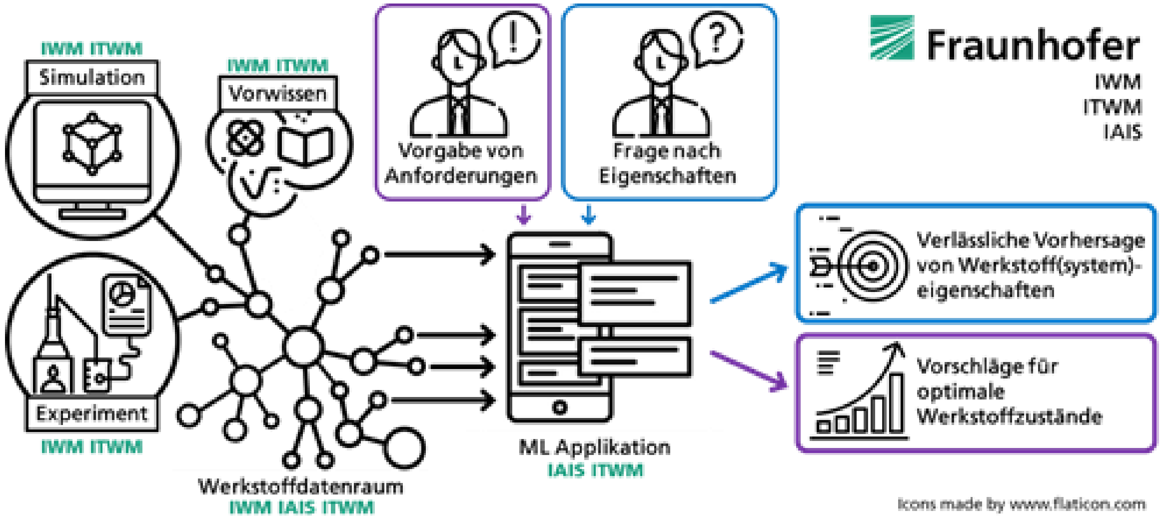
ONLINE-VERANSTALTUNG

Digital verfügbares Werkstoff- und Prozesswissen
Anwendungsbeispiel »Bewertung der Lebensdauer hochfester Stähle« im Überblick

Abschlusskolloquium
des Fraunhofer-Konsortiums »UrWerk«
zur Entwicklung von unternehmensspezifischen
Werkstoff(system)-Datenräumen



Moderation Dr. Michael Luke
Projektleiter »UrWerk«
Geschäftsfeldleiter »Bauteilsicherheit und Leichtbau«
am Fraunhofer-Institut für Werkstoffmechanik IWM

24.November 2022

Digital verfügbares Werkstoff- und Prozesswissen
Anwendungsbeispiel »Bewertung der Lebensdauer hochfester Stähle« im Überblick

24.11.2022

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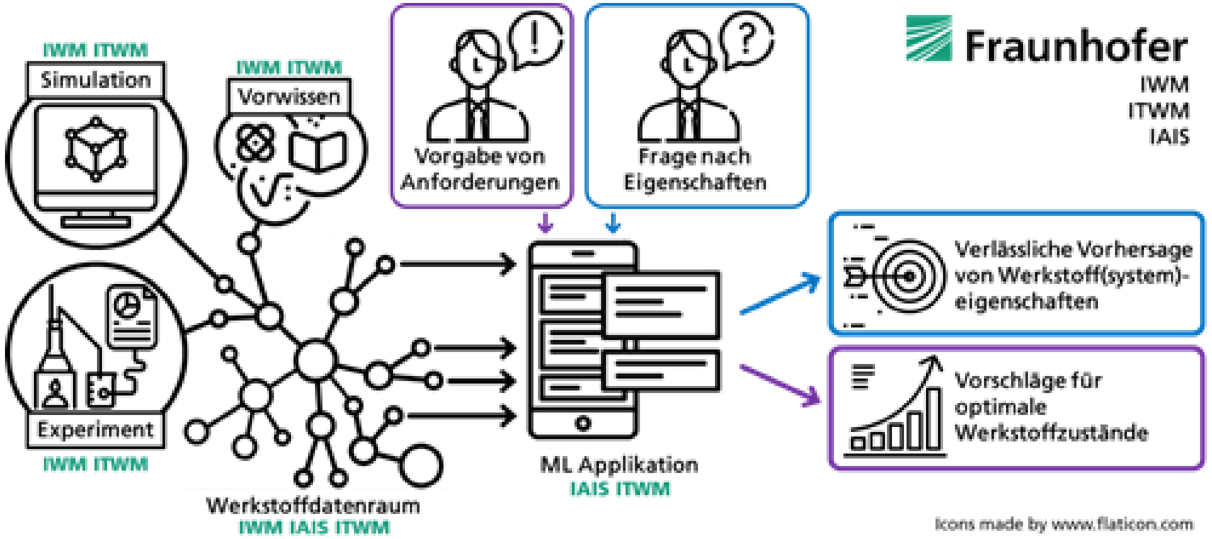
José Manuel Domínguez,
Gunar Ernis,
Joana Francisco Morgado,
Hans-Ulrich Kobialka,
Johannes Rosenberger,
Johannes Tlatlik

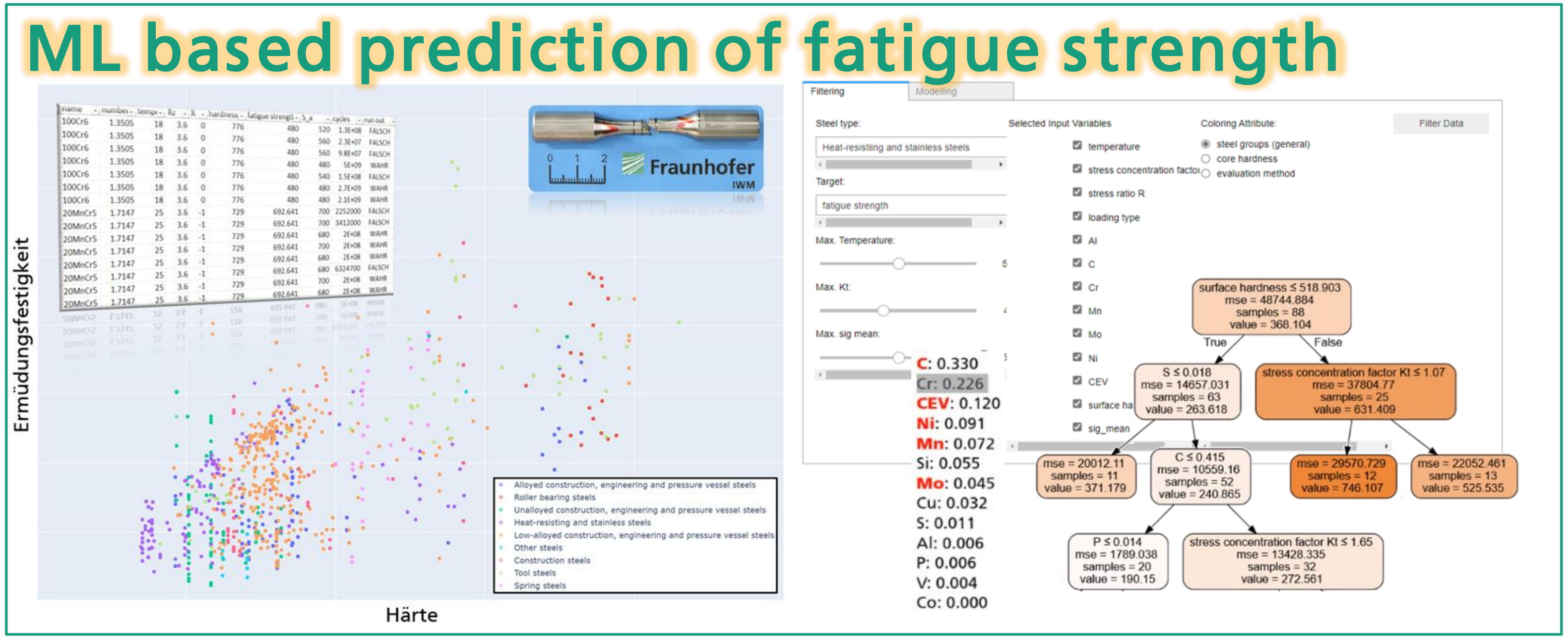


MAVO „UrWerk“ (2019 – 2022)
Unternehmensspezifische Werkstoff-Datenräume zur beschleunigten Produktentwicklung

sascha.fliegener@iwm.fraunhofer.de

Introduction

- The **fatigue strength of high strength steels** depends on a multitude of parameters: *chemical composition, heat treatment, surface condition (hardness, roughness), specimen geometry, load parameters (loading type, stress amplitude, R ratio etc) and microstructure (inclusion, pores…)*
- **Aim:** Digital methods can enable a **machine learning based prediction of fatigue strength** which complements or replaces material characterization experiments in the product design phase and thus enable significant cost savings



