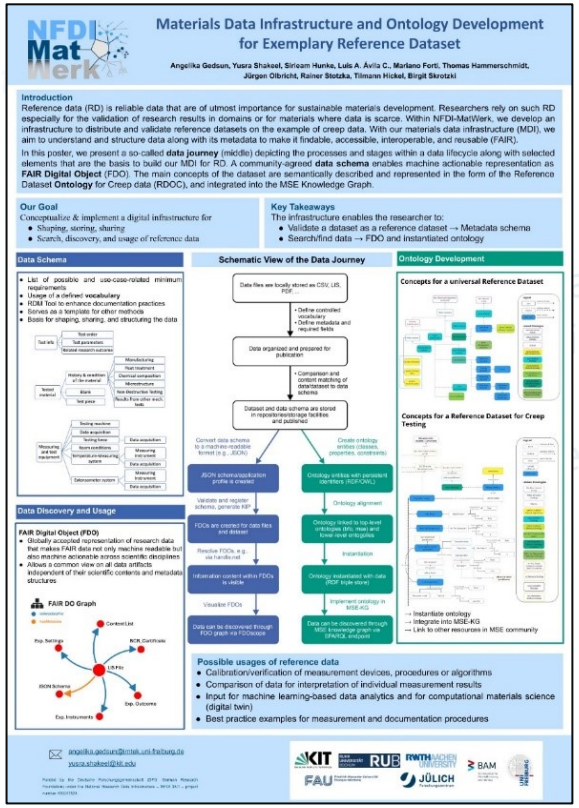
Overview of the Proposed Framework

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



- 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

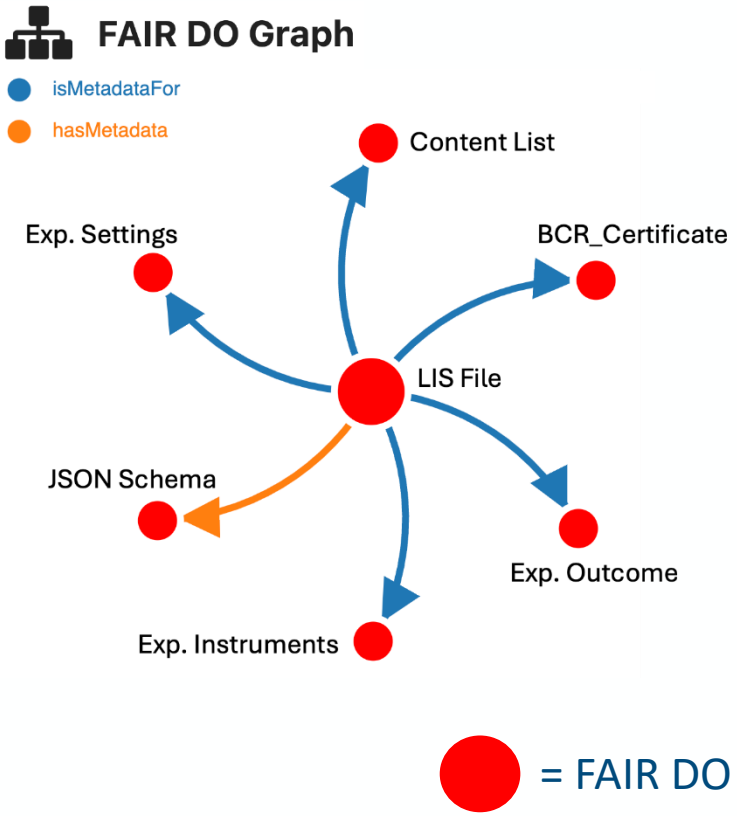
- Contact: Yusra Shakeel, KIT
- Globally accepted representation of research data as a sequence of bits (= a link)

PID	PID Profile	Type	Location URL	. . .

