Demonstration of the Infrastructure Use Case 02

Framework for curation and distribution of reference datasets

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Introduction and Motivation

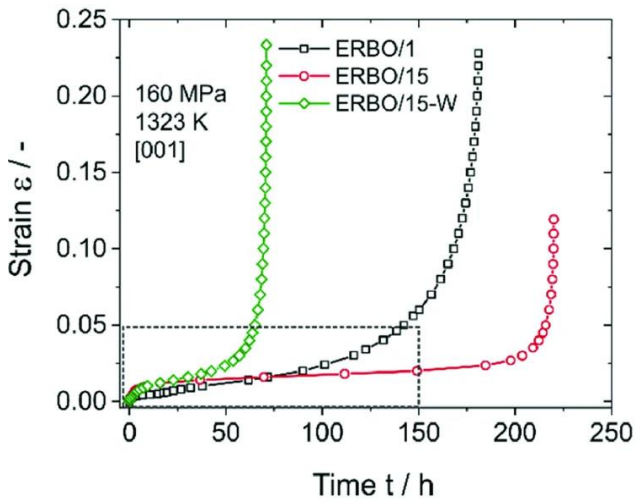
"The aim of IUC2 is to **develop a framework for reference material data sets** using creep properties of single- & polycrystalline Ni-based superalloy as example."

https://nfdi-matwerk.de/infrastructure-use-cases/iuc02-framework-for-curation-and-distribution-of-reference-datasets

- **User/User Journey**: Research task could be alloy design, optimization of mechanical properties (chemical composition, heat treatment strategy)
- **Data available**: Normal' data set (DS) e.g. from SFB/TRR 103 vs. reference data set (RDS) e.g. from BAM

- A **RDS** would be a DS used
  - as high quality data to correlate material properties and serve as baseline for the optimization process
  - to calibrate the experiments in the own lab
- Requirements (contents, shape, FAIR, accessibility)

Demonstrator at the booth at marketplace: GitLab (Notebook with data)
User Journey: https://app.conceptboard.com/board/x7zn-2yq0-eabn-piic-dbiu



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

IUC02 - Overview

“develop a framework for reference material data sets”

Reference Data Set

- Definition, criteria for reference data (material, equipment, procedures, results)
- … Community process needed → Poster
- Curation process

User/Usage Analytics

- Testing laboratories
- Researchers

Possible uses

- Comparison of data for interpretation of individual measurement results
- Calibration/verification of measurement devices
- … Community process needed → Poster

→ Different user cases derive different requirement profiles (for **content** and **shape** of data)

Creating the reference dataset

Content:

- MSE perspective or “Fit for purpose”[1]
- Agreement on content based on input from domain experts

Shape:

- RDM perspective or “Fit for use”[1]
- Creation, structuring and distribution of (creep) (meta)data: FAIR DOs

Distribution/Publishing of the Reference Data Set

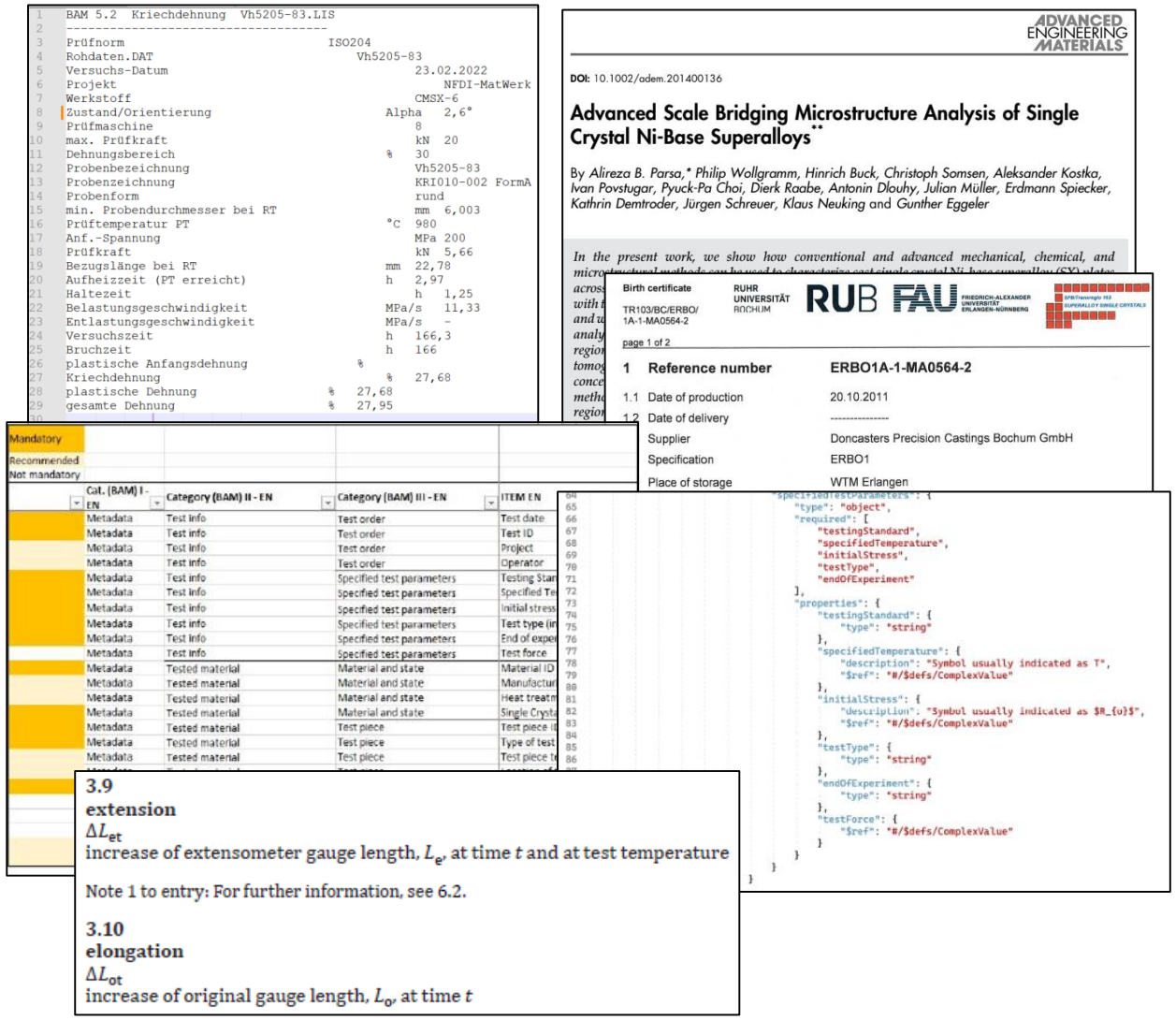
- Ontology, Licensing, DOI

[1] Ariza, Angela et al., Datennachnutzung in der Praxis; DOI: 10.5281/zenodo.7568266

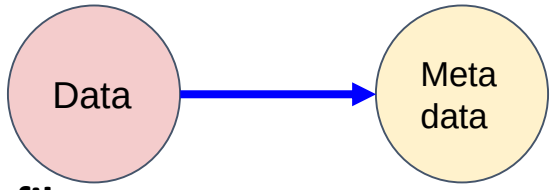
Agreement and Data Structuring

- **Agreement** on:
  - (meta)data and documentation, considering the existing datasets (BAM, RUB, SFB/TR 103)
  - data structure and vocabulary (ISO 204-standard on creep testing)
  - a “rating” of the (meta)data to define quality requirements in terms of contents

- Vision: Creation (a) data schema template(s) or check lists to be used by the community
(to generate RDS)



Shaping Exemplary Data Set: FAIR Digital Object



Data object

- Link to the location
  e.g. storage location of the **data file**
- Link(s) to metadata object(s)
- PID
- Type
- ….