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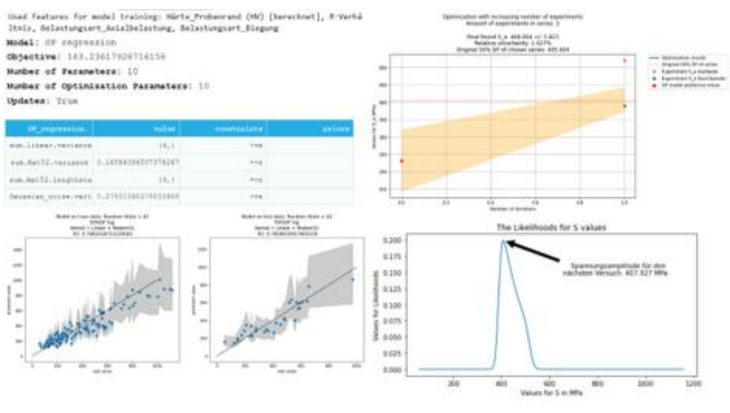
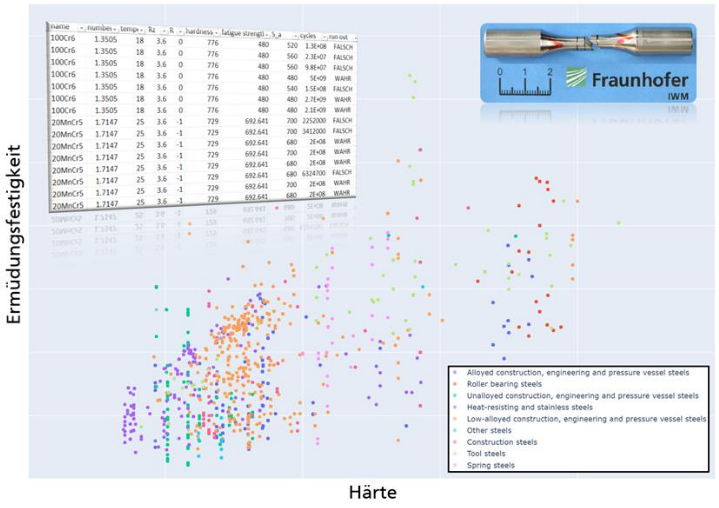
Overview of fatigue use case

- **1. Fatigue database** – data collection fatigue of high strength steels
- **2. Ontology and Dataspace** – Semantic description of fatigue data
- **3. Machine Learning** – Python based ML on fatigue database
- **4. DOE Tool** – Design of Experiments for fatigue use case

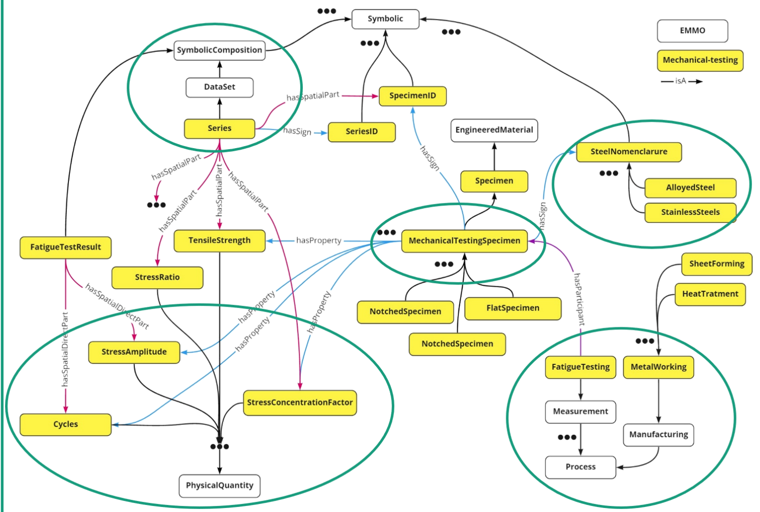
4. Design of Experiments



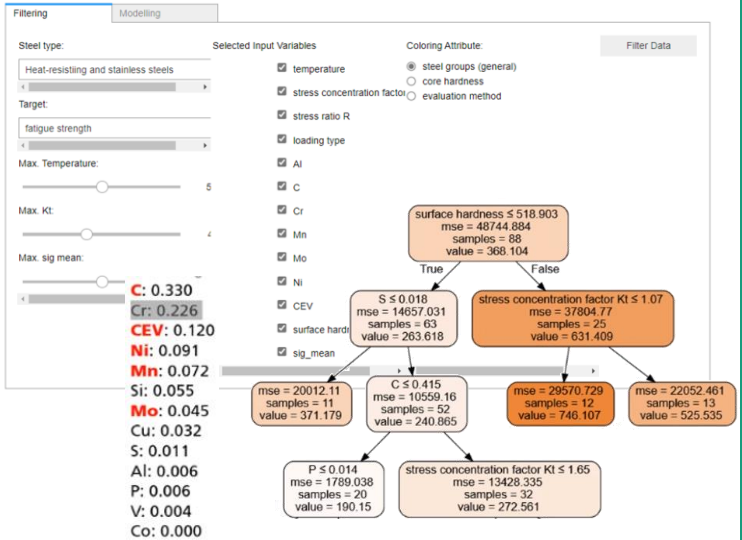
1. Fatigue Database



2. Ontology & Dataspace



3. Machine Learning



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UHRZEIT	PROGRAMMPUNKT
10:00 Uhr	Einführung »Digital verfügbares Werkstoff- und Prozesswissen für die beschleunigte Produktentwicklung« Prof. Dr. Chris Eberl, Dr. Michael Luke
10:10 Uhr	Anwendungsbeispiel »Bewertung der Lebensdauer hochfester Stähle« im Überblick Dr. Sascha Fliegener
10:30 Uhr Thema 1,2	Live Demo der Nutzung von Datenraum-Werkzeugen (Ontologie, Prozessgraph, Abfragen) Dr. Sascha Fliegener, José Dominguez, Dr. Joana Morgado, Johannes Rosenberger
11:00 Uhr	Diskussion; alle

11:15 Uhr Thema 3	Live Demo der Nutzung von Machine Learning Analysen zur Vorhersage der Ermüdungsfestigkeit von hochfesten Stählen Dr. Hans-Ulrich Kobialka, Dr. Sascha Fliegener, Johannes Rosenberger
11:45 Uhr	Diskussion
12:00 Uhr	Lunch break
13:00 Uhr Thema 4	Live Demo der Nutzung von Design of Experiments für die Planung von Lebensdauerversuchen (Treppenstufenverfahren) Dr. Gunar Ernis
13:15 Uhr	Diskussion

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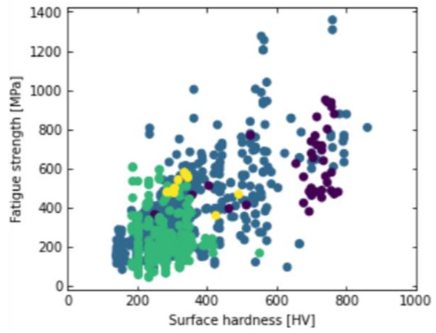
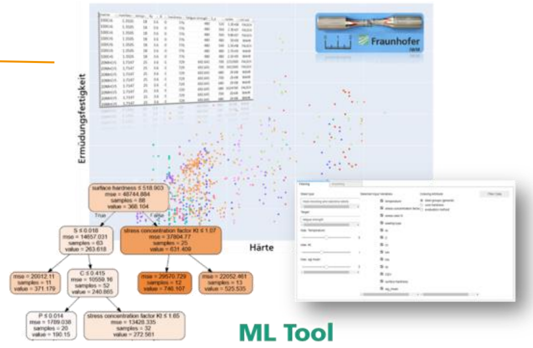
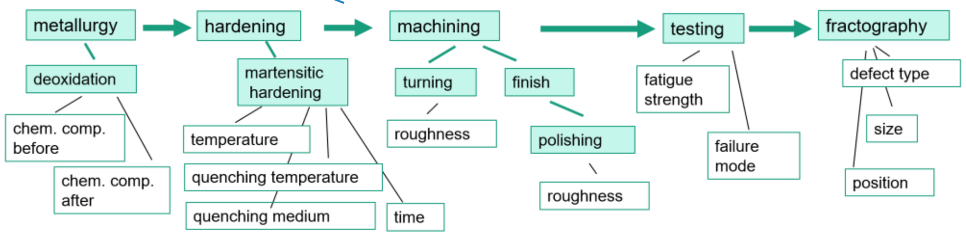
Agenda