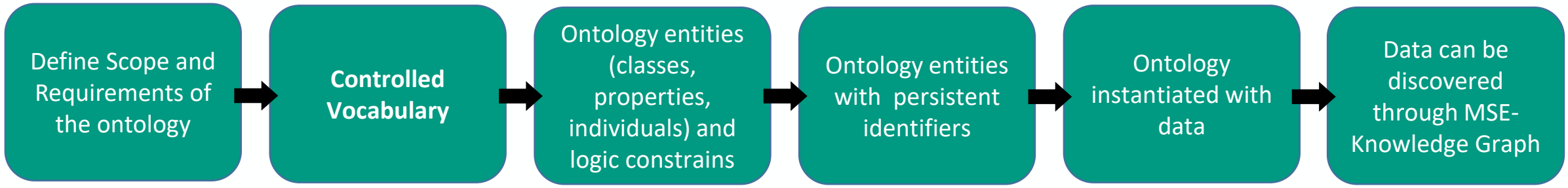
- Contains all information towards FAIR

- 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 interoperabilty



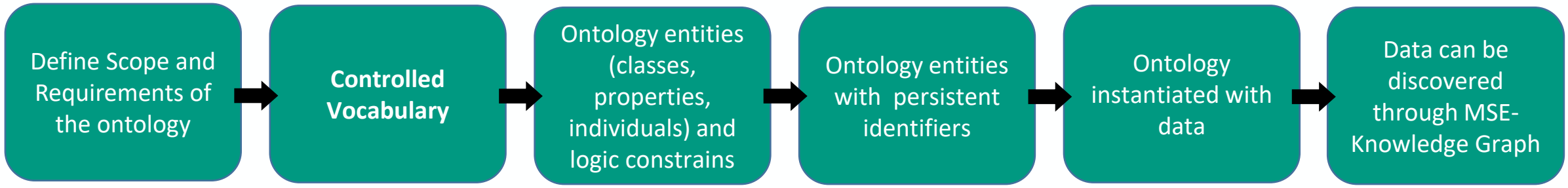
Semantic Structuring and Ontology development