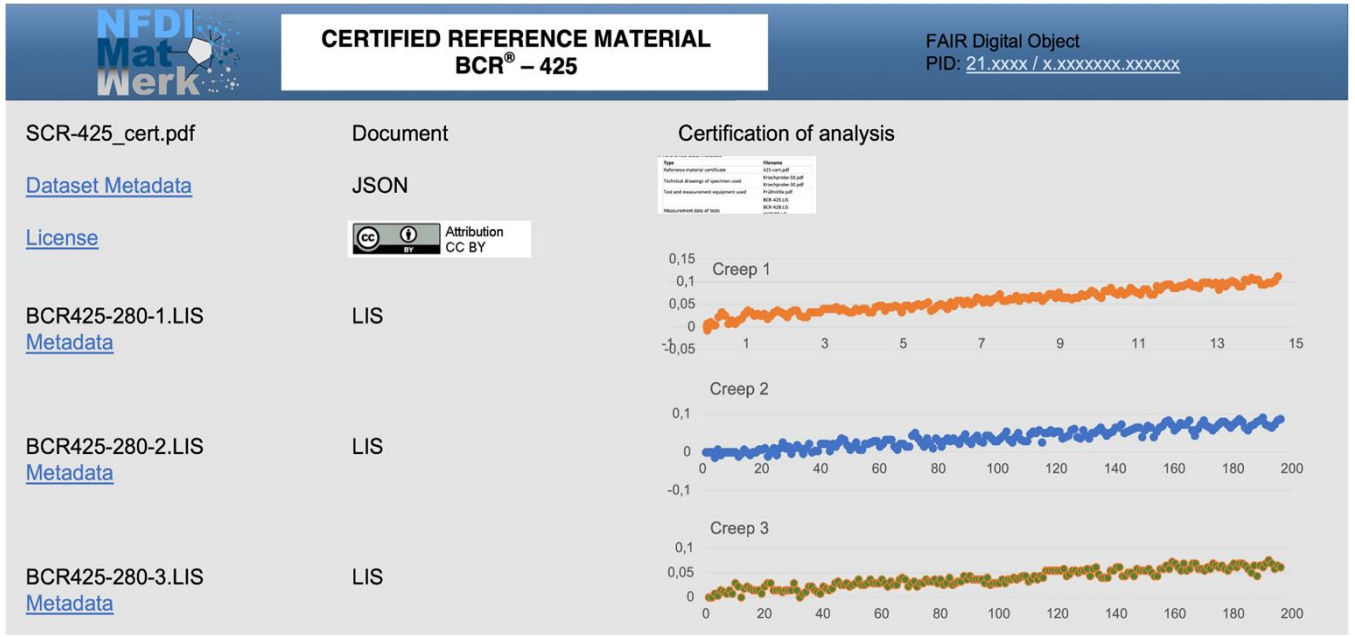
Metadata object

- Link to the location
  e.g. storage location of the **metadata document**
- PID
- Type
- ….

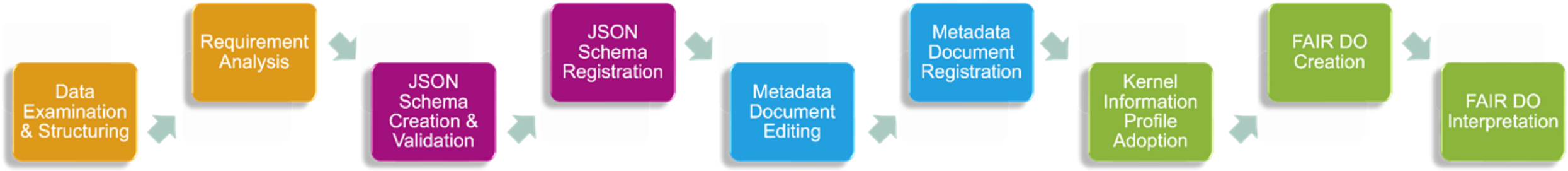
FAIR Digital Object:

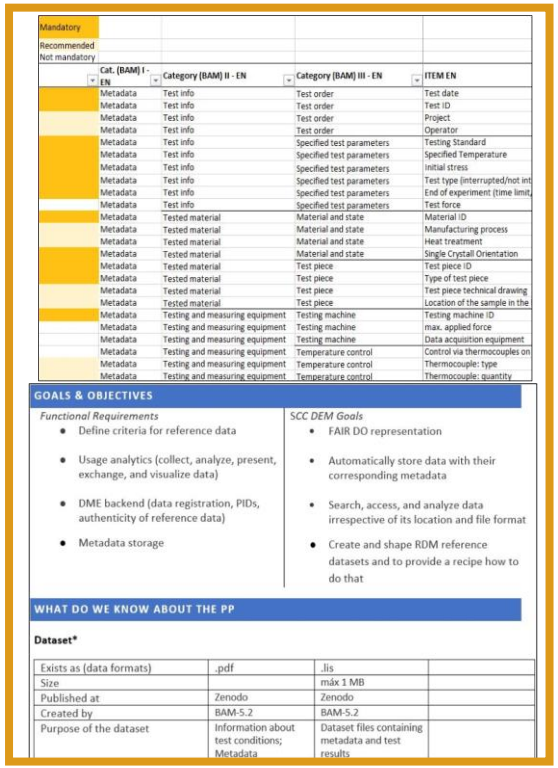
- Representation of data
- Contains all information towards FAIR
- Conception: technology agnostic
- Bridges between data repositories, disciplines, etc.
- Implementation
  - Handle PID
  - Information Record

PID	PID Profile	Type	Location URL	. . .



Exemplary RDM Reference Data Set: Technical Process Overview





Mandatory
Recommended
Not mandatory

Cat. (BAM) I - EN	Category (BAM) II - EN	Category (BAM) III - EN	ITEM EN
Metadata	Test info	Test order	Test date
Metadata	Test info	Test order	Test ID
Metadata	Test info	Test order	Project
Metadata	Test info	Test order	Operator
Metadata	Test info	Specified test parameters	Testing Standard
Metadata	Test info	Specified test parameters	Specified Temperature
Metadata	Test info	Specified test parameters	Initial stress
Metadata	Test info	Specified test parameters	Test type (interrupted/not int
Metadata	Test info	Specified test parameters	End of experiment (time limit,
Metadata	Test info	Specified test parameters	Test force
Metadata	Tested material	Material and state	Material ID
Metadata	Tested material	Material and state	Manufacturing process
Metadata	Tested material	Material and state	Heat treatment
Metadata	Tested material	Material and state	Single Crystall Orientation
Metadata	Tested material	Test piece	Test piece ID
Metadata	Tested material	Test piece	Type of test piece
Metadata	Tested material	Test piece	Test piece technical drawing
Metadata	Tested material	Test piece	Location of the sample in the
Metadata	Testing and measuring equipment	Testing machine	Testing machine ID
Metadata	Testing and measuring equipment	Testing machine	max. applied force
Metadata	Testing and measuring equipment	Testing machine	Data acquisition equipment
Metadata	Testing and measuring equipment	Temperature control	Control via thermocouples on
Metadata	Testing and measuring equipment	Temperature control	Thermocouple: type
Metadata	Testing and measuring equipment	Temperature control	Thermocouple: quantity