- Introduction
- Fatigue database and machine learning
  - Assembling a fatigue database from literature data and previous projects
  - ML tool: property predictions using the data set
- Ontology and knowledge graph
  - Use cases
    (1) large fatigue database
    (2) process & manufacturing history of 100Cr6
  - Knowledge graph, domain ontology, data mapping workflow
  - Example: Query the heat treatment history (SPARQL)
- Conclusions, Outlook



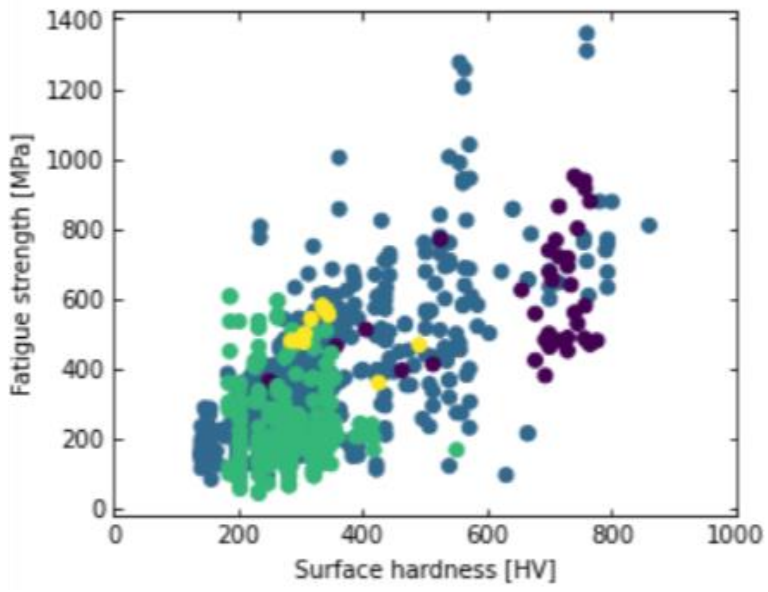




Fatigue Database
Assembling the database

- **Fatigue data from different data sources** (literature, existing database collections, previous projects etc.)
- **Fatigue parameters:** fatigue strength, slope SN curve, knee point
- **Properties:** chemical composition, hardness, specimen geometry (stress concentration factor), load parameters, surface condition (e.g. roughness) etc.
- Raw Experimental data (i.e. stress amplitude and number of cycles for each specimen of a test series) was evaluated in a **standardized way** with the software „JuroJin" [1] to get the fatigue properties (SN curve) for each testing series

Series property (fatigue strength)
Source1, Source2, Source3, Source4



- **Final database version:** 110 materials, 1100 testing series), 22 000 experiments
- **Data curation**, e.g. hardness / tensile strength conversion, derived roughness values, steel categories…

[1] https://www.itwm.fraunhofer.de/de/abteilungen/mf/produkte-und-leistungen/jurojin.html

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Fatigue Database
Final version of the database

110 materials

1100 testing series

22 000 experiments

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Fatigue Database

Data Analytics / Machine Learning

- **UseCase 1: Hardness prediction for steels** depending on their chemical composition
  - Validation of material science knowledge with a „real“ database (see table*)
  - Aim: Establish confidence in the analysis method
- **UseCase 2: Fatigue strength prediction for high strength steels**
  - Industrial use case, influence of chemical elements, hardness, roughness and other parameters

*Quelle: Vorlesung „Metallische Werkstoffe“, Ernst Fleischmann, Universität Bayreuth

Übersicht: Einfluß der Legierungselemente auf die Eigenschaften des Stahls

Werkstoffe

	Mechanische Eigenschaften																Magnet.Eigensch.				
Legierungs-element	Härte	Festigkeit	Streck-grenze	Dehnung	Einschnürung	Kerbschlag-zähigkeit	Elastizität	Warm-festigkeit	Abkühlge-schwindigkeit	Karbid-bildung	Verschleiß-festigkeit	Schmied-barkeit	Zerspan-barkeit	Verzunderung	Nitrier-barkeit	Rostbe-ständigkeit	Hysteresis	Permeabilität	Koerzitivkraft	Remanenz	el. Leistungs-verlust
Si	↑	↑	↑↑	↓	~	↓	↑↑↑	↑	↓	↓	↓↓↓	↓	↓	↓	↓	–	↓↓	↑↑	↓↓	–	↓↓
Mn In perlit. Stählen	↑	↑	↑	~	~	~	↑	~	↓	~	↓↓	↑	↓	~	~	–					
Mn In austenit. Stählen	↓↓↓	↑	↓	↑↑↑	~	–	–	–	↓↓	–	–	↓↓↓	↓↓↓	↓↓	–	–	unmagnetisch not magnetic non magnétique				
Cr	↑↑	↑↑	↑↑	↓	↓	↓	↑	↑	↓↓↓	↑↑	↑	↓	–	↓↓↓	↑↑	↑↑↑			↑	↑↑	
Ni In perlit. Stählen	↑	↑	↑	~	~	~	–	↑	↓↓	–	↓↓	↓	↓	↓	–	–			↑↑	↑↑	
Ni In austenit. Stählen	↓↓	↑	↓	↑↑↑	↑↑	↑↑↑	–	↑↑↑	↓↓	–	–	↓↓↓	↓↓↓	↓↓	–	↑↑	unmagnetisch not magnetic non magnétique				
Al	–	–	–	–	↓	↓	–	–	–	–	–	↓↓	–	↓↓	↑↑↑	–			↑↑	↑↑	
W	↑	↑	↑	↓	↓	~	–	↑↑↑	↓↓	↑↑	↑↑↑	↓↓	↓↓	↓↓	↑	–			↑↑↑	↑↑↑	
V	↑	↑	↑	~	~	↑	↑	↑↑	↓↓	↑↑↑↑	↑↑	↑	–	↓	↑	↑					
Co	↑	↑	↑	↓	↓	↓	–	↑↑	↑↑	–	↑↑↑	↓	~	↓	–	–		↑↑	↑↑↑	↑↑↑	
Mo	↑	↑	↑	↓	↓	↑	–	↑↑	↓↓	↑↑↑	↑↑	↓	↓	↑↑	↑↑	–			↑		
Cu	↑	↑	↑↑	~	~	~	–	↑	–	–	–	↓↓↓	~	~	–	↑					
S	–	–	–	↓	↓	↓	–	–	–	–	–	↓↓↓	↑↑↑	–	–	↓					
P	↑	↑	↑	↓	↓	↓↓↓	–	–	–	–	–	↓	↑↑	–	–	–					

↑ Erhöhung ↓ Erniedrigung ~ gleichbleibend - nicht charakteristisch oder unbekannt Mehrere Pfeile = verstärkte Wirkung

Ernst Fleischmann, Metallische Werkstoffe 138 Metallische Halbzeuge

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Fatigue Database: Machine Learning