- 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

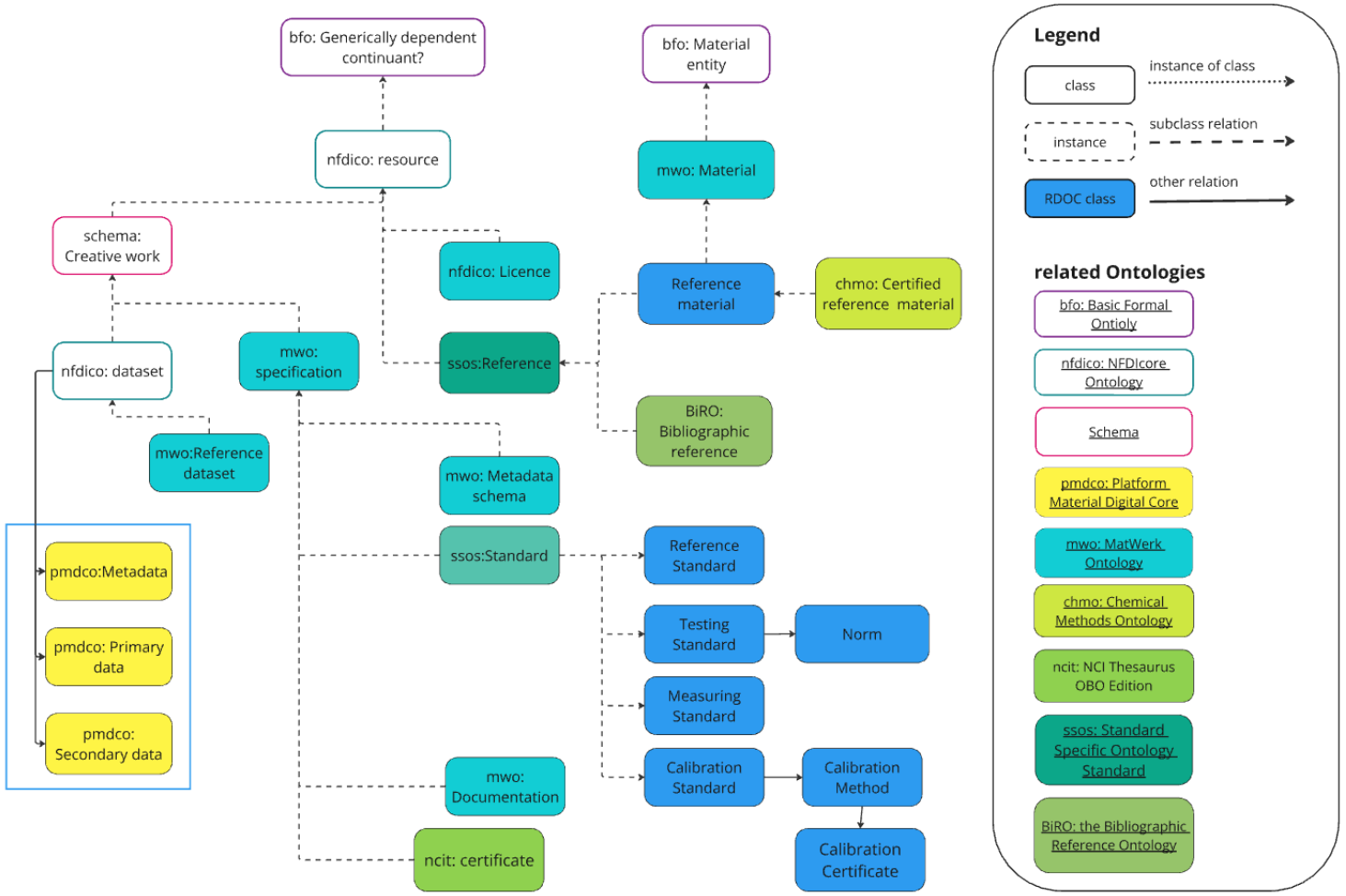


- Contact: Angelika Gedsun, Uni Freiburg
- Connect/Reuse existing ontologies:
  - SSOS: Standard Specific Ontology Standard, BFO: Basic Formal Ontology, NFDIcore Ontology, MWO: MatWerk Ontology
  - TTO (PMD) Tensile Test Ontology from PMD, HTO (PMD) Heat Treatment Ontology PMD, SSOS Standards-Specific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

