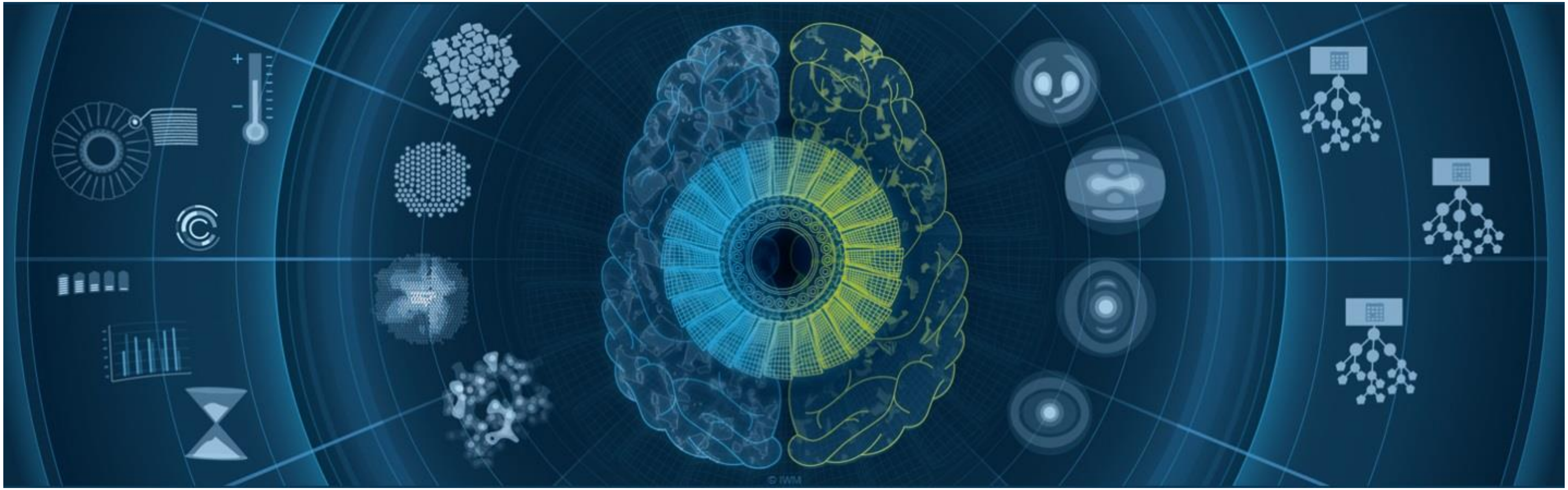
# Digital transformation in materials science and the role of a common ontologie

C. Eberl, et al., Regensburg, 2019



Digital transformation in materials science and engineering:

# Boundary conditions for manufacturers in Europe

- Materials expenses for industrial manufacturing are 56.7 % (personnel expenses 18.6, destatis Germany 2014) – improving on materials efficiency has a 10-fold higher impact than energy efficiency or 30-fold higher than logistics improvement.
- Ressource-rich countries use their commodities strategically (z.B. Steel, Cu, Rare Earth Metals, Oil).
- The global competition shifts from a productivity challenge to a purchase market – although they are connected!
- Climate changes, ressource scarcity and the increasing population need political as well as technological solutions.
- Technological shifts have been accelerating, new tools have been made available, especially in the big data community

**Speed, flexibility and adaptivity in product development depends on the ability to develop novel materials and bring them into production will be key to compete in the future market.**

Digital transformation in materials science and engineering:

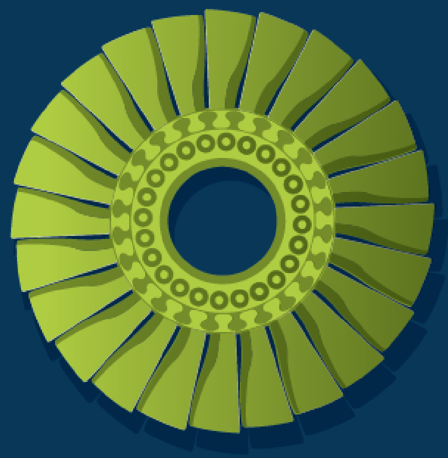
# Make materials behavior available in a digital form

- Connecting product develoment to materials development
- Through Industry 4.0: Connecting materials information into the processing chain
- Higher safety, reliability, functionality and adaptivity to market changes

► Beschleunigte Materialentwicklung

► Flexiblere Produktion

► Zuverlässiger Bauteileinsatz





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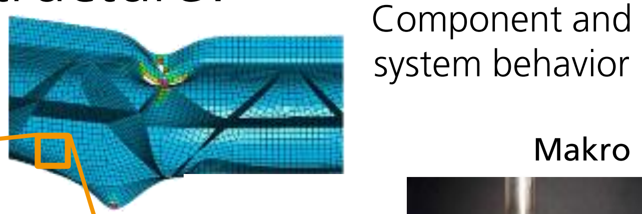
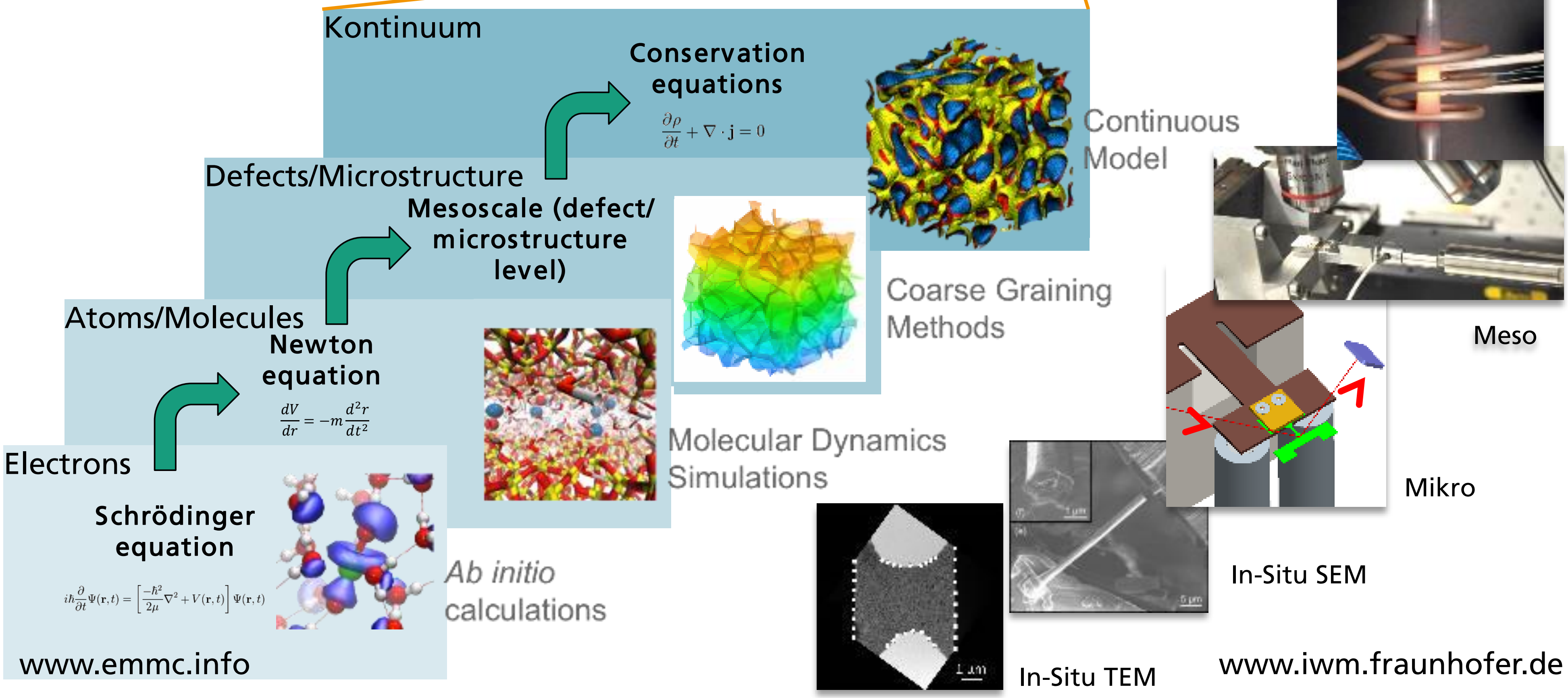
# Matter has a hierarchical structure in time and space – a digital materials representation must have the same structure!