GOALS & OBJECTIVES

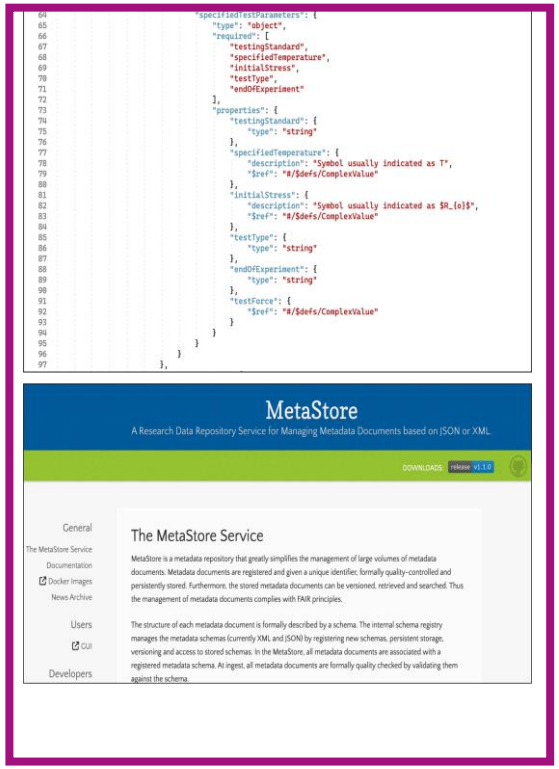
Functional Requirements
- Define criteria for reference data
- Usage analytics (collect, analyze, present, exchange, and visualize data)
- DME backend (data registration, PIDs, authenticity of reference data)
- Metadata storage

SCC DEM Goals
- FAIR DO representation
- Automatically store data with their corresponding metadata
- Search, access, and analyze data irrespective of its location and file format
- Create and shape RDM reference datasets and to provide a recipe how to do that

WHAT DO WE KNOW ABOUT THE PP

Dataset*

Exists as (data formats)	.pdf	.lis	
Size		máx 1 MB	
Published at	Zenodo	Zenodo	
Created by	BAM-5.2	BAM-5.2	
Purpose of the dataset	Information about test conditions; Metadata	Dataset files containing metadata and test results	




```
"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 $R_{o}$",
      "$ref": "#/$defs/ComplexValue"
    },
    "testType": {
      "type": "string"
    },
    "endOfExperiment": {
      "type": "string"
    },
    "testForce": {
      "$ref": "#/$defs/ComplexValue"
    }
  }
}
},
```


MetaStore
A Research Data Repository Service for Managing Metadata Documents based on JSON or XML.

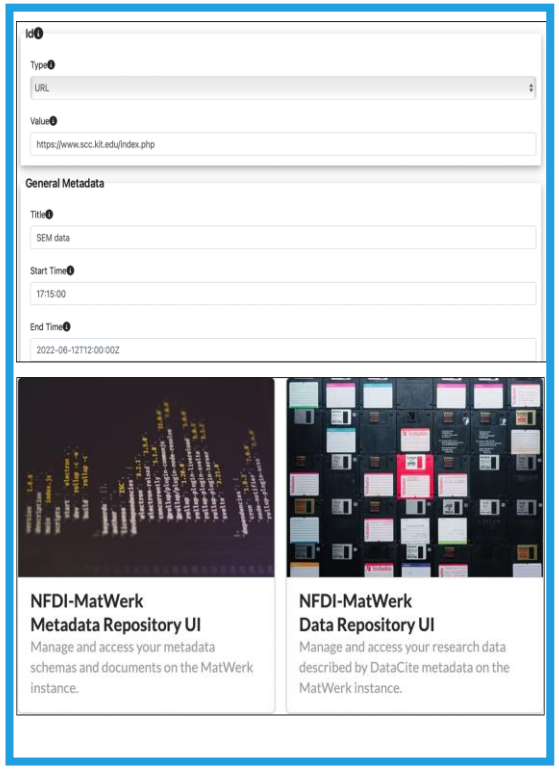
DOWNLOADS release v1.1.0

General
The MetaStore Service
Documentation
Docker Images
News Archive
Users
GUI
Developers

The MetaStore Service

MetaStore is a metadata repository that greatly simplifies the management of large volumes of metadata documents. Metadata documents are registered and given a unique identifier, formally quality-controlled and persistently stored. Furthermore, the stored metadata documents can be versioned, retrieved and searched. Thus the management of metadata documents complies with FAIR principles.

The structure of each metadata document is formally described by a schema. The internal schema registry manages the metadata schemas (currently XML and JSON) by registering new schemas, persistent storage, versioning and access to stored schemas. In the MetaStore, all metadata documents are associated with a registered metadata schema. At ingest, all metadata documents are formally quality checked by validating them against the schema.



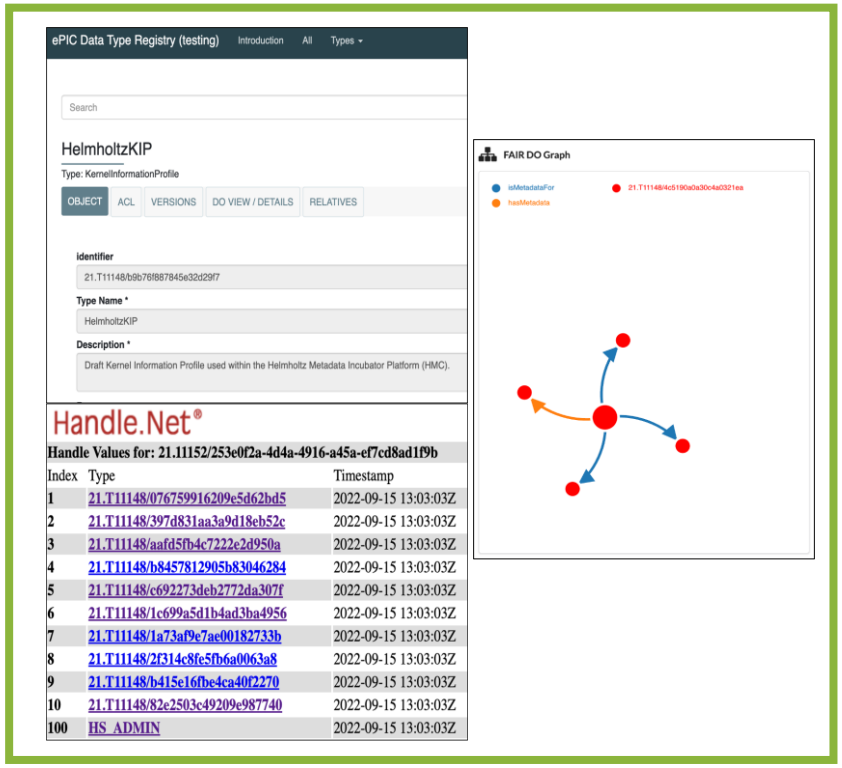
Id
Type
URL
Value
https://www.scc.kit.edu/index.php

General Metadata

Title
SEM data
Start Time
17:15:00
End Time
2022-06-12T12:00:00Z

NFDI-MatWerk Metadata Repository UI
Manage and access your metadata schemas and documents on the MatWerk instance.