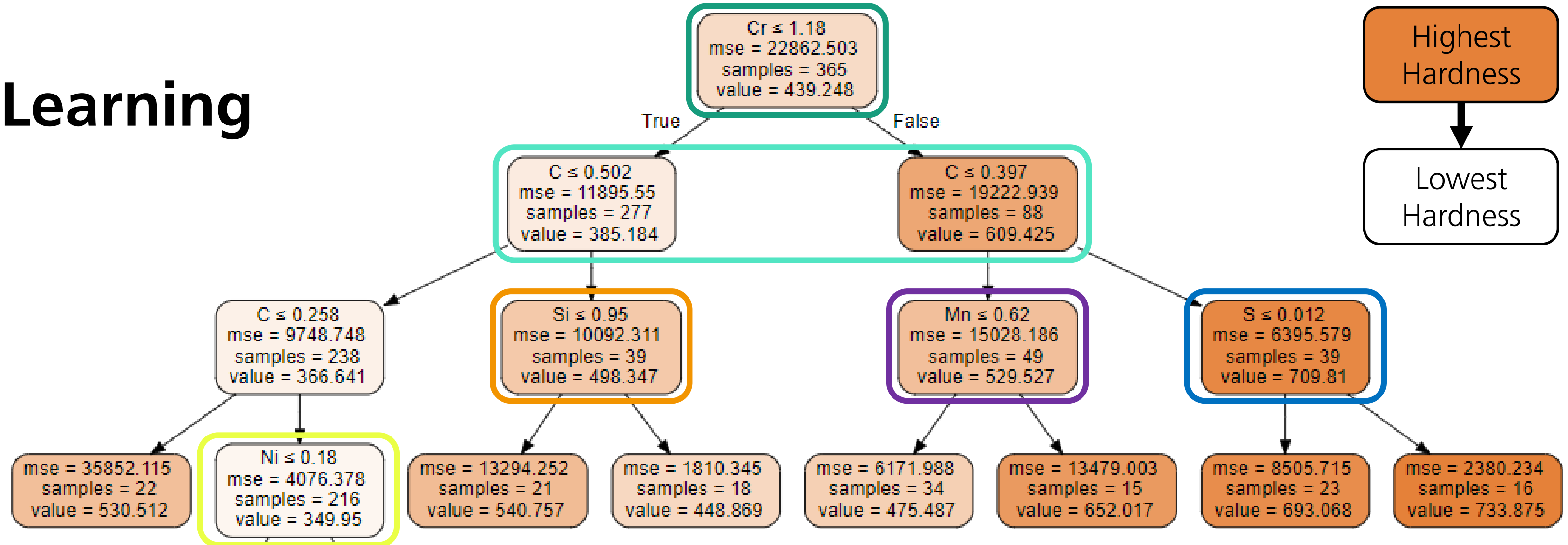
Hardness prediction

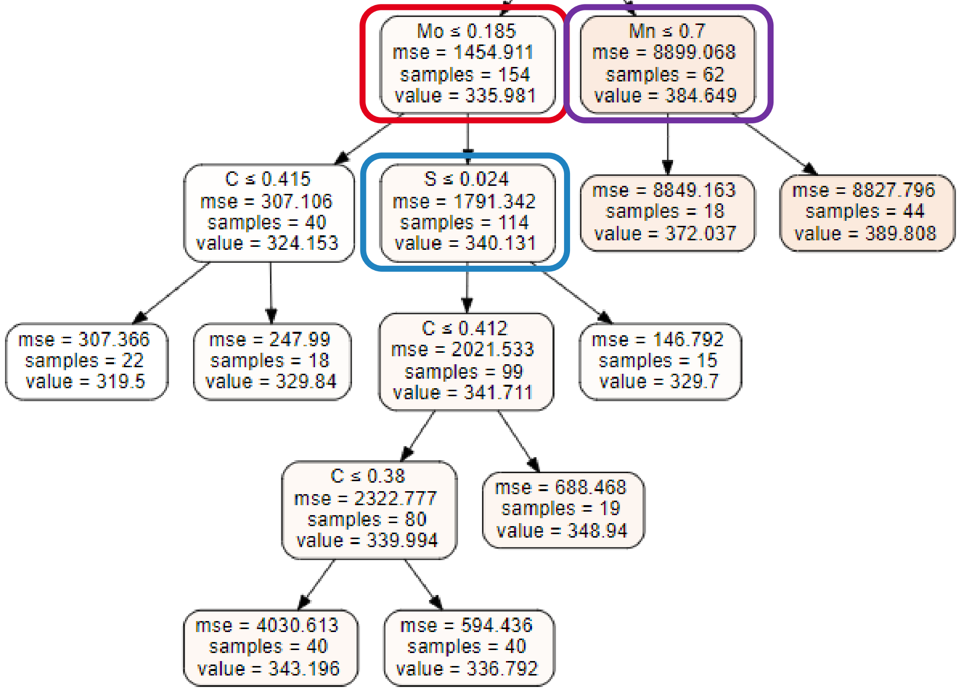
Exisiting material science knowledge
(effect of alloying elements on hardness)
vs.
Machine learning prediction
(feature importance list)

Legierungs-element		Härte
Si		↑
Mn	In perlit. Stählen	↑
Mn	In austenit. Stählen	↓↓↓
Cr		↑↑
Ni	In perlit. Stählen	↑
Ni	In austenit. Stählen	↓↓
Al		–
W		↑
V		↑
Co		↑
Mo		↑
Cu		↑
S		–
P		↑

from [1]

```
Cr: 0.471
C: 0.300
Ni: 0.066
Cu: 0.033
Si: 0.033
Mo: 0.031
Mn: 0.031
N: 0.023
S: 0.005
Al: 0.003
P: 0.003
V: 0.002
Co: 0.000
```





- Machine learning analysis based on random forest regression
- Aim: reproduce well known correlations from material science with real data to verify the analysis procedure
- Here: influence of different alloying elements on hardness

[1] Quelle: Vorlesung „Metallische Werkstoffe“, Ernst Fleischmann, Universität Bayreuth

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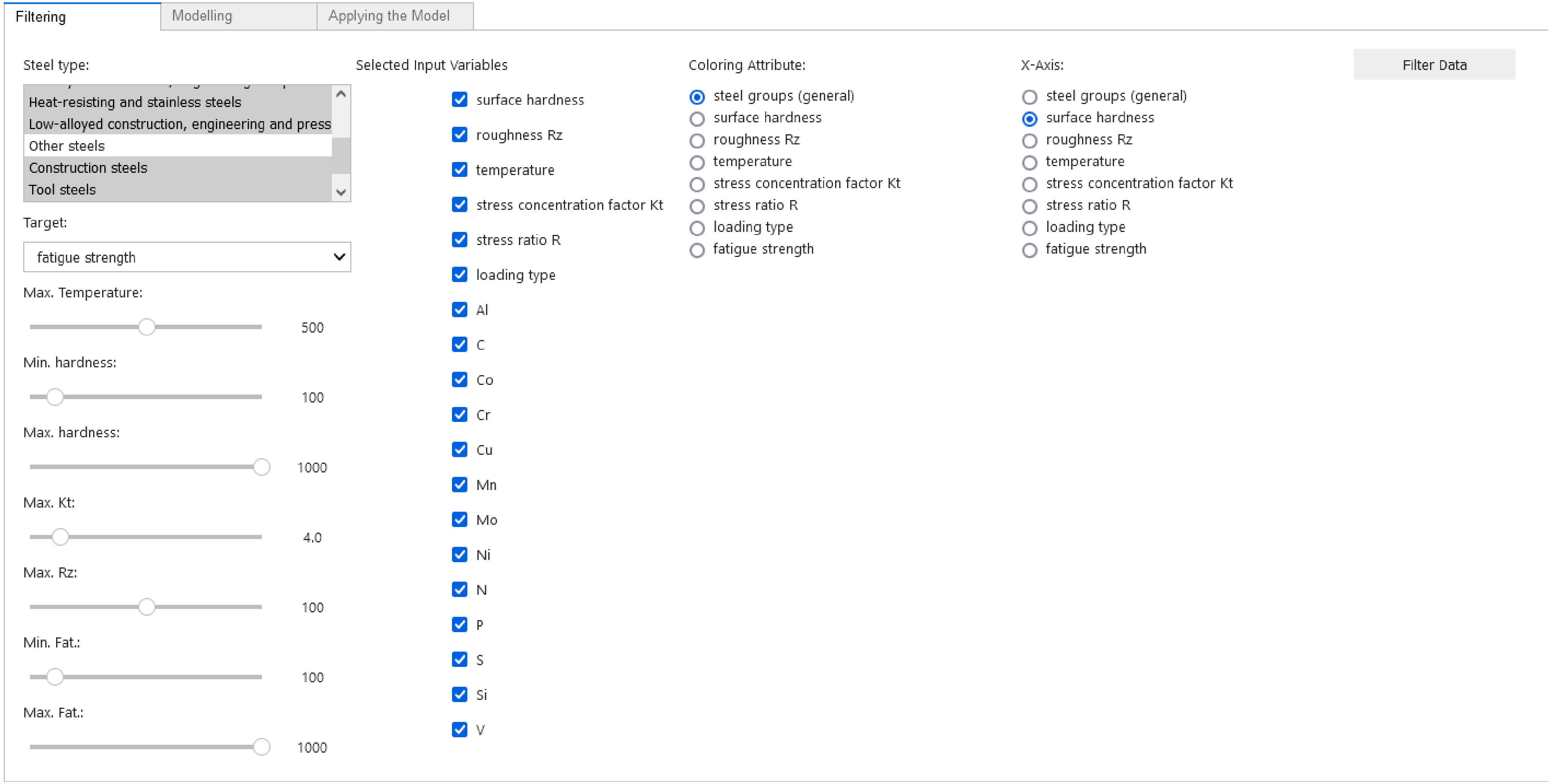
Fatigue Database: Machine Learning