Materials behavior is determined by the interaction of the active mechanisms which can be numerous under realistic loading conditions.







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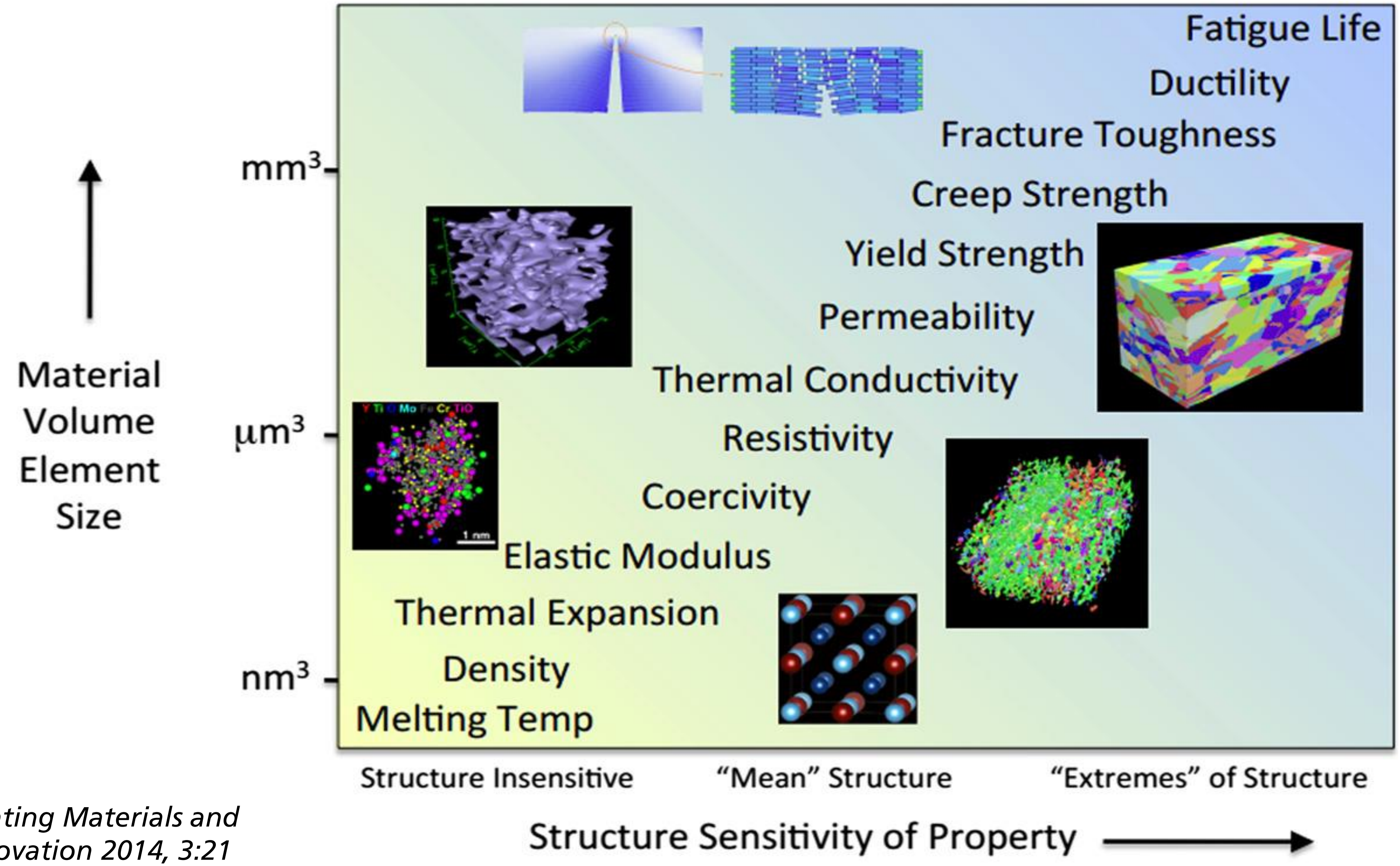
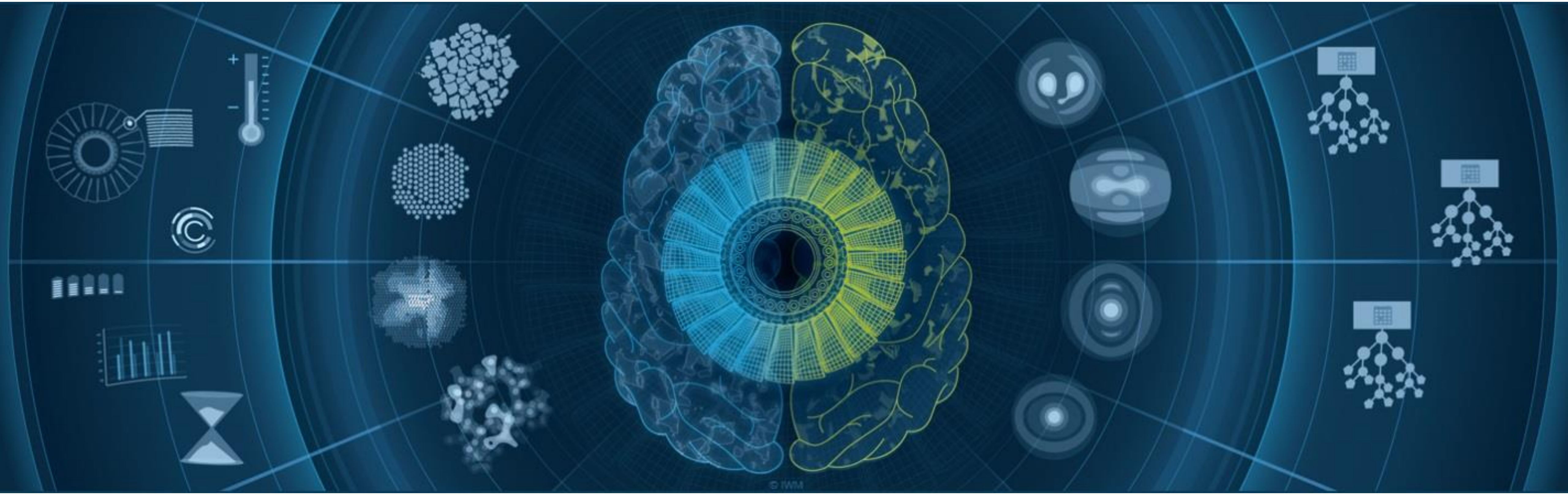
McLean P Echlin*, William C Lenthe and Tresa M Pollock

# The size of the representative volume element - RVE




Echlin *et al. Integrating Materials and Manufacturing Innovation 2014, 3:21*

Vision meets pragmatism
# The digital representation of materials



- Holistic approach versus relevant materials information
- Availability of materials behavior during processing and in applications
- Information on processing and loading history to predict behavior



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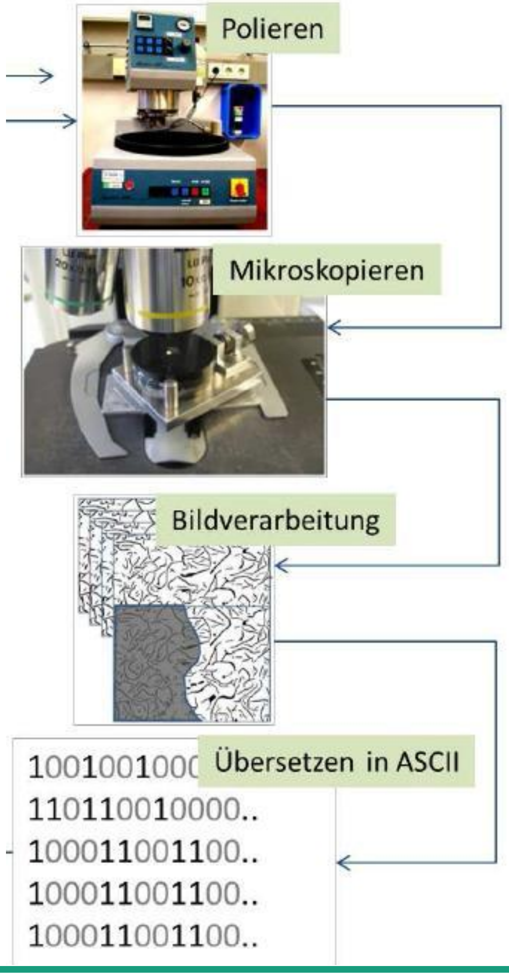
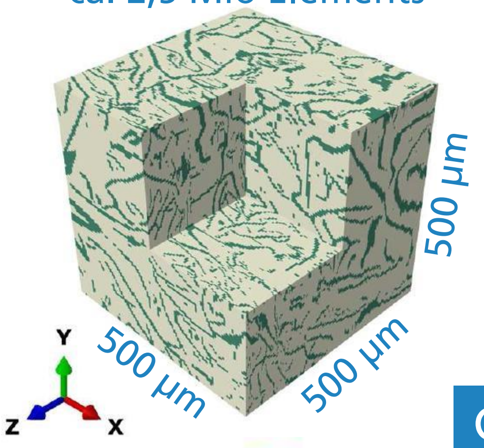
# Development of microstructure-property relation in lamellar cast iron