NFDI-MatWerk Data Repository UI
Manage and access your research data described by DataCite metadata on the MatWerk instance.



ePIC Data Type Registry (testing) Introduction All Types

Search

HelmholtzKIP
Type: KernelInformationProfile

OBJECT ACL VERSIONS DO VIEW / DETAILS RELATIVES

Identifier
21.T11148/b9b76f887845e32d29f7

Type Name *
HelmholtzKIP

Description *
Draft Kernel Information Profile used within the Helmholtz Metadata Incubator Platform (HMC).

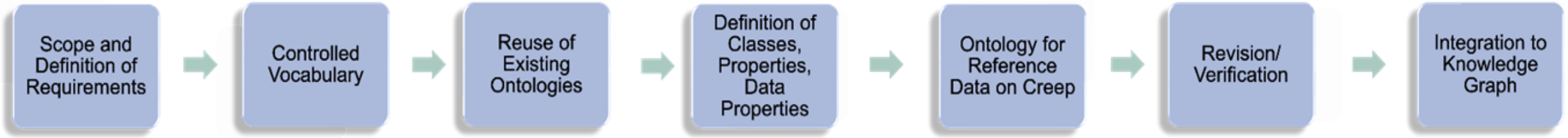
Handle.Net®

Handle Values for: 21.11152/253e0f2a-4d4a-4916-a45a-ef7cd8ad1f9b

Index	Type	Timestamp
1	21.T11148/076759916209e5d62bd5	2022-09-15 13:03:03Z
2	21.T11148/397d831aa3a9d18eb52c	2022-09-15 13:03:03Z
3	21.T11148/aafd5fb4c7222e2d950a	2022-09-15 13:03:03Z
4	21.T11148/b84578129O5b83046284	2022-09-15 13:03:03Z
5	21.T11148/c692273deb2772da307f	2022-09-15 13:03:03Z
6	21.T11148/1c699a5d1b4ad3ba4956	2022-09-15 13:03:03Z
7	21.T11148/1a73af9e7ae00182733b	2022-09-15 13:03:03Z
8	21.T11148/2f314c8fe5fb6a0063a8	2022-09-15 13:03:03Z
9	21.T11148/b415e16fbe4ca40f2270	2022-09-15 13:03:03Z
10	21.T11148/82e2503c49209e987740	2022-09-15 13:03:03Z
100	HS_ADMIN	2022-09-15 13:03:03Z

FAIR DO Graph
isMetadataFor
hasMetadata
21.T11148/4c5190a0a30c4a0321ea

Towards Ontology for Creep Data (Reference Data Set)
Ongoing work



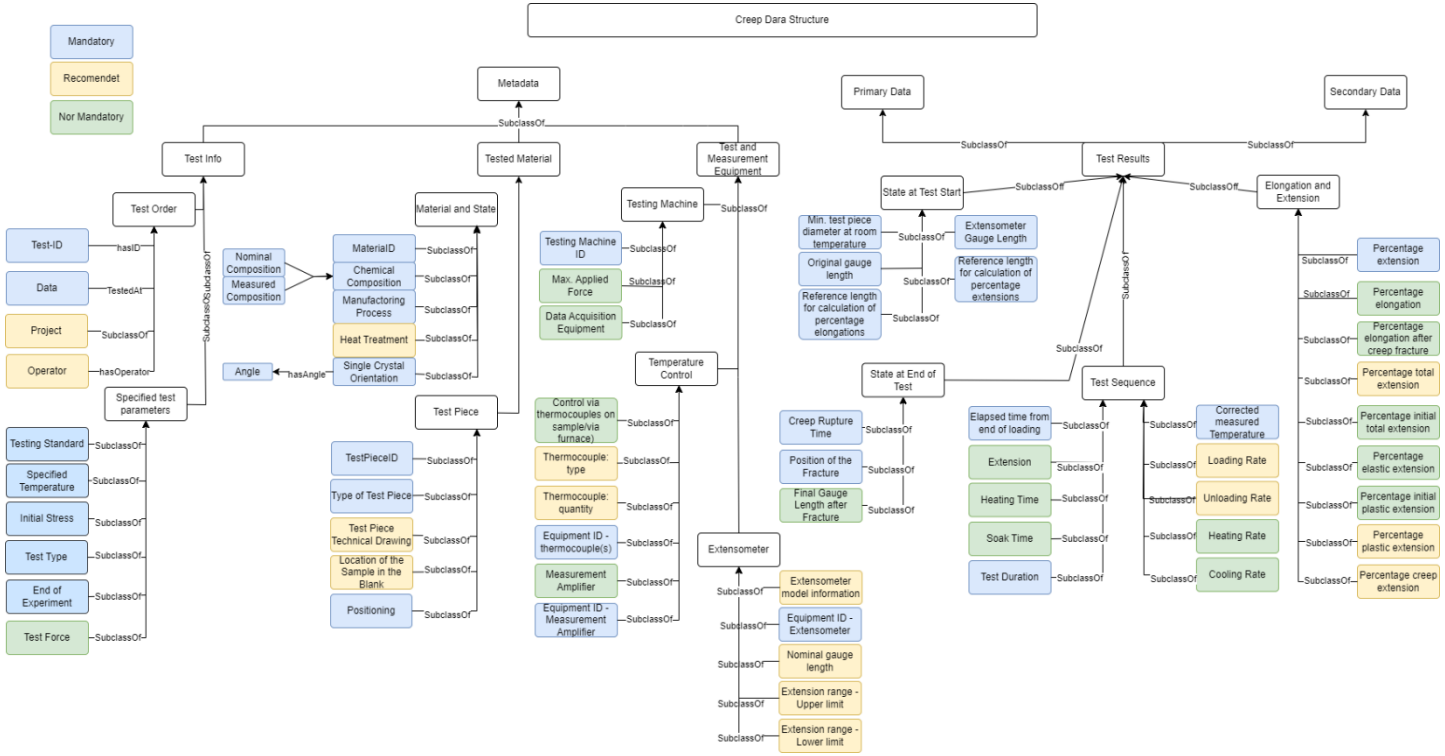
- Domain: MSE (High temperature application/ creep testing)

- Requirements:
  - Representation of creep testing in a conceptual way for a reference material and based on a testing standard/norm