ML Tool - Overview

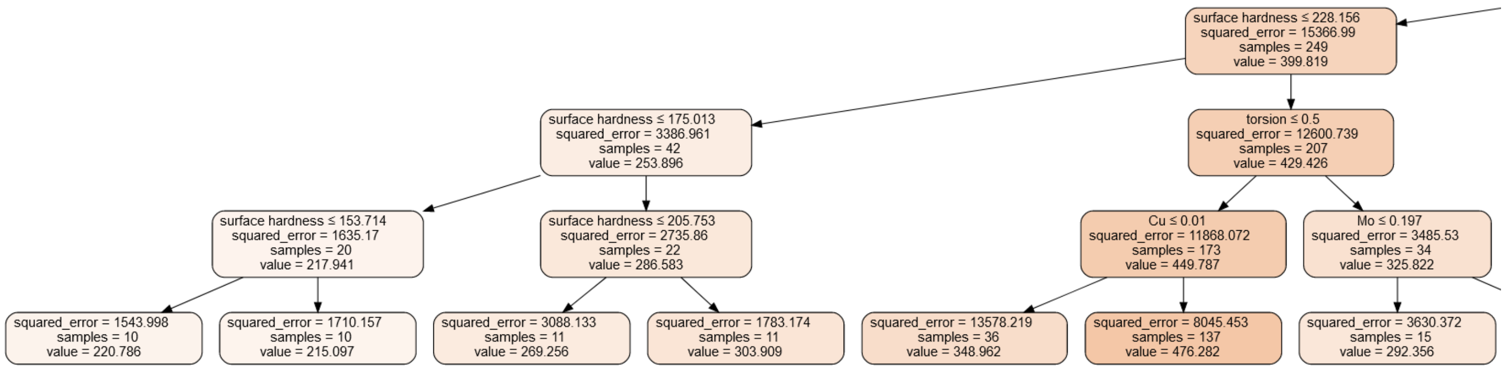


Fatigue Database: Machine Learning
ML Tool – Training and Cross Validation

Feature importance

```
surface hardness: 0.573
stress concentration factor Kt: 0.222
stress ratio R: 0.053
Cu: 0.035
S: 0.022
torsion: 0.022
Mn: 0.020
roughness Rz: 0.009
Si: 0.009
Ni: 0.006
rotating bending: 0.005
Cr: 0.004
C: 0.004
Mo: 0.004
V: 0.004
P: 0.002
temperature: 0.001
Al: 0.001
tension/compression: 0.001
bending: 0.001
N: 0.001
superposition: 0.000
Co: 0.000
```

```
None
R2 score on training data is 0.698427498657641
R2 score on log training data is 0.7337726117332948
```



Fatigue Database: Machine Learning

ML Tool – Applying the Model

Filtering | Modelling | Applying the Model

Initial Setting of Input Variables

100Cr6

Initial Series Selection

IWM_26

Input Variables

surface har...	765.00
roughness Rz	1.60
temperature	18.00
stress conc...	1.00
stress ratio R	-1.00
loading type	tension/compression
Al	0.00
C	0.95
Co	0.00
Cr	1.44
Cu	0.07
Mn	0.37
Mo	0.02

Model Prediction

799.4027

Apply model

```
Prediction for Target:
fatigue strength
Input values:
surface hardness                 765.0000
roughness Rz                       1.6000
temperature                       18.0000
stress concentration factor Kt     1.0000
stress ratio R                    -1.0000
Al                                 0.0025
C                                  0.9500
Co                                 0.0000
Cr                                 1.4400
Cu                                 0.0710
Mn                                 0.3710
Mo                                 0.0180
Ni                                 0.0000
N                                  0.0000
P                                  0.0150
S                                  0.0070
Si                                 0.3090
V                                  0.0000
bending                            0.0000
rotating bending                   0.0000
superposition                      0.0000
tension/compression                0.0000
torsion                            0.0000
dtype: float64
```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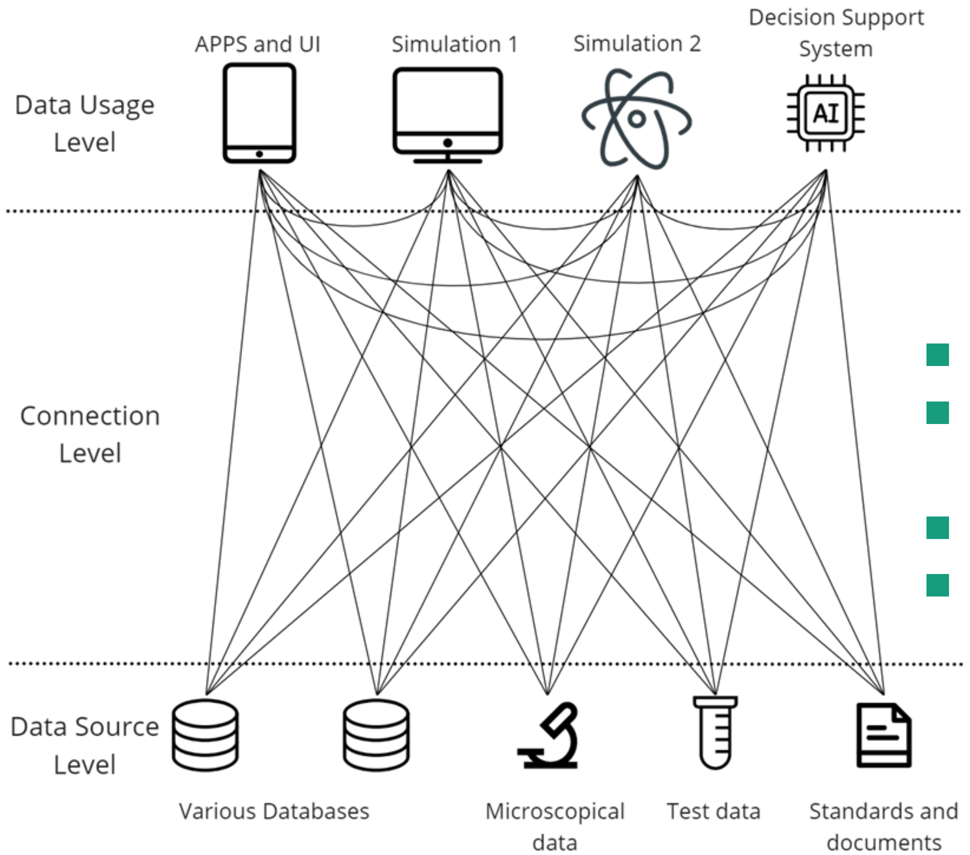
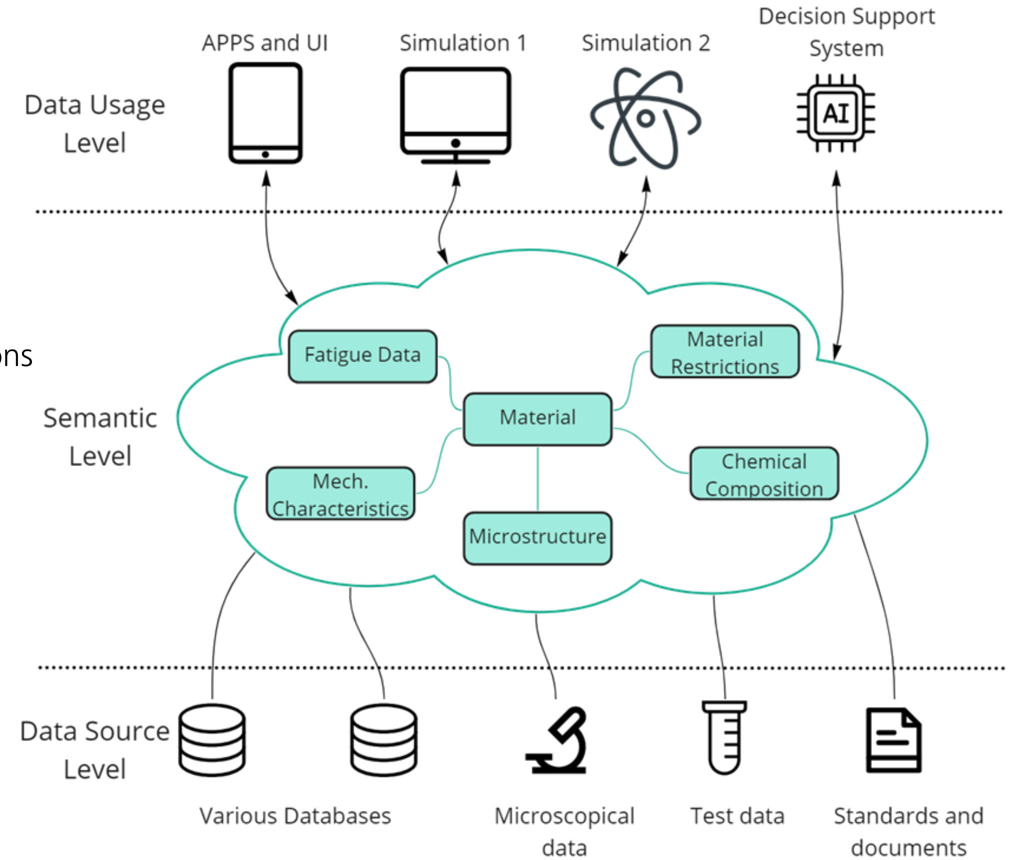
Ontology and Knowledge Graph
Motivation

Why use Knowledge Graphs?