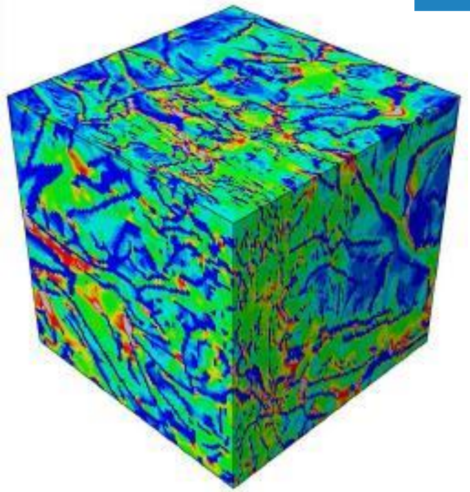
## Digitizing microstructure




## Finite Elemente Modell

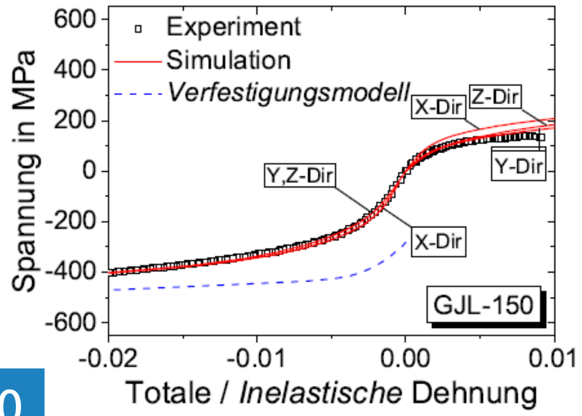
ca. 2,5 Mio Elements

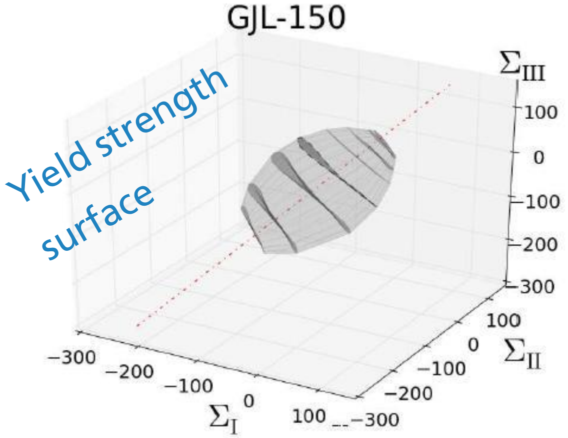


GJL-150

## Calculation and Validation




M. Metzger, C. Schweizer et al.





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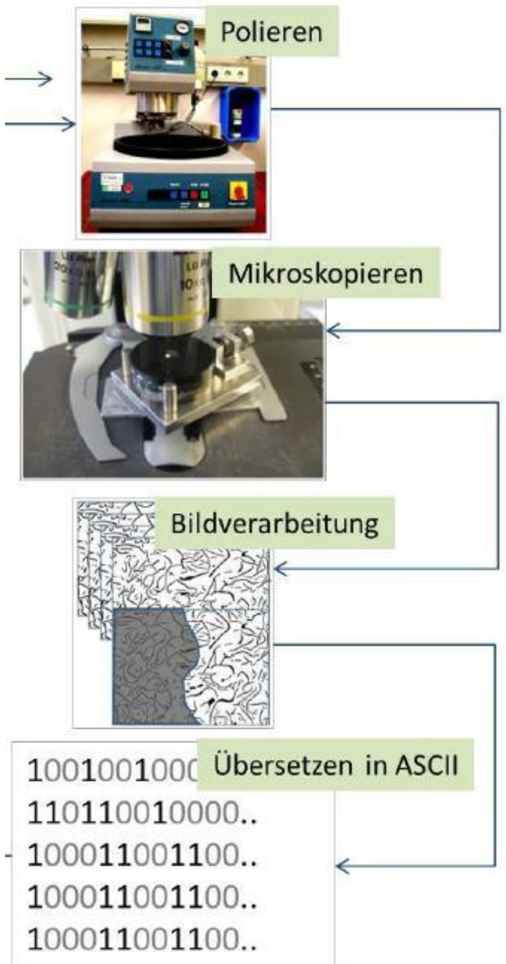
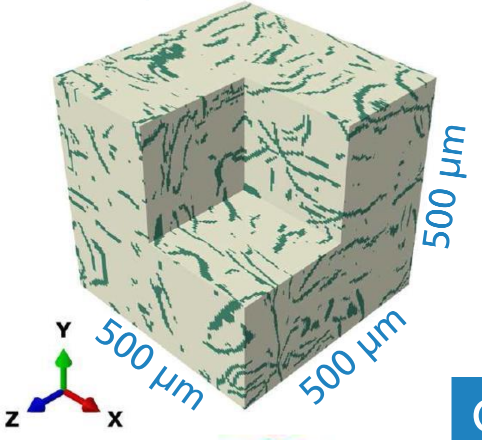
# Development of microstructure-property relation in lamellar cast iron