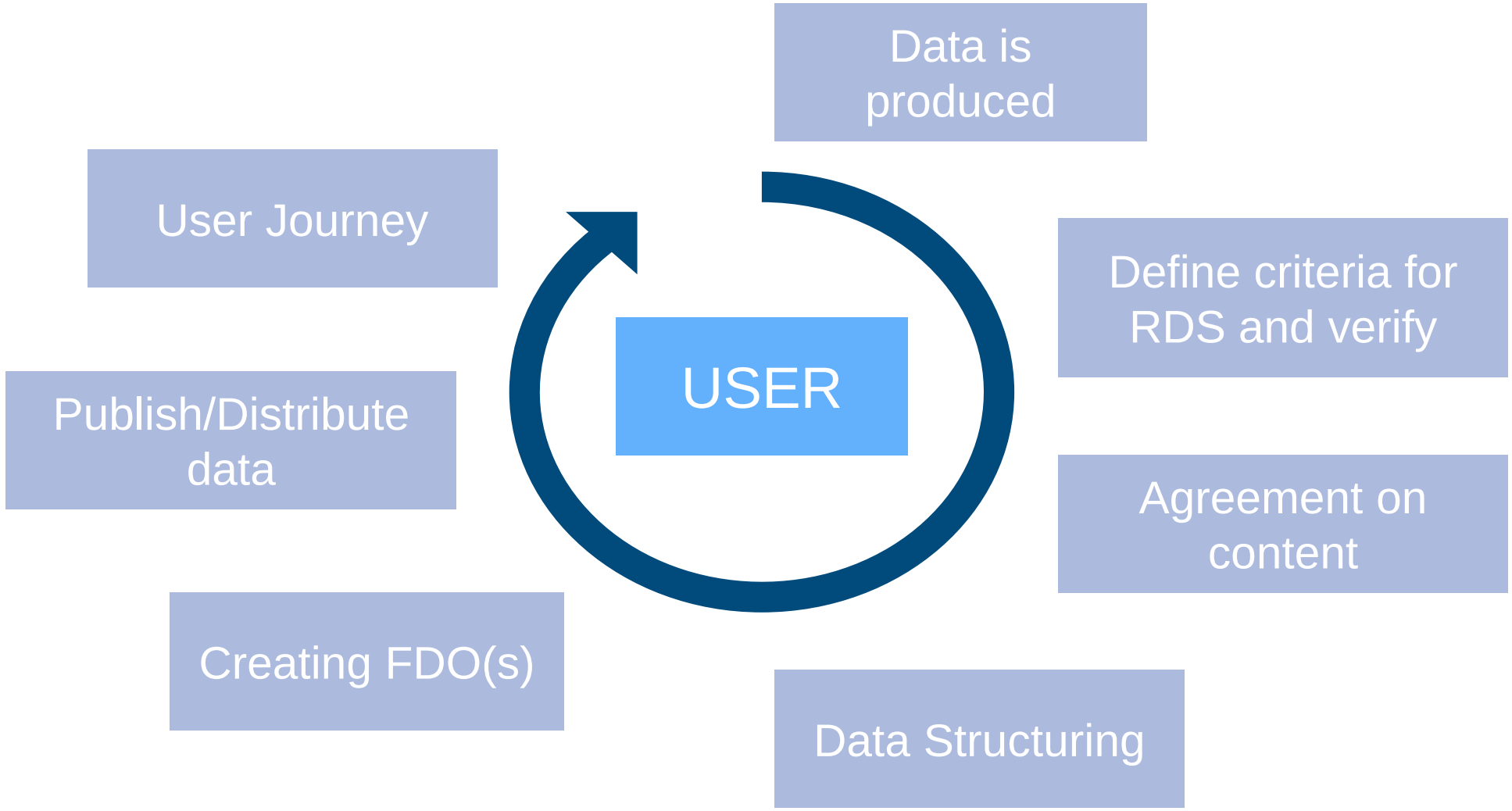
  → user can transfer the concepts in their own work

- Status: Metadata annotation /agreement on controlled vocabulary (with BAM/RUB)

- Reuse:
  - NFDIcore
  - PMDcore Ontology on tensile testing



Key Takeaway



Back-Up slides

Application for data schema and control vocabulary

A reference dataset is available. It provides:

- Data schema
- Example data

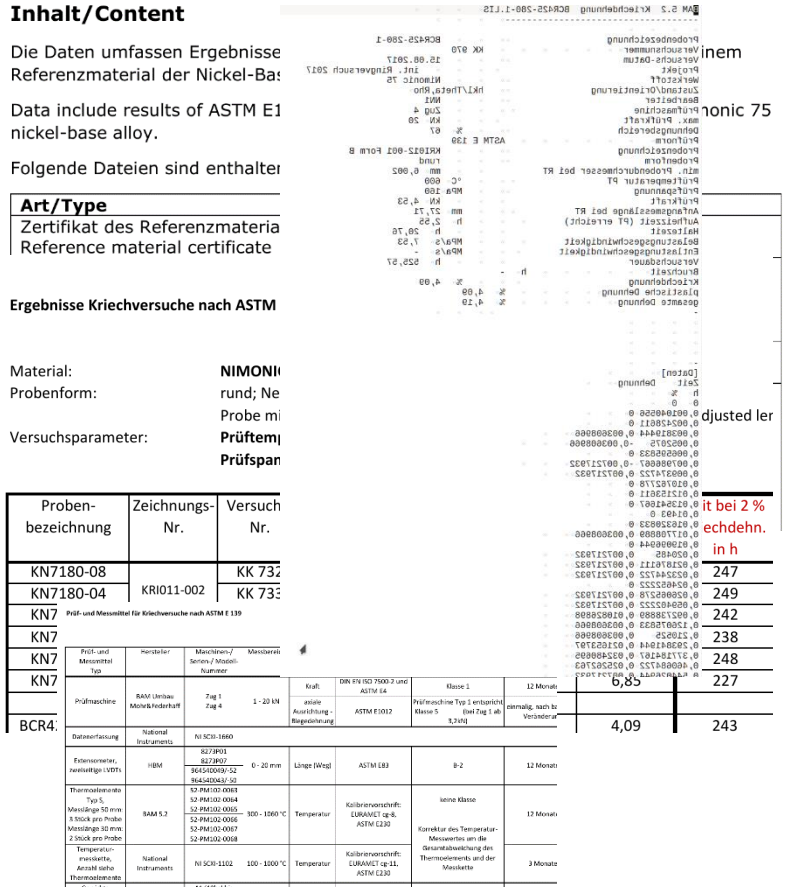
A group wants to publish data related to previous publication. They follow the next steps:

- get the data schema
- Prepare their data for schema compatibility
- Fill the data schema with their data
- compare the data with reference dataset to check completeness

Application for data schema and control vocabulary

Data schema / vocabulary from experts + Reference data → Structured reference data