Situation **before** the use of Knowledge Graphs

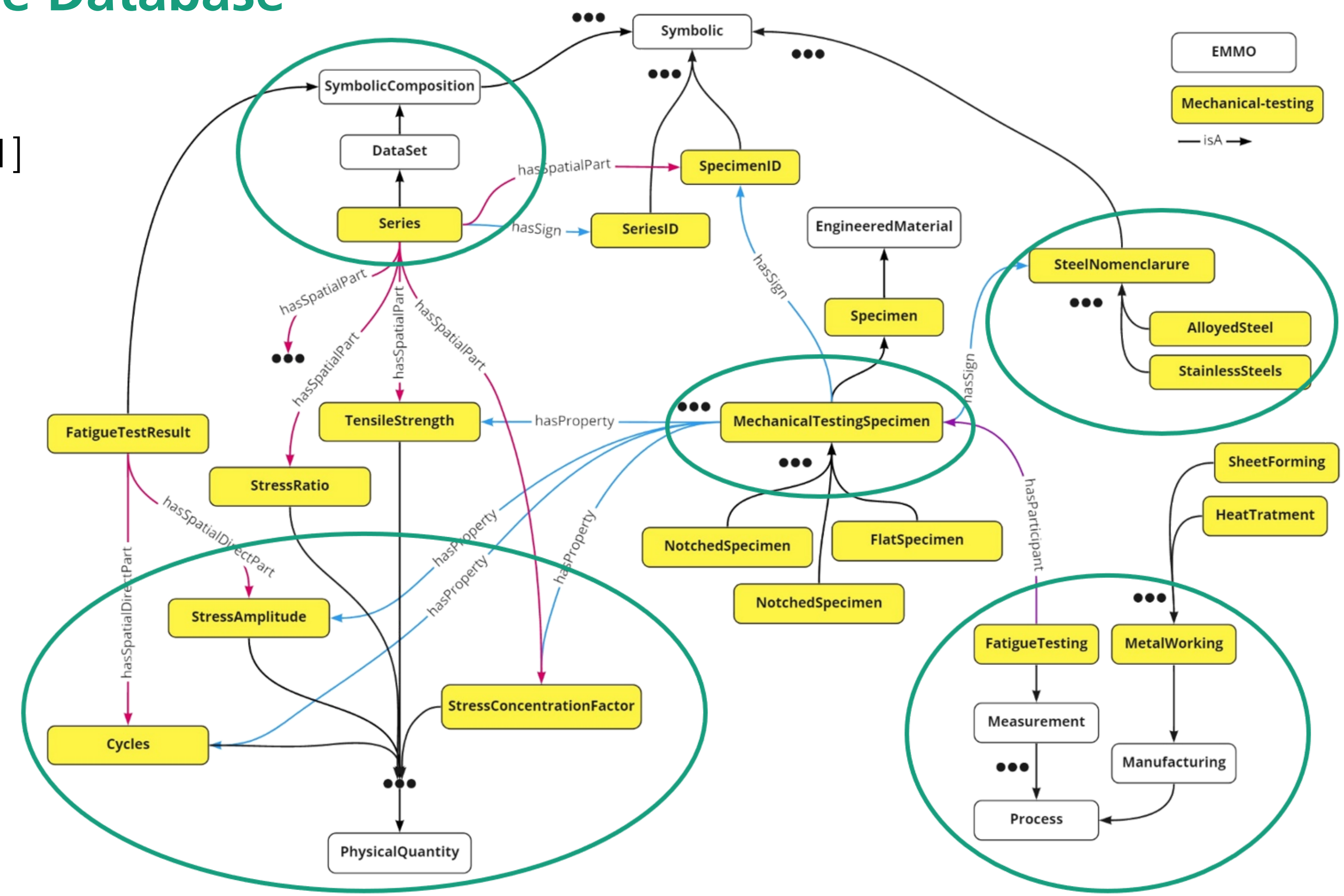
- Enrich Data by relations
- Integration of Data Sources
- Interoperability
- Data-Driven



Situation **after** the use of Knowledge Graphs

Ontology and Knowledge Graph
Use Case 1: Large Fatigue Database

- Fatigue „vocabulary" defined in EMMO Mechanical Testing [1]
- Knowledge graph describing
  - steel nomenclature
  - specimen types
  - fatigue testing: *loading parameters resulting SN curve*
  - heat treatment
- Properties attached to series or specimen object



[1] Elemental Multiperspective Material Ontology (EMMO)
Mechanical Testing Domain Ontology: https://github.com/emmo-repo/domain-mechanical-testing

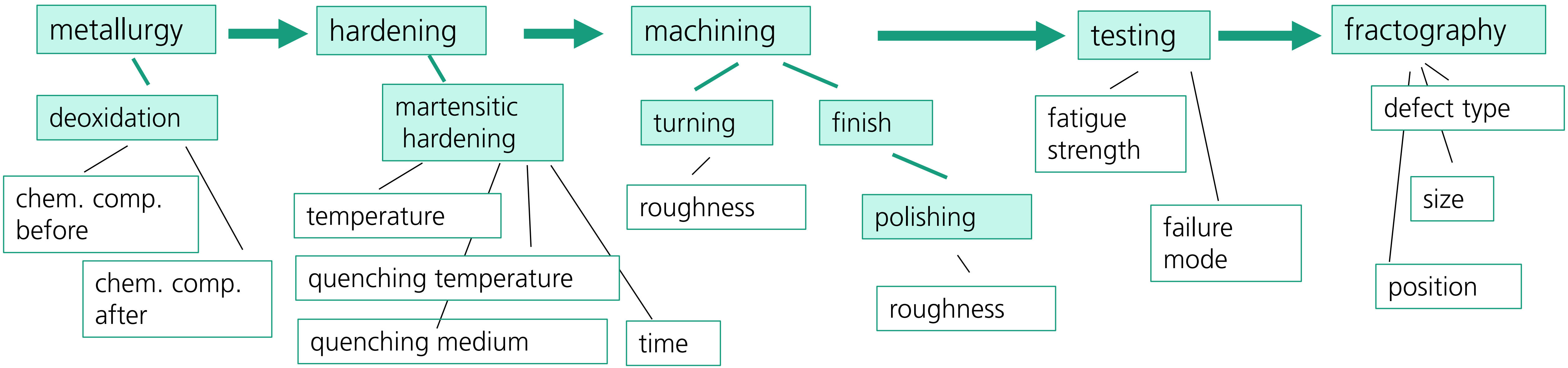
Fraunhofer ITWM | Fraunhofer IAIS | Fraunhofer IWM process steps

parameters / numerical values

Ontology and Knowledge Graph

Use Case 2: Process / manufacturing history of 100Cr6

- Draft of a process graph (specifically for 100Cr6)
- Modular approach: Combination of top-level (e.g. „hardening“) and subprocesses (e.g. „martensitic hardening“) for each material variant
- Implementation in EMMO Domain ontology module „Mechanical Testing“ [1]