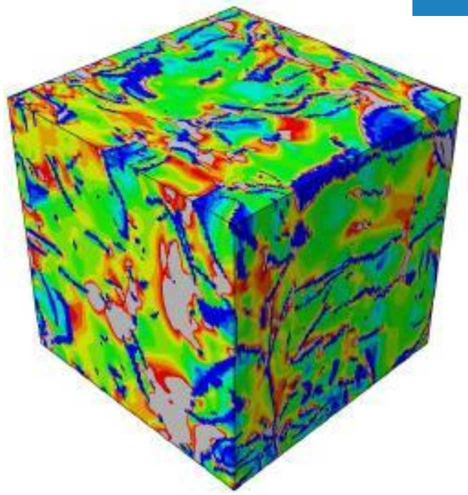
## Digitizing microstructure




## Finite Elemente Modell

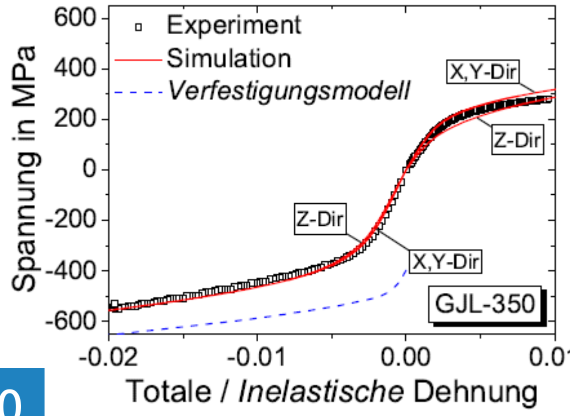
ca. 2,5 Mio Elemente

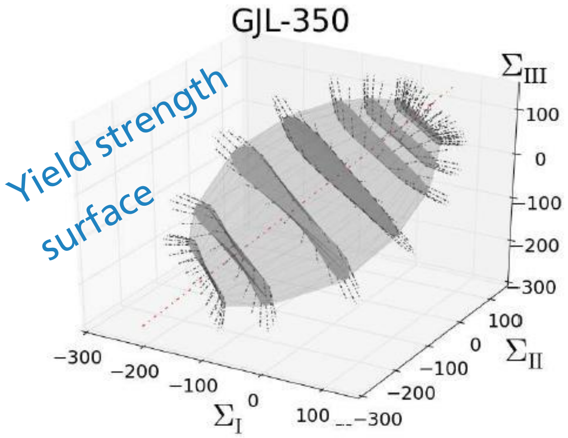


GJL-350

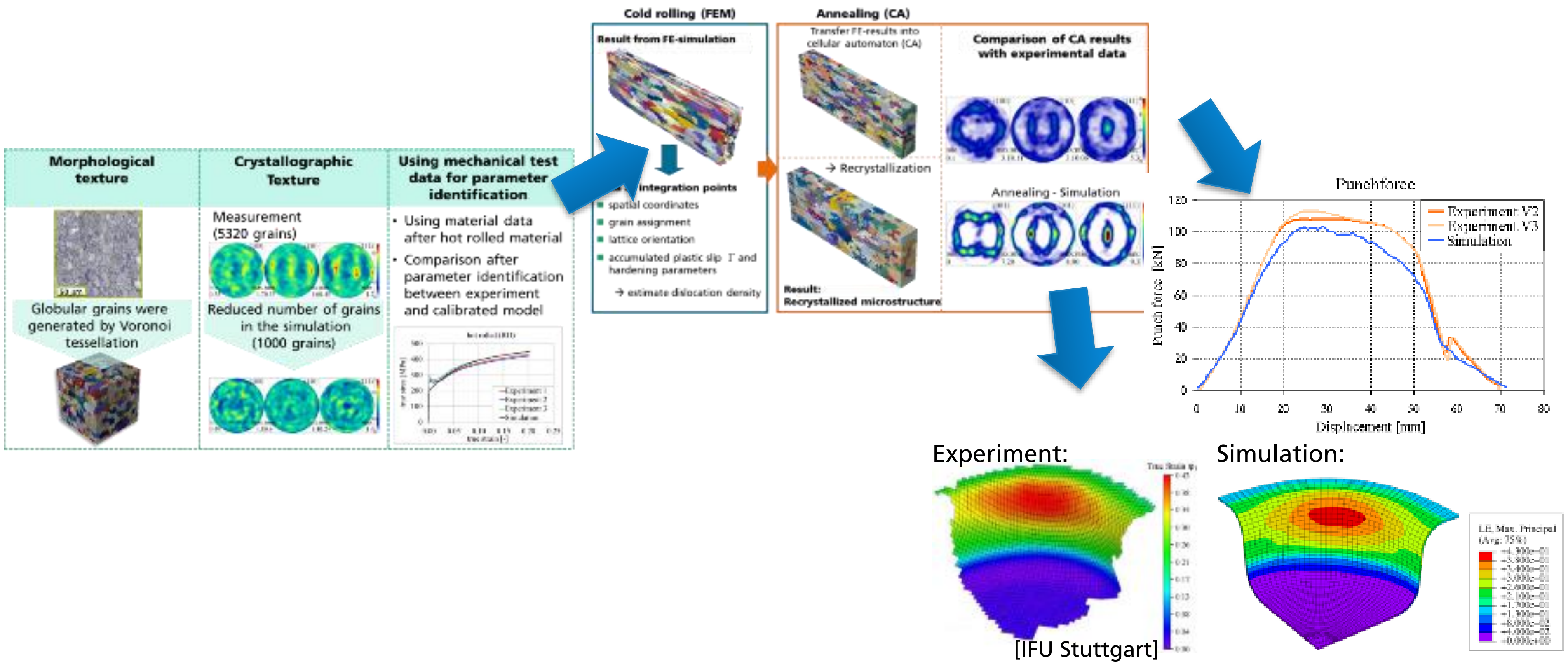
## Calculation and Validation




M. Metzger, C. Schweizer et al.

# Transient behavior based on the simulation of the microstructural evolution

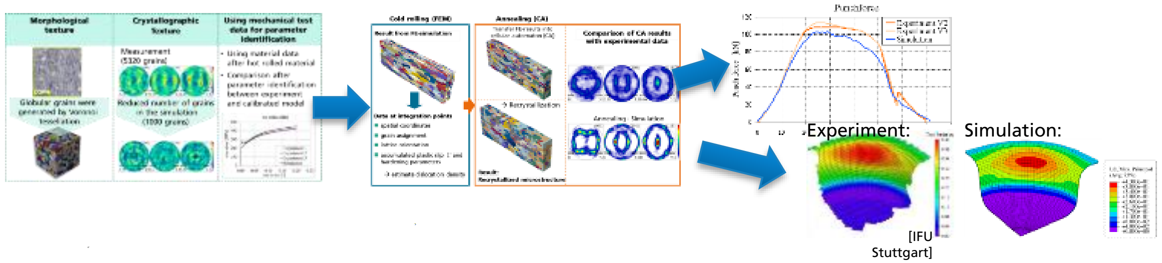



**Materials Data Space:**
**Experimental and sensor raw- and meta data, physical and data based materials models,**

D. Helm et al.

Adaptive materials processing is based on materials knowledge

# Digitizing Materials within the Industry 4.0 Initiative

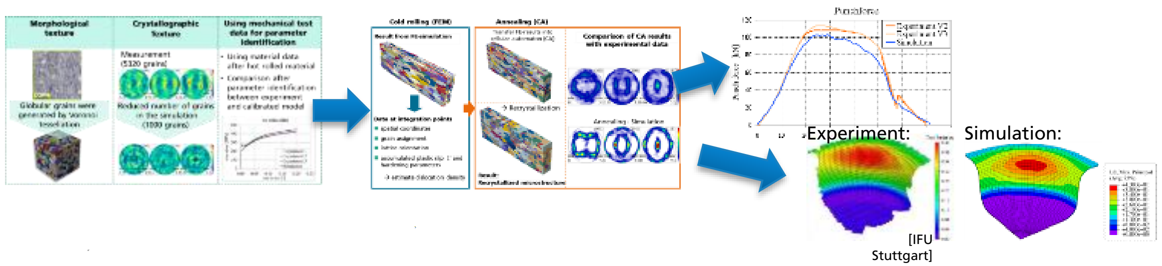



Sensor Input

Sensors will describe the materials state better in the future – development of specific sensors motivated by the materials experts

Materials Data Space:
Experimental and sensor raw- and meta data, physical and data based materials models,

# Digitizing Materials within the Industry 4.0 Initiative




## The key performance indicators change!

Sensor Input

*Real time* physical/statistical material modells, e.g.: neural networks trained with data from the **Materials Data Space**

Materials Data Space:
Experimental and sensor raw- and meta data, physical and data based materials models,



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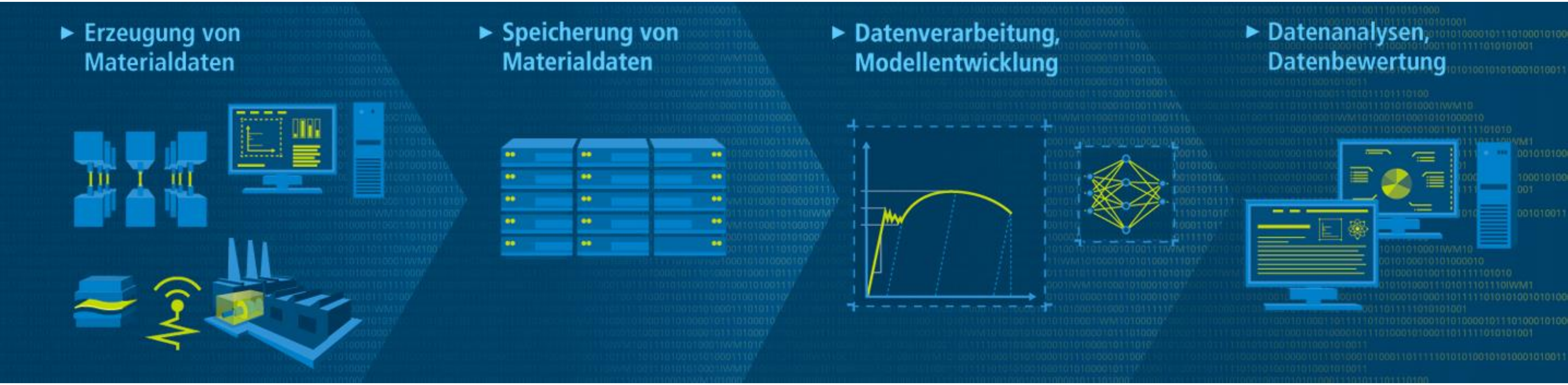
Digital Workflows

# We need to develop the digital infrastructure




- Automated data generation: processing , experimentation and simulation
- Automated 3D microstructural analysis
- Filling in missing materials data through virtual testing
- Establishing materials data spaces containing the materials history and predict ist future behavior
- Development of real time materials models through machine learning