Miro-board for collaboration

Semantic Structuring and Ontology development

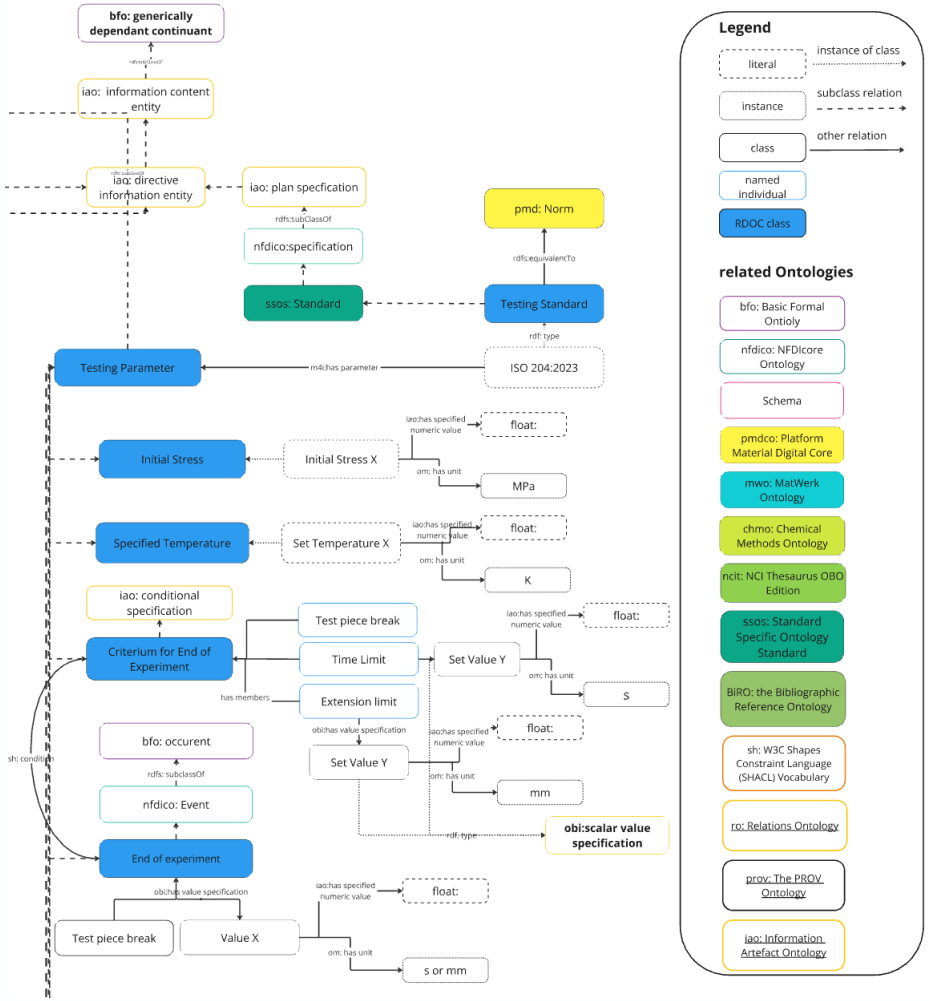
- Concepts for an universal reference dataset



Miro-board for collaboration

Semantic Structuring and Ontology development

- Reference Dataset Ontology – Creep (RDOC)



Miro-board for collaboration

Key Takeaways

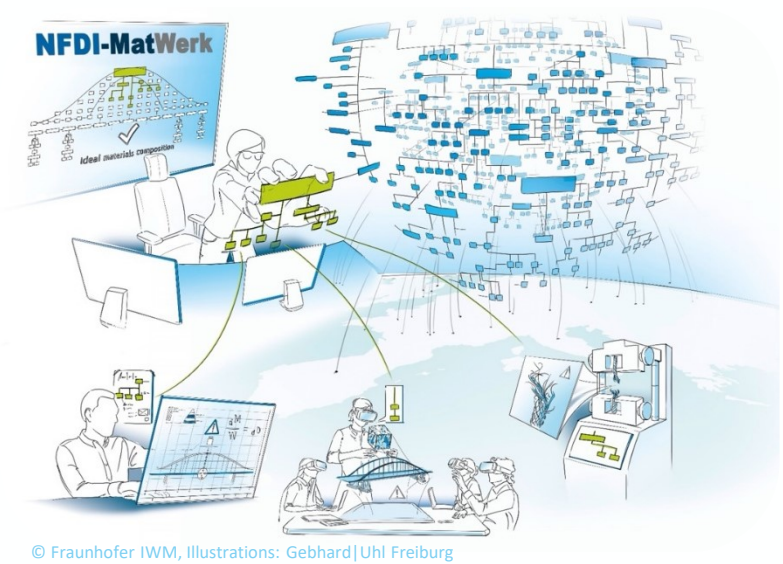
- Framework for RD covering the data generation, provision, identification and usage
- The proposed framework considers from the very beginning the intended use of the data
- Community-agreed definition for reference data (RD) in the MSE domain and a (extendable) data schema (template) for creep (of 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. Shakeel[2], A. Gedsun[3], M. Forti[4], S. Hunke[5], Hammerschmidt[4], R. Aversa[2], J. Olbricht[1], M. Chmielowski[6], R. Stotzka[2], E. Bitze[6]

In Revision

[1] Bundesanstalt für Materialforschung und -prüfung, 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



Thank you for your Attention!!

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