[1] Elemental Multiperspective Material Ontology (EMMO)
Mechanical Testing Domain Ontology: https://github.com/emmo-repo/domain-mechanical-testing

process steps

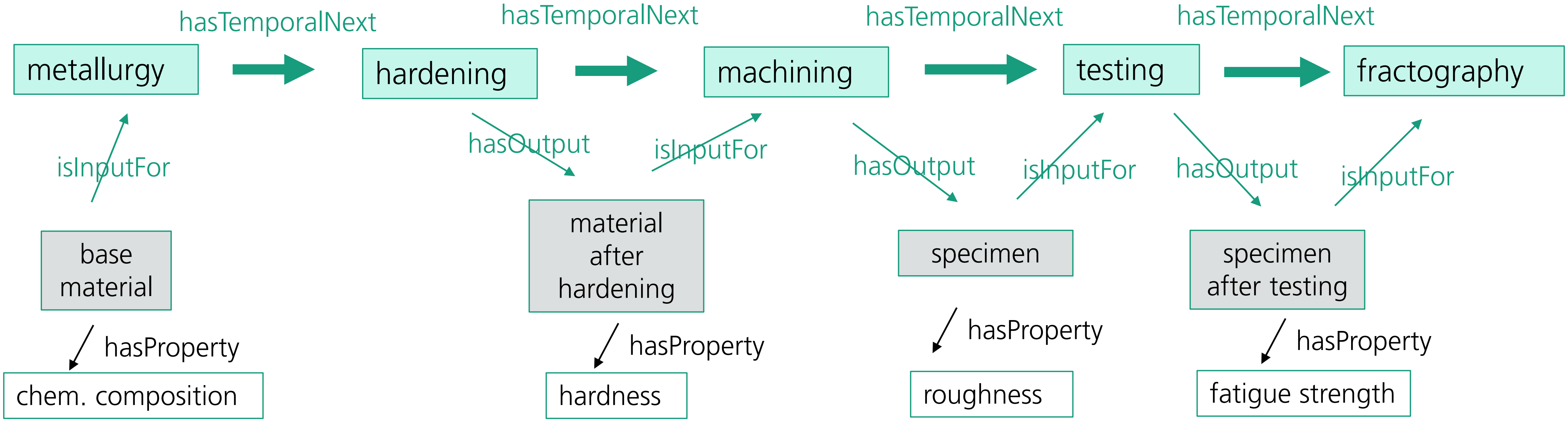
material state

parameters / numerical values

Ontology and Knowledge Graph

Use Case 2: Process / manufacturing history of 100Cr6

- Sequence of processes is modelled with „hasTemporalNext“ relations
- Different material states after each subprocess
- Specific properties attached to differnt material states



Ontology and Knowledge Graph

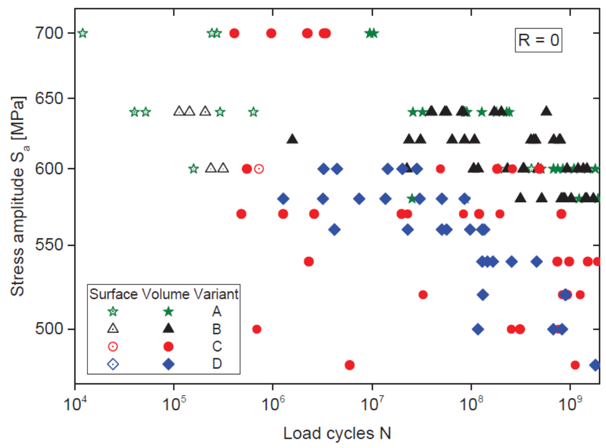
Use Case 2: Process / manufacturing history of 100Cr6

- **100Cr6 dataset**
  - **In total 10 series of 100Cr6 data** (last review meeting Feb 2022: 1 variant)
  - E.g. data from Burkart 2017 [1]: 100Cr6 material from **4 different processing routes**:
    A – standard processing route (Al for deoxidization)
    B – deoxidized by silicon, high oxidic cleanliness
    C – ingot casting with highly improved isotropic properties
    D – vacuum melting / remelting (VIM-VAR)

Variant	mass %								ppm	
	C	Cr	Si	Mn	Cu	Al	S	P	O	N
A	0.95	1.33	0.24	0.41	0.10	0.010	0.005	0.013	4	77
B	0.95	1.43	0.35	0.33	0.07	0.003	0.006	0.011	5	83
C	0.94	1.50	0.29	0.26	0.04	0.027	0.001	0.003	2	67
D	1.00	1.49	0.29	0.33	0.06	0.022	0.002	0.020	2	28

Table 1: Chemical composition of the four steel heats

from [1]



from [1]

Fig. 1: Failed specimens at stress ratio R = 0 differentiated according to surface and volume failure

[1] Burkart K et al, Evaluation of multiple-flaw failure of bearing steel 52100 in the VHCF regime and description of the single-flaw behavior, Stiftung Inst. für Werkstofftechnik (IWT), Bremen 2017

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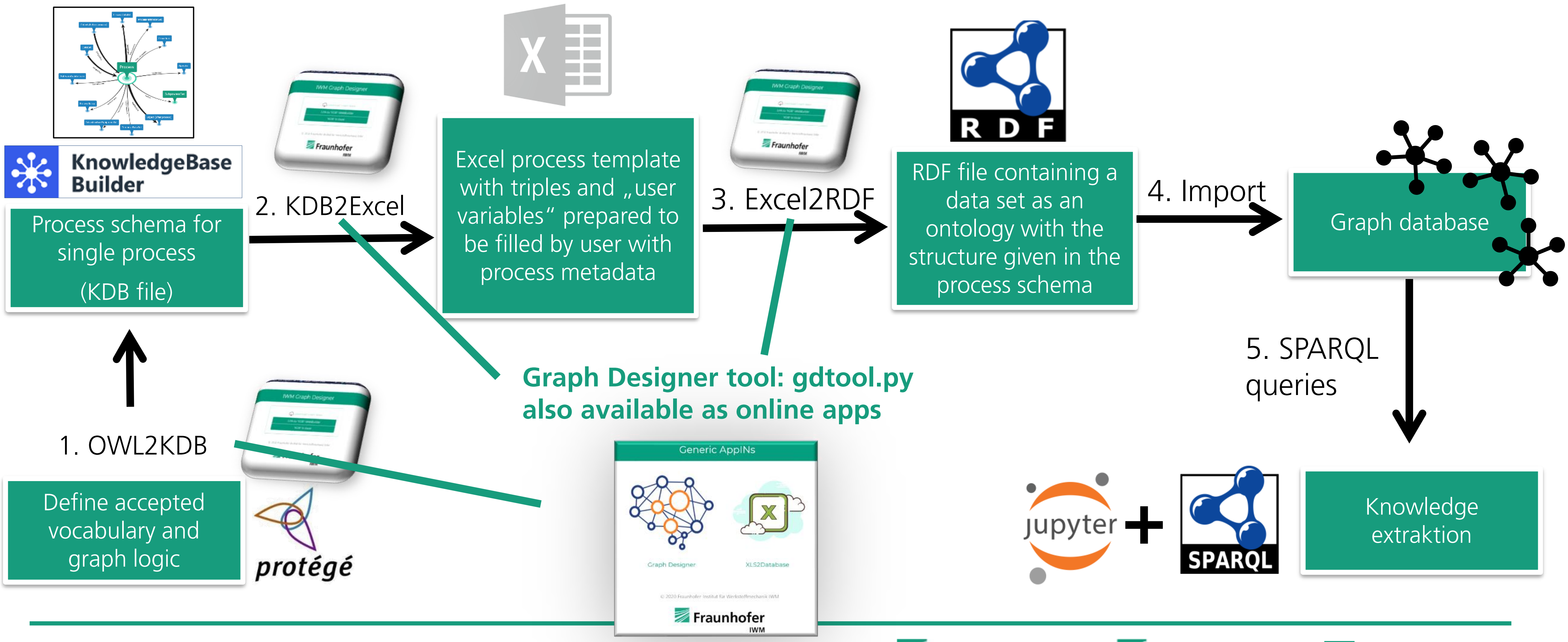
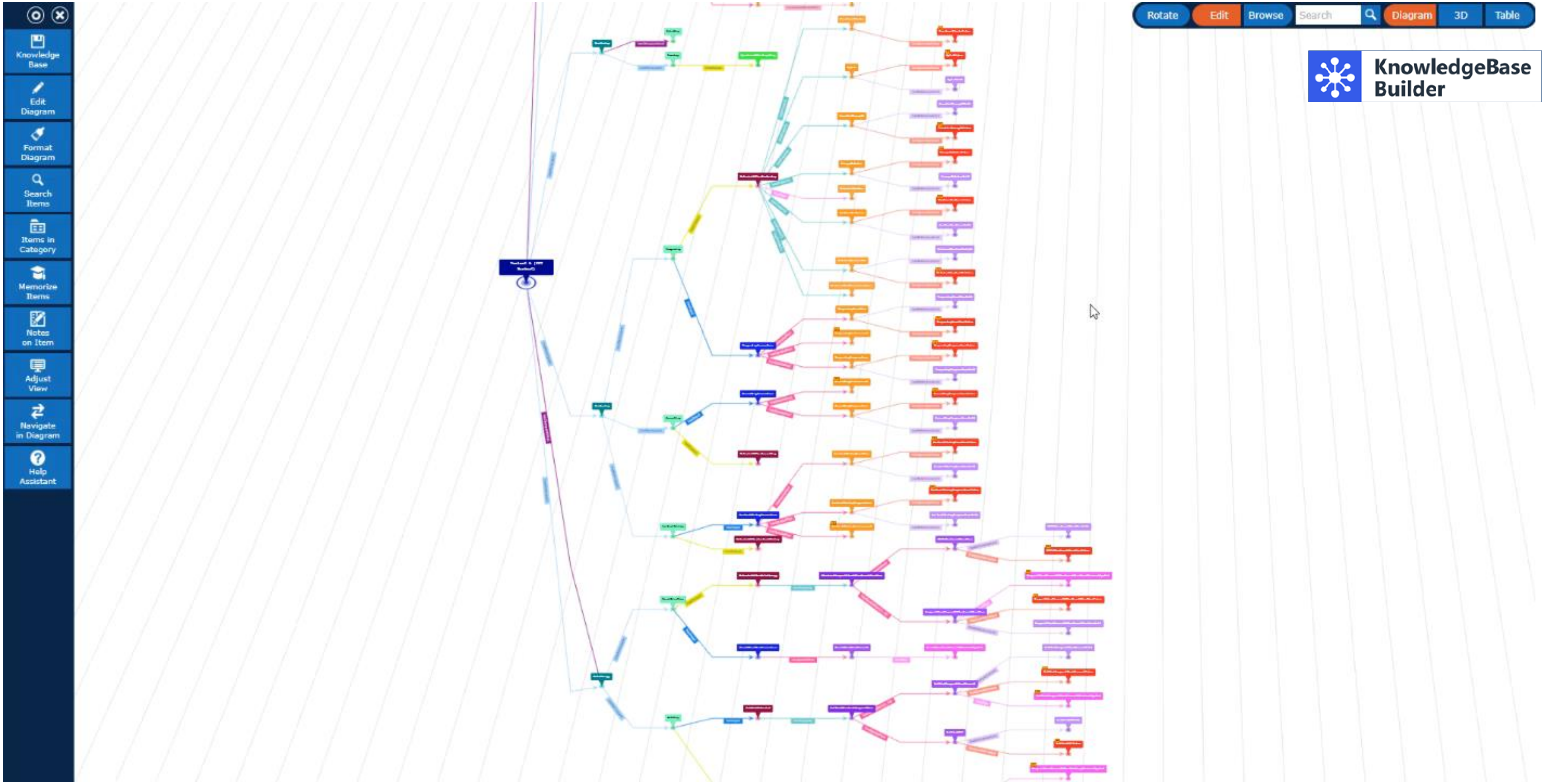
Ontology and Knowledge Graph
Workflow: process graph modeling and mapping of data