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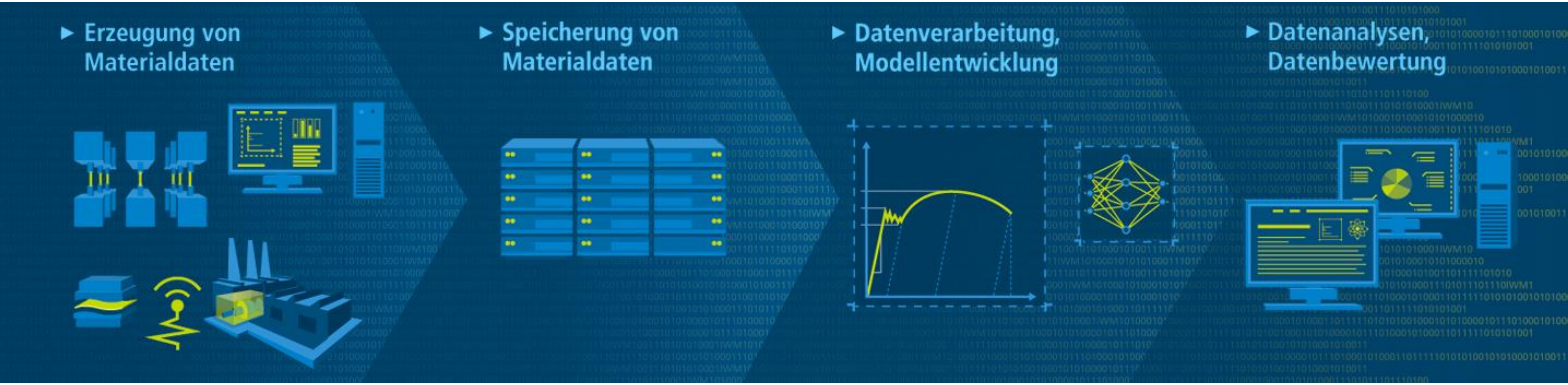
## Digital Workflows

# Digital infrastructure needs a common ontology




The European Materials Ontology is out and we can start implementing:

- https://github.com/emmo-repo
- https://emmc.info/wp-content/uploads/2019/06/1-Gerhard-Goldbeck-EMMO.pdf
- https://emmc.info/wp-content/uploads/2019/04/Part_1_Ontology_Intro.pdf
- https://emmc.info/wp-content/uploads/2019/04/Part_2_EMMO_Intro.pdf
- https://emmc.info/wp-content/uploads/2019/04/Part_3_Interoperability_Intro.pdf

## Developing a structured data space (not yet EMO)

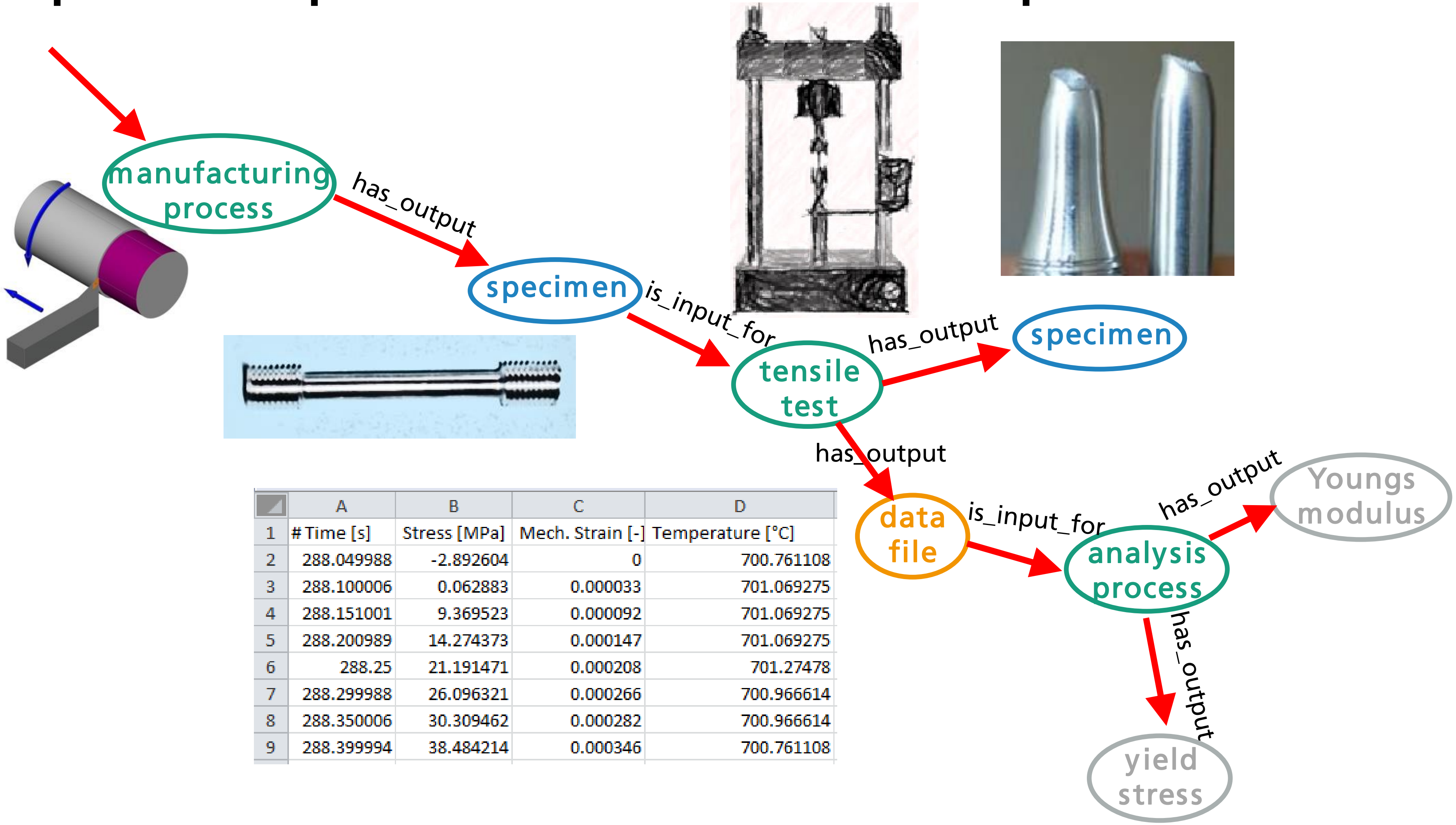
# From single process steps towards a structured data space

object

process

information
content entity

quality




| | A | B | C | D |
|---|---|---|---|---|
| 1 | # Time [s] | Stress [MPa] | Mech. Strain [-] | Temperature [°C] |
| 2 | 288.049988 | -2.892604 | 0 | 700.761108 |
| 3 | 288.100006 | 0.062883 | 0.000033 | 701.069275 |
| 4 | 288.151001 | 9.369523 | 0.000092 | 701.069275 |
| 5 | 288.200989 | 14.274373 | 0.000147 | 701.069275 |
| 6 | 288.25 | 21.191471 | 0.000208 | 701.27478 |
| 7 | 288.299988 | 26.096321 | 0.000266 | 700.966614 |
| 8 | 288.350006 | 30.309462 | 0.000282 | 700.966614 |
| 9 | 288.399994 | 38.484214 | 0.000346 | 700.761108 |