Category I - EN	Category II - DE	Category II	Category III - DE	Category III - EN	ITEM DE	ITEM EN	Symbol	Unit
Metadaten Metadata	Versuchsinfo	Test info			Bibliographische Information	Bibliographic information		
Metadaten Metadata	Versuchsinfo	Test info	Prüfauftrag	Test order	Versuchsdatum	Test date		
Metadaten Metadata	Versuchsinfo	Test info	Prüfauftrag	Test order	Versuchs-ID	Test ID		
Metadaten Metadata	Versuchsinfo	Test info	Festgelegte Prüfpar	specified test parameters	Prüfnorm	Testing Standard		
Metadaten Metadata	Versuchsinfo	Test info	Festgelegte Prüfpar	specified test parameters	festgelegte Prüftemperatur	Specified Temperature	T	°C
Metadaten Metadata	Versuchsinfo	Test info	Festgelegte Prüfpar	specified test parameters	Prüfspannung (should we add whether constant force or constant st	Initial stress	R_u	MPa
Metadaten Metadata	Versuchsinfo	Test info	Festgelegte Prüfpar	specified test parameters	Versuchsart (unterbrochen/nicht unterbrochen)	Test type (interrupted/not interrupted)		
Metadaten Metadata	Versuchsinfo	Test info	Festgelegte Prüfpar	specified test parameters	Versuchsende (Zeitvorgabe/Probenbruch/Dehnungsvorgabe)	End of experiment (time limit/test piece break/extension limit)		
Metadaten Metadata	Versuchsinfo	Test info	Festgelegte Prüfpar	specified test parameters	Prüfkraft	Test force		kN
Metadaten Metadata	geprüfter Werksto	Tested materi	Werkstoff und Zus	Material and state	Werkstoffbezeichnung	Material ID		
Metadaten Metadata	geprüfter Werksto	Tested materi			Bibliographische Information	Bibliographic information		
Metadaten Metadata	geprüfter Werksto	Tested materi	Werkstoff und Zus	Material and state	Werkstoffbezeichnung	Material ID		
Metadaten Metadata	geprüfter Werksto	Tested materi	Werkstoff und Zus	Material and state	Herstellung: Schmelzen	Manufacturing: Melting		
Metadaten Metadata	geprüfter Werksto	Tested materi	Werkstoff und Zus	Material and state	Herstellung: Gießen	Manufacturing: Casting		
Metadaten Metadata	geprüfter Werksto	Tested materi	Werkstoff und Zus	Material and state	Herstellung: Umschmelzen	Manufacturing: Remelting		
Metadaten Metadata	geprüfter Werksto	Tested materi	Werkstoff und Zus	Material and state	Herstellung: Atmosphäre	Manufacturing: Atmosphere		
Metadaten Metadata	geprüfter Werksto	Tested materi	Werkstoff und Zus	Material and state	Herstellung: Ein- oder Polykristall erstarrt	Manufacturing: Single or polycrystal solidified		
Metadaten Metadata	geprüfter Werksto	Tested materi	Werkstoff und Zus	Material and state	Herstellung: Thermomechanische Behandlung	Manufacturing: Thermomechanical treatment		
Metadaten Metadata	geprüfter Werksto	Tested materi	Werkstoffzustand	same as condition? Ausg	Zustand: wärmebehandelt / wie gefertigt	Condition: Heat treated / as manufactured		
Metadaten Metadata	geprüfter Werksto	Tested materi	Werkstoff und Zus	Material and state	Wärmebehandlung: Atmosphäre	Heat treatment: Atmosphere		
Metadaten Metadata	geprüfter Werksto	Tested materi	Werkstoff und Zus	Material and state	Auslagerung durchgeführt?	Ageing applied?		
Metadaten Metadata	geprüfter Werksto	Tested materi	Werkstoff und Zus	Material and state	Chemische Zusammensetzung, nominal	Chemical composition, nominal		
Metadaten Metadata	geprüfter Werksto	Tested materi	Werkstoff und Zus	Material and state	Chemische Zusammensetzung, gemessen (inkl. Messunsicherheit)	Chemical composition, measured (including precision)		
Metadaten Metadata	geprüfter Werksto	Tested materi	Werkstoff und Zus	Material and state	Angaben zum Rohling: Lieferant	Geometry/dimensions of blank		
Metadaten Metadata	geprüfter Werksto	Tested materi	Werkstoff und Zus	Material and state	Angaben zum Rohling: Geometrie/Abmessungen	Blank: Geometry/Dimensions		
Metadaten Metadata	geprüfter Werksto	Tested materi	Werkstoff und Zus	Material and state	Angaben zum Rohling: Lieferdatum	Blank: date of supply		
Metadaten Metadata	geprüfter Werksto	Tested materi	Werkstoff und Zus	Material and state	Angaben zum Rohling: Auftragnummer	Blank: order number		
Metadaten Metadata	geprüfter Werksto	Tested materi	Werkstoff und Zus	Material and state	Angaben zum Rohling: Probenbezeichnung vom Lieferant	Blank: supplier sample ID		
Metadaten Metadata	geprüfter Werksto	Tested materi	Werkstoff und Zus	Material and state	Mikrogefüge: Wärmebehandlungszustand (lösungsgeglüht, ausgehär	Microstructure: Heat treatment condition (annealed, hardened, ...)		
Metadaten Metadata	geprüfter Werksto	Tested materi	Werkstoff und Zus	Material and state	Zugversuchskennwerte bei festgelegter Prüftemperatur vorhanden?	Tensile properties at testing temperature available?		
Metadaten Metadata	geprüfter Werksto	Tested materi	Werkstoff und Zus	Material and state	Nachweis der Einkristallinität	Proof of single crystallinity		
Metadaten Metadata	geprüfter Werksto	Tested materi	Werkstoff und Zus	Material and state	Einkristallorientierung	Single Crystall Orientation		hkl/Theta,R
Metadaten Metadata	geprüfter Werksto	Tested materi	Werkstoff und Zus	Material and state	Winkelorientierung	Angle orientation		
Metadaten Metadata	geprüfter Werksto	Tested materi	Werkstoff und Zus	Material and state	Angaben zu Rissprüfung	Crack inspection details		
Metadaten Metadata	geprüfter Werksto	Tested materi	Werkstoff und Zus	Material and state	Röntgenfilm?	X-Ray film?		
Metadaten Metadata	geprüfter Werksto	Tested materi	Werkstoff und Zus	Material and state	Korndefektkarten?	Grain Defects maps?		
Metadaten Metadata	geprüfter Werksto	Tested materi	Probe	Test piece	Probenbezeichnung	Test piece ID		
Metadaten Metadata	geprüfter Werksto	Tested materi	Probe	Test piece	Probenform	Type of test piece		
Metadaten Metadata	Prüf- und Messmitt	Testing and m	Prüfmaschine	Testing machine	Bibliographische Information	Bibliographic information		
Metadaten Metadata	Prüf- und Messmitt	Testing and m	Prüfmaschine	Testing machine	Prüfmaschinenbezeichnung	Testing machine ID		
Metadaten Metadata	Prüf- und Messmitt	Testing and m	Prüfmaschine	Testing machine	max. Prüfkraft	max. applied force		kN
Metadaten Metadata	Prüf- und Messmitt	Testing and m	Prüfmaschine	Testing machine	Datenerfassungsgerät	Data acquisition equipment		
Metadaten Metadata	Prüf- und Messmitt	Testing and m	Temperatur-Regel	Temperature control	Regelung über Thermoelementen an Probe/über Ofen	Control via thermocouples on sample/via furnace)		
Metadaten Metadata	Prüf- und Messmitt	Testing and m	Temperatur-Regel	Temperature control	Geräteummer-Thermoelement(e)	Equipment ID - thermocouple(s)		