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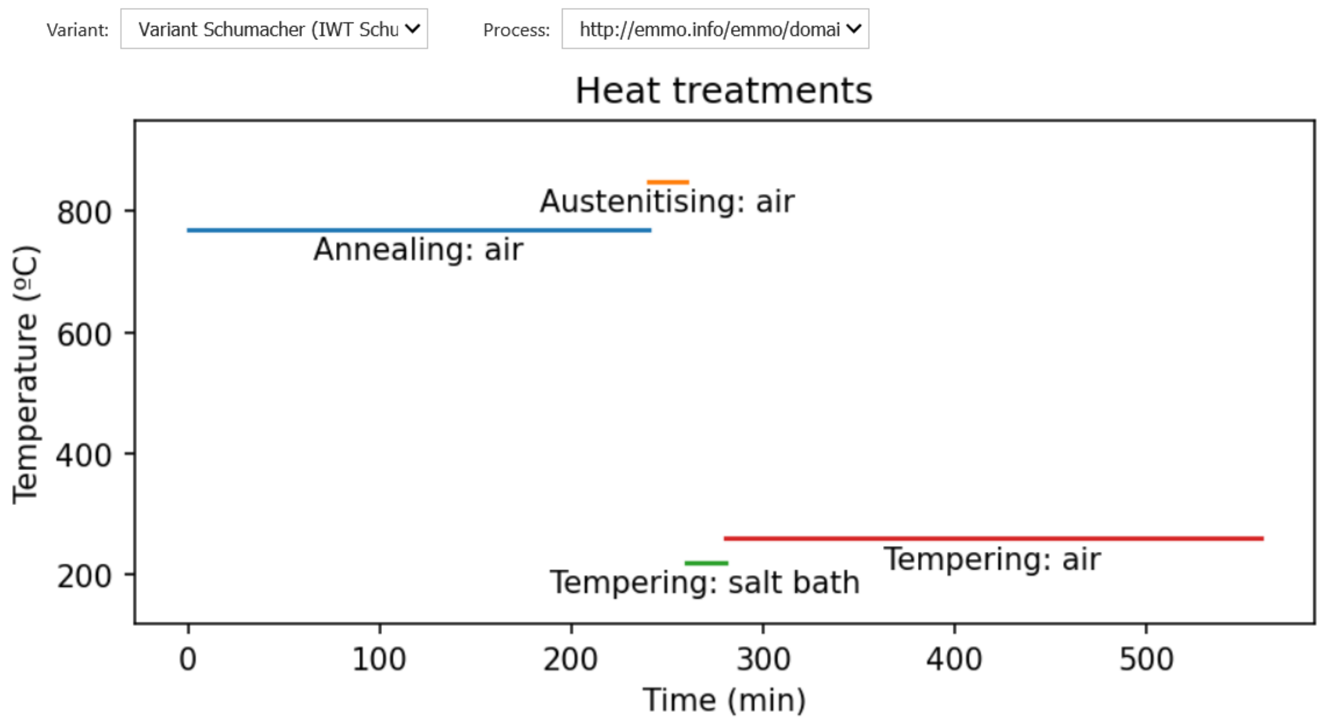
Ontology and Knowledge Graph

Example: Query the heat treatment history (SPARQL)

- Querying the heat treatment temperatures along the process chain with SPARQL




```
query = f"""
SELECT ?top_process ?top_process_label ?process ?process_label ?process_type ?parent_process ?predecess

  # Specific manufacturing/measurement subprocess and "top" process it is part of (whole manufacturing l
  {{
    SELECT DISTINCT ?process ?process_label ?process_type ?top_process ?top_process_label WHERE {{
      # The process must be a manufacturing or measurement process
      ?process rdf:type ?process_type .
      {{ FILTER ( ?process_type = <{manufacturing.Manufacturing.iri}> ) }} UNION {{ ?process_type rdfs::
      {{ FILTER ( ?process_type = <{properties.Measurement.iri}> ) }} UNION {{ ?process_type rdfs:subCla

      # The process must have a specimen or material either as output or as input
      # ?process <{mechanical.hasInput.iri}>|^<{mechanical.hasInput.iri}>|<{mechanical.hasOutput.iri}>
      # ?specimen rdf:type/rdfs:subClassOf* <{manufacturing.EngineeredMaterial.iri}> .

      # It must be possible to navigate backwards to the top process (whole manufacturing history).
      # The top process serves also as a way to uniquely identify the material being manufactured and cl
      ?process (^<{emmo.hasTemporalNext.iri}>|^<{emmo.hasTemporalFirst.iri}>)* ?top_process .
      ?top_process rdf:type/rdfs:subClassOf* <{holistic.Process.iri}> .
      FILTER NOT EXISTS {{ # The top process is not part of another parent process.
        ?other_process rdf:type/rdfs:subClassOf* <{holistic.Process.iri}> .
        ?other_process ?predicate ?top_process .
      }}
      OPTIONAL {{
          ?top_process rdfs:label|skos:prefLabel ?top_process_label .
      }}

      OPTIONAL {{
          ?process_type skos:prefLabel ?process_label .
      }}
    }}
  }}
```

- See presentation of J.M. Domínguez

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Conclusions and Outlook

- **Fatigue database and machine learning**
  - fatigue database with ~ 22 000 specimens, 1100 series, 110 materials
  - ML-tool enables prediction of properties
- **Ontology and knowledge graph**
  - domain ontology implemented in EMMO mechanical testing
  - semi-automized workflows for knowledge graphs and data mapping
  - use cases:
    (1) large fatigue database (110 materials)
    (2) process history of 10 different 100Cr6 steel processing routes
- **Outlook**
  - Enable ML on knowledge graph (considering sequence effects)
  - Our vision: „Fatigue apps" connected to fatigue dataspace

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