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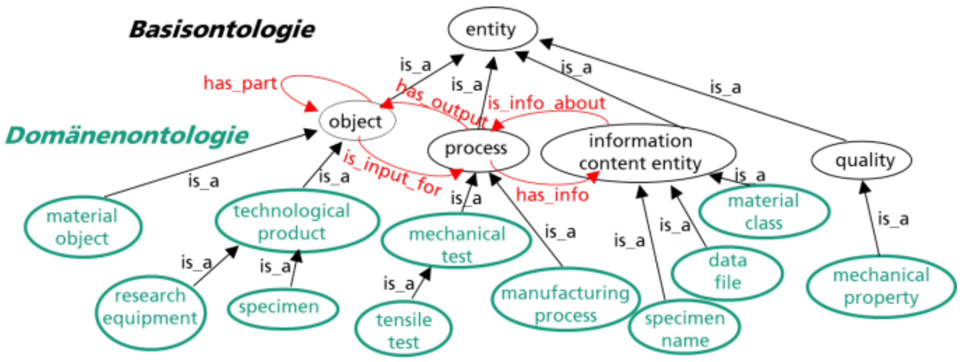
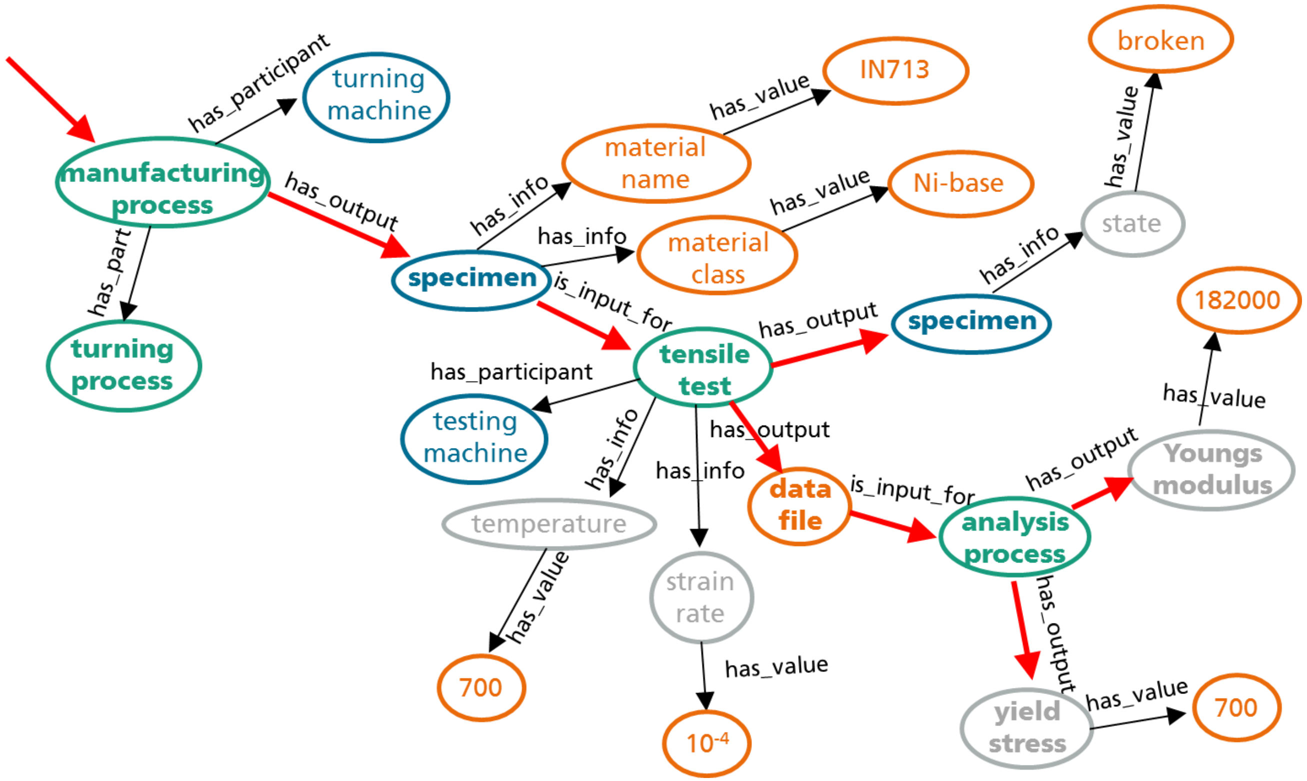
# How to structure knowledge and data? (not yet EMO)

## Materials ontology implemented into knowledge graphs




object process information content entity quality

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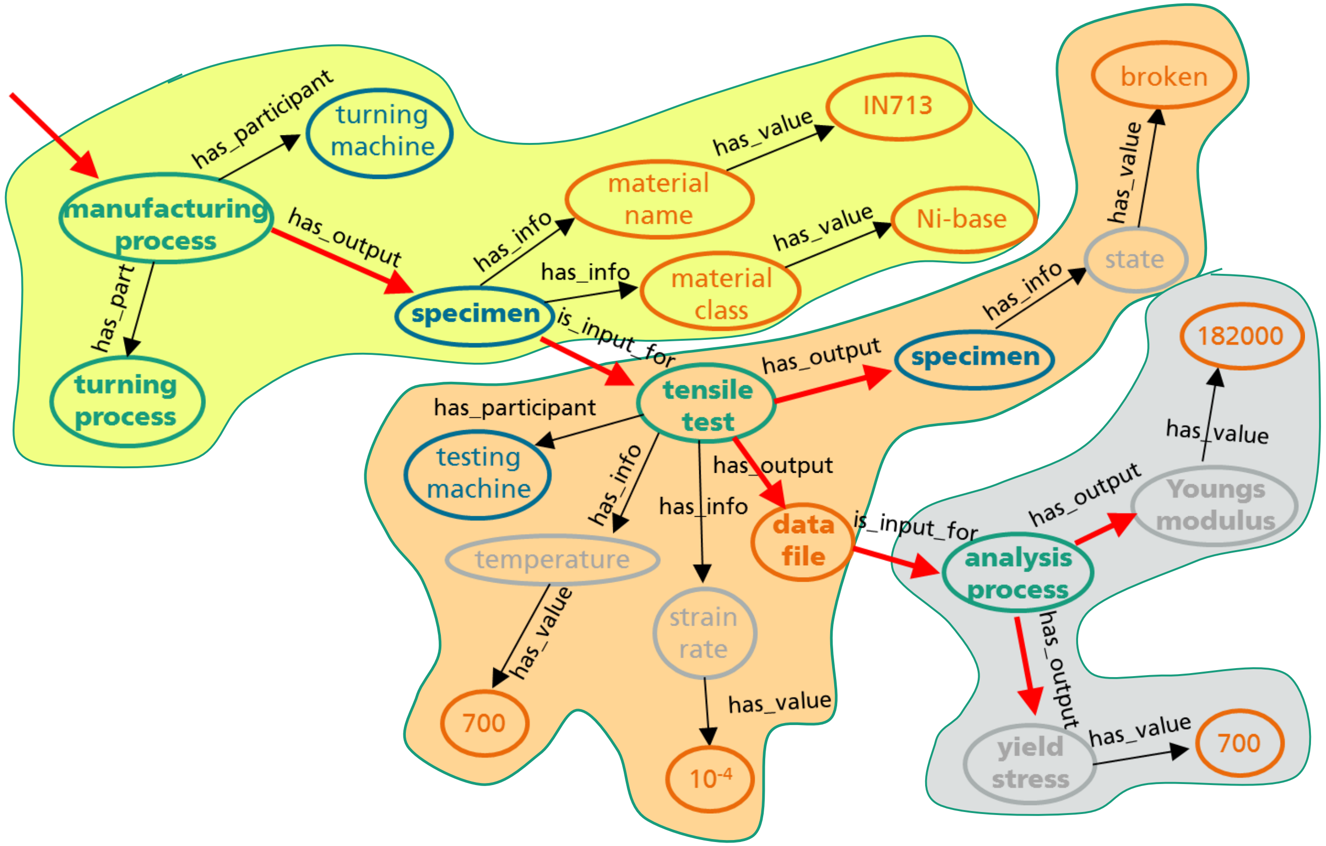