Inhalt/Content

Die Daten umfassen Ergebnisse … Referenzmaterial der Nickel-Ba… nem

Data include results of ASTM E1… nickel-base alloy. …onic 75

Folgende Dateien sind enthalte…

Art/Type
Zertifikat des Referenzmateria…
Reference material certificate

Ergebnisse Kriechversuche nach ASTM …

Material: **NIMONI…**

Probenform: rund; Ne… Probe mi…

Versuchsparameter: **Prüftem… Prüfspan…**

djusted ler…

Proben-bezeichnung	Zeichnungs-Nr.	Versuch Nr.		
KN7180-08		KK 732		
KN7180-04	KRI011-002	KK 733		
KN7…				
KN7…				
KN7…				
KN7…				
			6,85	227
BCR4…			4,09	243

it bei 2 % echdehn. in h

247	
249	
242	
238	
248	

Prüf- und Messmittel für Kriechversuche nach ASTM E 139

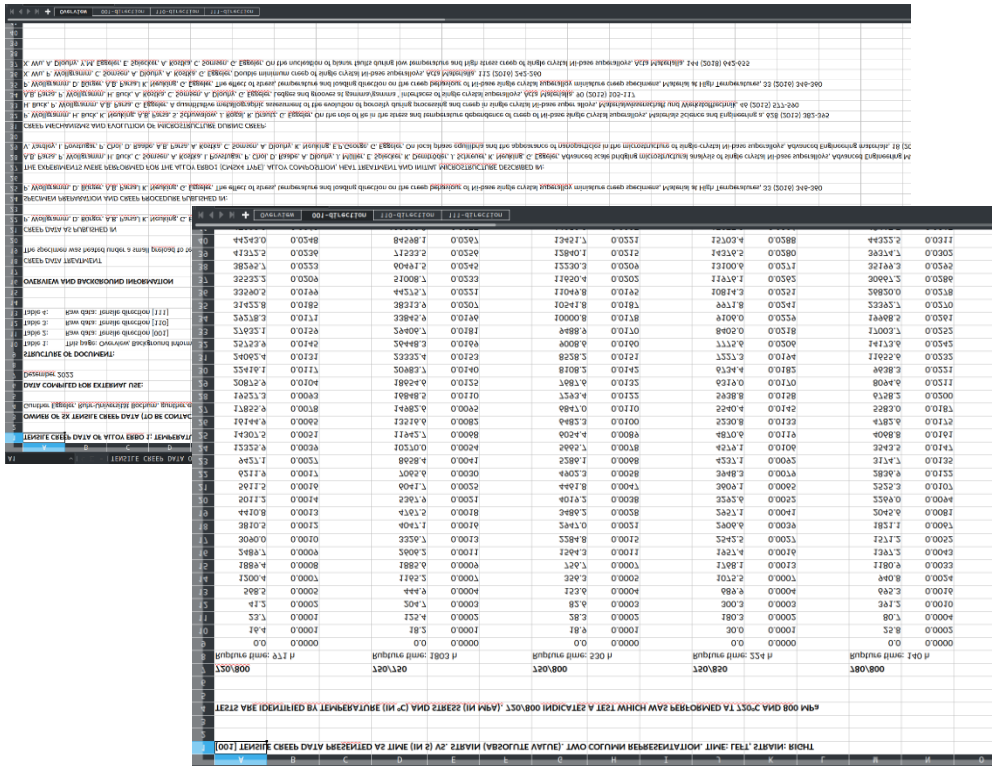
Prüf- und Messmittel Typ	Hersteller	Maschinen-/ Serien-/ Modell-Nummer	Messbereich				
Prüfmaschine	BAM Umbau Mohr&Federhaff	Zug 1 Zug 4	1 - 20 kN	Kraft: axiale Ausrichtung - Biegeeinstellung	DIN EN ISO 7500-2 und ASTM E4 ASTM E1012	Klasse 1 Prüfmaschine Typ 1 entspricht Klasse 5 (bei Zug 1 ab 9,7kN)	12 Monate einmalig, nach be… Veränderu…
Datenerfassung	National Instruments	NI SCXI-1600					
Extensometer, zweiseitige LVDTs	HBM	8273P01 8273P07 3645400430-52 3645400431-50	0 - 20 mm	Länge [Weg]	ASTM E83	B-2	12 Monate
Thermoelemente Typ S, Messlänge 50 mm 3 Stück pro Probe Messlänge 30 mm 2 Stück pro Probe	BAM 5.2	52-PM102-0063 52-PM102-0064 52-PM102-0065 52-PM102-0066 52-PM102-0067 52-PM102-0068	300 - 1060 °C	Temperatur	Kalibriervorschrift: EURAMET cg-8, ASTM E230	keine Klasse Korrektur des Temperatur-Messwertes um die Gesamtabweichung des Thermoelements und der Messkette	12 Monate
Temperatur-messkette, Anzahl siehe Thermoelemente	National Instruments	NI SCXI-1102	100 - 1000 °C	Temperatur	Kalibriervorschrift: EURAMET cg-11, ASTM E230		3 Monate

```
▾ Metadata:
  ▾ Test info:
    ▸ Bibliographic information:
    ▾ Test order:
      ▾ Test date:
          Value: "15.08.2017"
          Unit: ""
          Symbol: ""
      ▾ Test ID:
          Value: "KK 970"
          Unit: ""
          Symbol: ""
      ▾ Project:
          Value: "int. Ringversuch 2017"
          Unit: ""
          Symbol: ""
      ▾ Operator:
          Value: "NN1"
          Unit: ""
          Symbol: ""
  ▾ Specified test parameters:
    ▾ Testing Standard:
        Value: "ASTM E 139"
        Unit: ""
        Symbol: ""
    ▾ Specified Temperature:
        Value: "600"
        Unit: "°C"
        Symbol: "T"
    ▸ Initial stress:
    ▸ Test type (interrupted/not interrupted):
    ▸ End of experiment (time limit/test piece break/extension limit):
    ▸ Test force:
  ▸ Tested material:
  ▸ Testing and measuring equipment:
▸ Primary data:
▸ Secondary data:
```

Notebook 00_GetSchema
Notebook 01_BAM_to_schema

Application for data schema and control vocabulary

Data from working group → Mappings → data schema / data structure → Structured user data



- Metadata:
  - Test info:
  - Tested material:
  - Testing and measuring equipment:
- Primary data:
  - Test results:
    - Bibliographic information:
    - State at test start:
    - Test sequence:
    - State at end of test :
    - raw_elongations:
    - raw_times:
- Secondary data:
  - Test results:
    - Test sequence:
      - Corrected measured temperature:
      - Loading rate:
      - Unloading rate:
      - Heating speed:
      - Cooling speed:
    - Elongation and extension:

- Metadata:
  - Test info:
    - Bibliographic information:
    - Specified test parameters:
      - End of experiment (time limit/test piece break/extension limit):
      - Initial stress:
        - Symbol: "R0"
        - Unit: "MPa"
        - Value: "800"
      - Specified Temperature:
        - Symbol: "T"
        - Unit: "°C"
        - Value: "720"
      - Test force:
      - Test type (interrupted/not interrupted):
      - Testing Standard:
    - Test order:
      - Operator:
      - Project:
        - Symbol: ""
        - Unit: ""
        - Value: "SFB/TR103"
      - Test ID:
      - Test date:
  - Tested material:
    - Bibliographic information:
    - Material and state:
      - Ageing applied?:
      - Angle orientation:
        - Blank: Geometry/Dimensions: "Plate"
        - Blank: date of supply: "20.10.2011"
      - Blank: order number:
      - Blank: supplier sample ID:
      - Chemical composition, measured (including precision):
      - Chemical composition, nominal:
      - Crack inspection details:
      - Geometry/dimensions of blank:
      - Grain Defects mapzos?:
      - Heat treatment: Atmosphere:

Notebook 02_GetRubTables
Notebook 03_Rub_to_schema

Application for data schema and control vocabulary

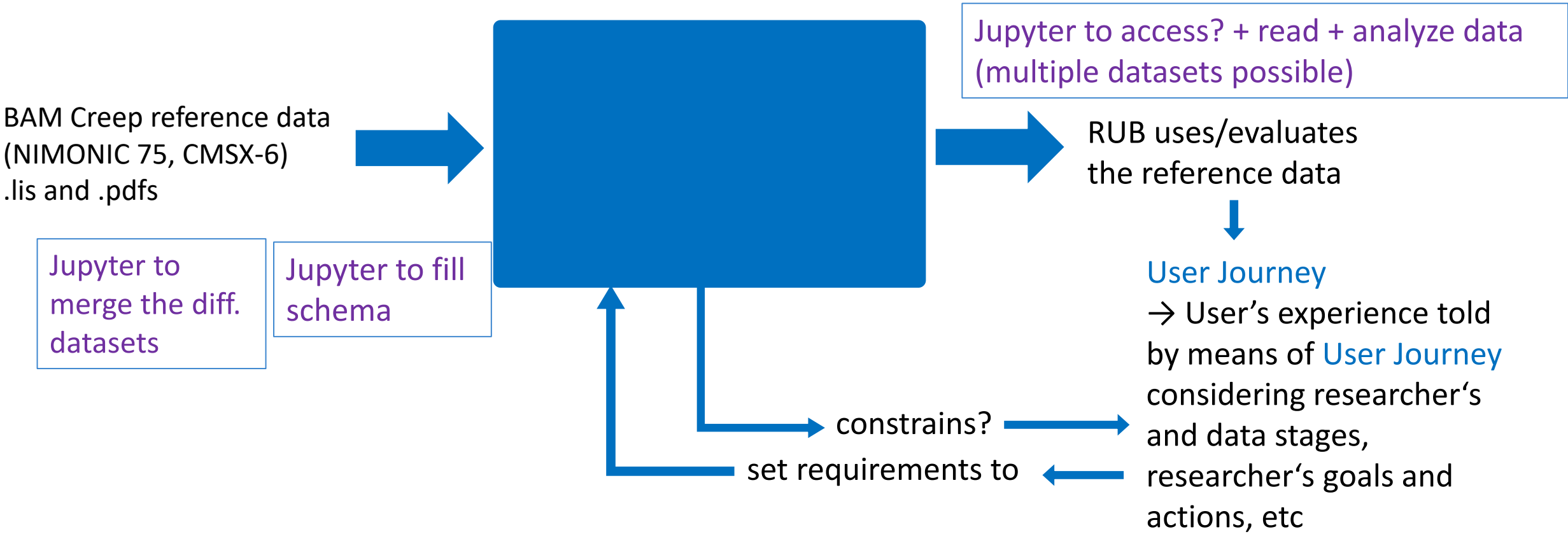
User 1 data + User 2 data → Direct comparison of data (automated)

	BAM			RUB		
	Value	Unit	Symbol	Value	Unit	Symbol
Testing Standard	ISO 204			MISSING		
Specified Temperature	600	°C	T	720	°C	T
Initial stress	MISING	MPa	R0	800	MPa	R0
Test type (interrupted/not interrupted)	MISSING			MISSING		
End of experiment (time limit/test piece break/extension limit)	MISSING - Time limit ?			MISSING - Time limit ?		
Test force	4,53	kN		MISSING		

	BAM			RUB		
	Value	Unit	Symbol	Value	Unit	Symbol
Test date	15.08.2017			MISSING		
Test ID	KK 970			MISSING		
Project	int. Ringversuch 2017			SFB/TR103		
Operator	NN1			MISSING		

Notebook 04_CompareDataSources

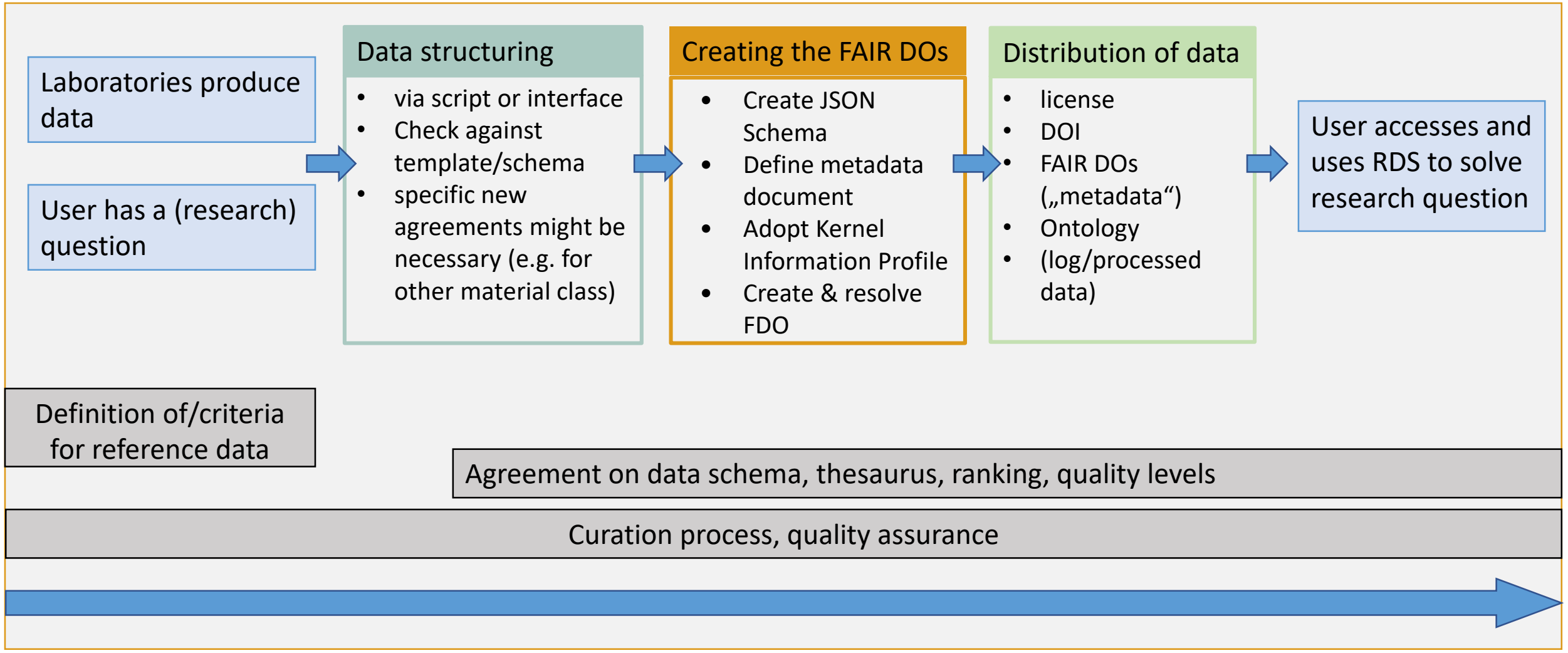
Demonstrator sche



Merging of the vocabulary (diff. data entries), Glossary

User Journey:
https://app.conceptboard.com/board/x7zn-2yq0-eabn-piic-dbiu

Summary


Laboratories produce data
User has a (research) question
Data structuring
• via script or interface
• Check against template/schema
• specific new agreements might be necessary (e.g. for other material class)
Creating the FAIR DOs
• Create JSON Schema
• Define metadata document
• Adopt Kernel Information Profile
• Create & resolve FDO
Distribution of data
• license
• DOI
• FAIR DOs („metadata“)
• Ontology
• (log/processed data)
User accesses and uses RDS to solve research question
Definition of/criteria for reference data
Agreement on data schema, thesaurus, ranking, quality levels
Curation process, quality assurance