object process

information content entity

quality


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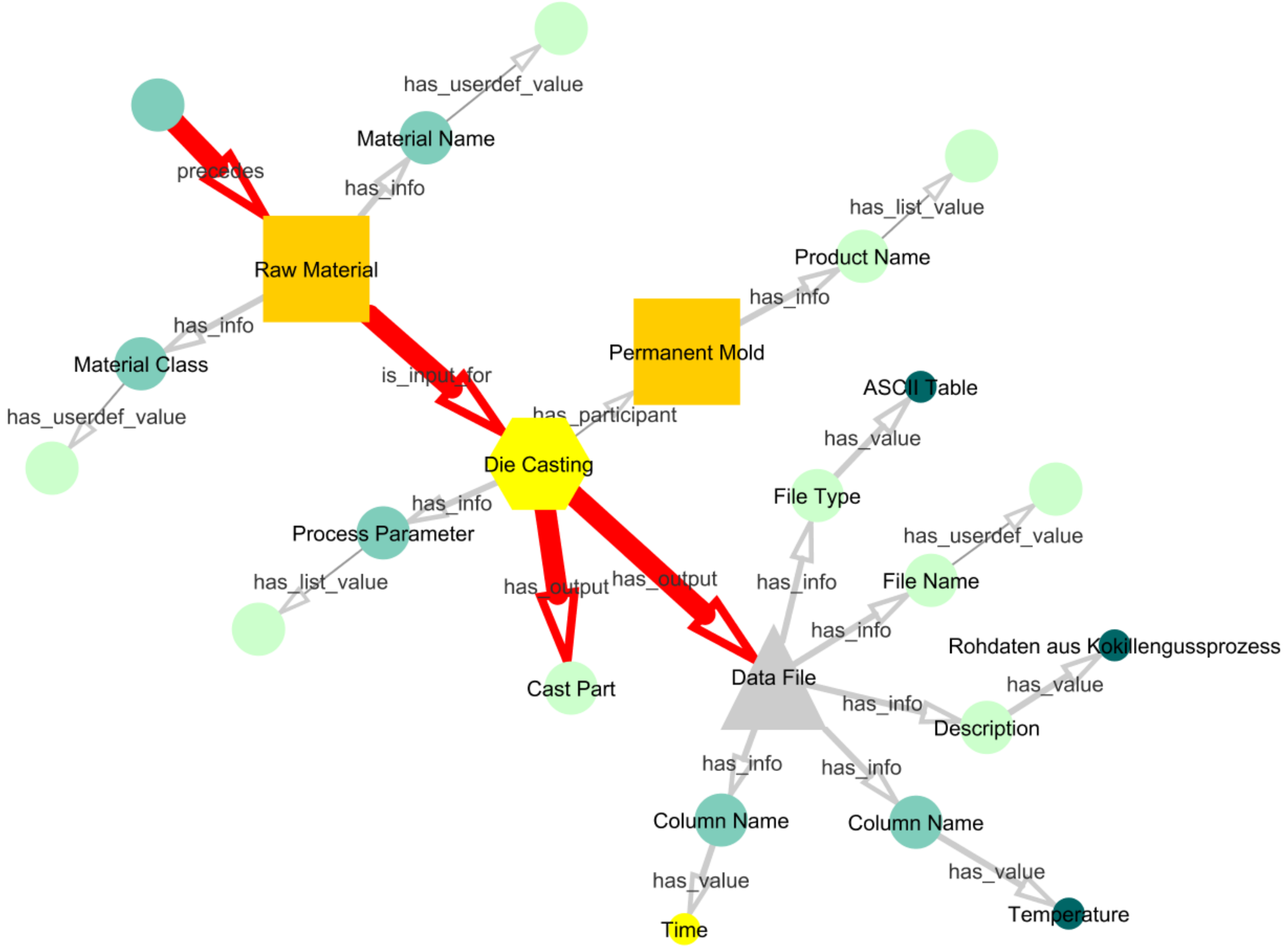
# Example work flow: Casting process

- Guss-prozess
- Sägen
- Einbetten
- Polieren
- Ätzen
- Mikrosko-pieren




(not yet EMO)





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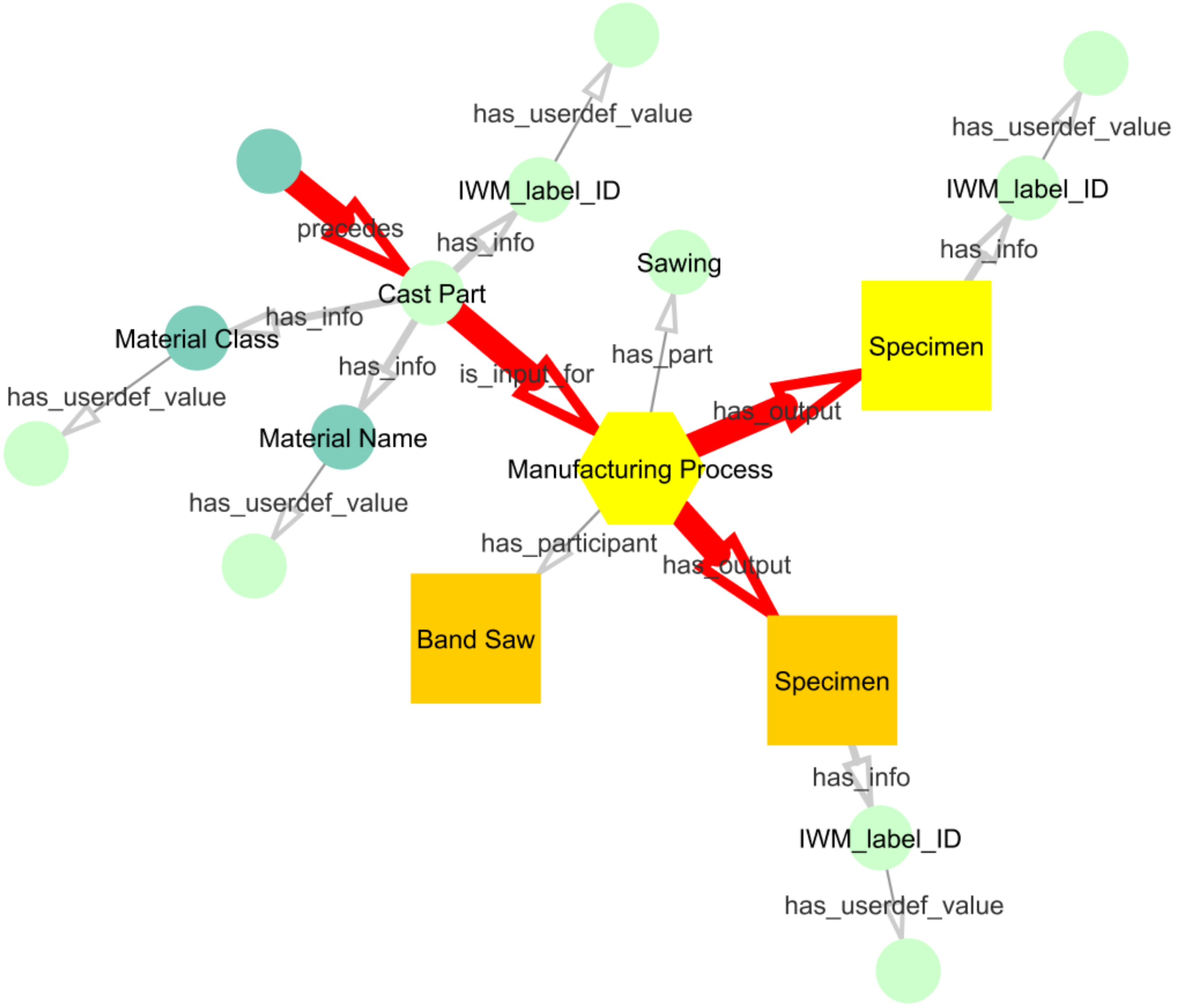
# Example work flow: Casting process - sawing

- Guss-prozess
- Sägen
- Einbetten
- Polieren
- Ätzen
- Mikrosko-pieren




(not yet EMO)



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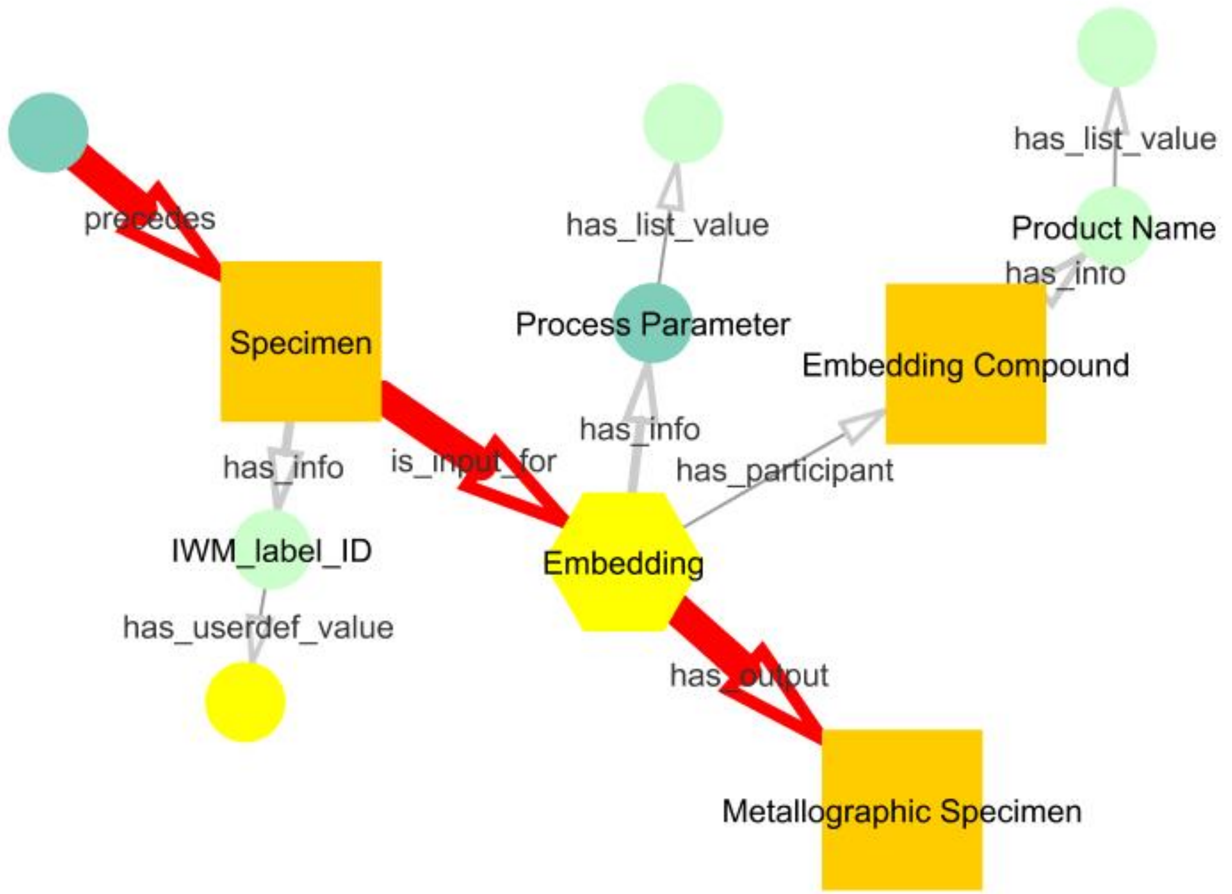
# Example work flow: Casting process - embedding

- Guss-prozess
- Sägen
- **Einbetten**
- Polieren
- Ätzen
- Mikrosko-pieren







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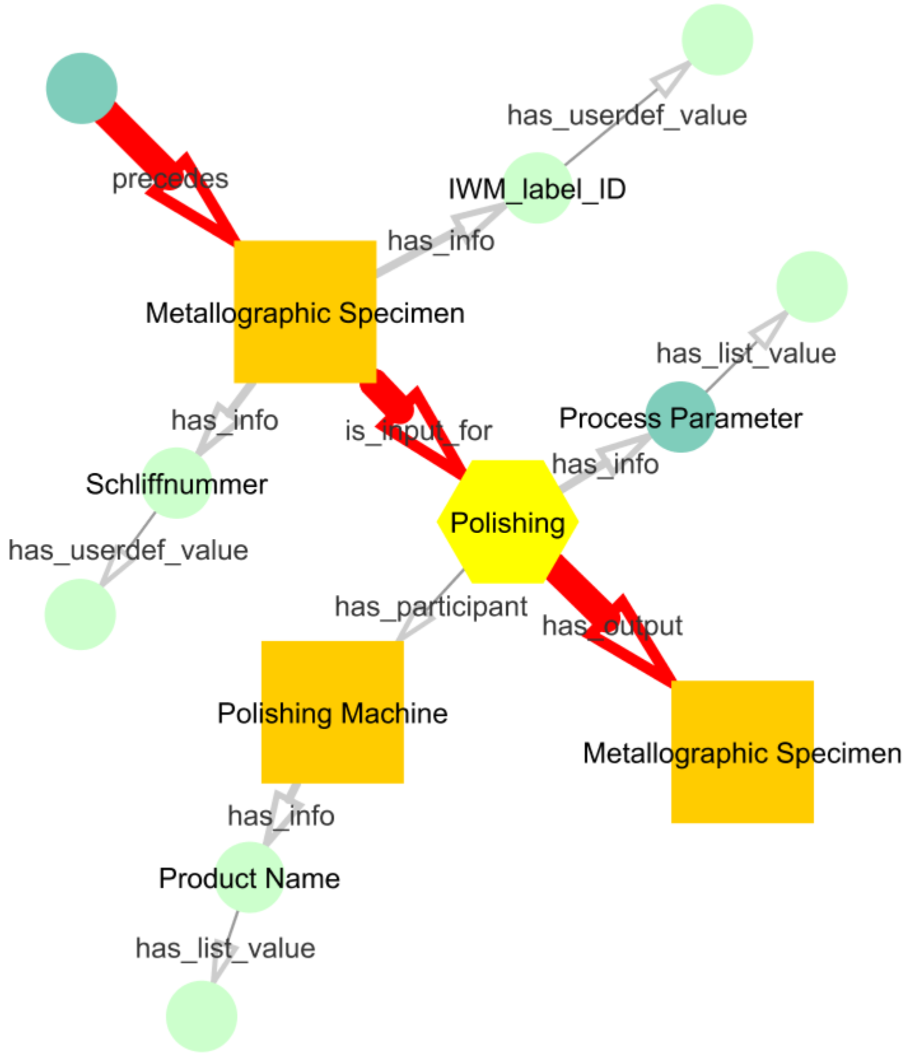
# Example work flow: Casting process - polishing



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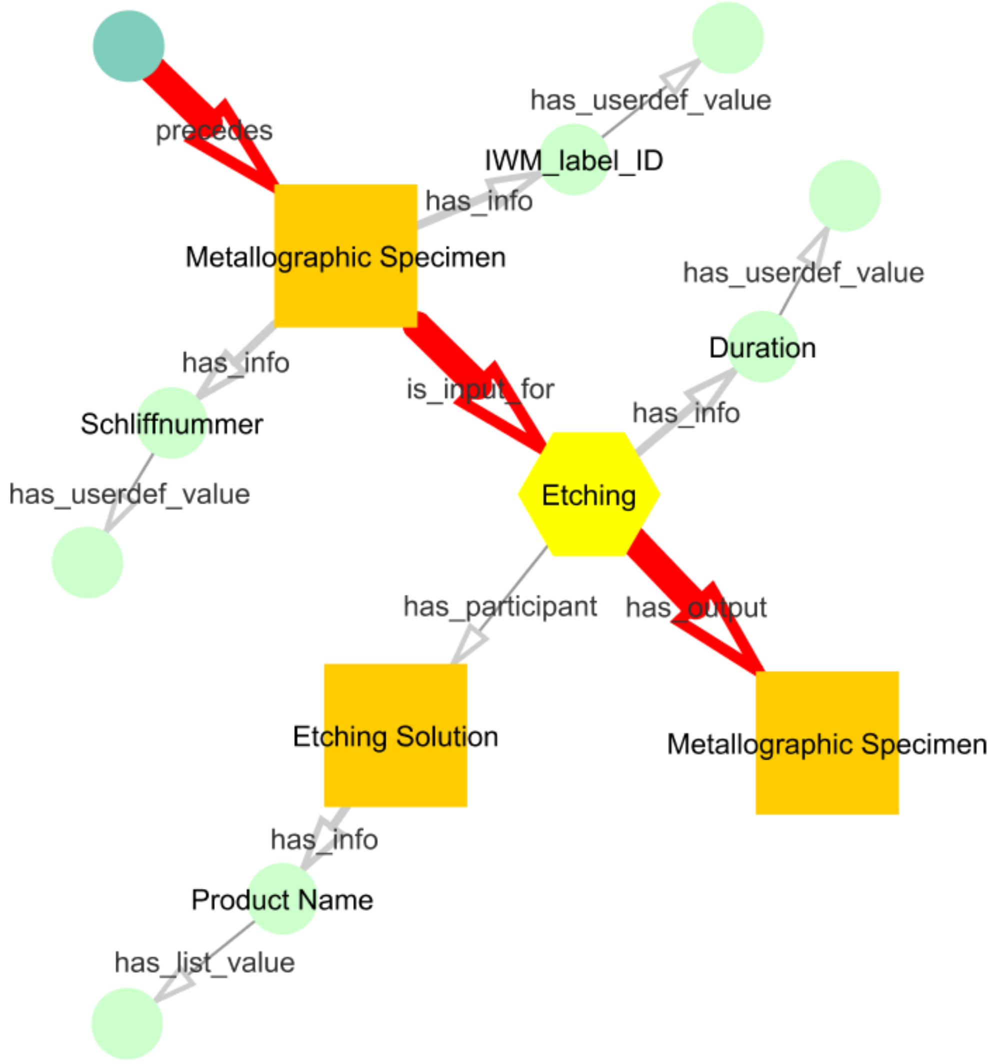
# Example work flow: Casting process - etching


(not yet EMO)

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# Example work flow: Casting process - microscopy

Guss-
prozess

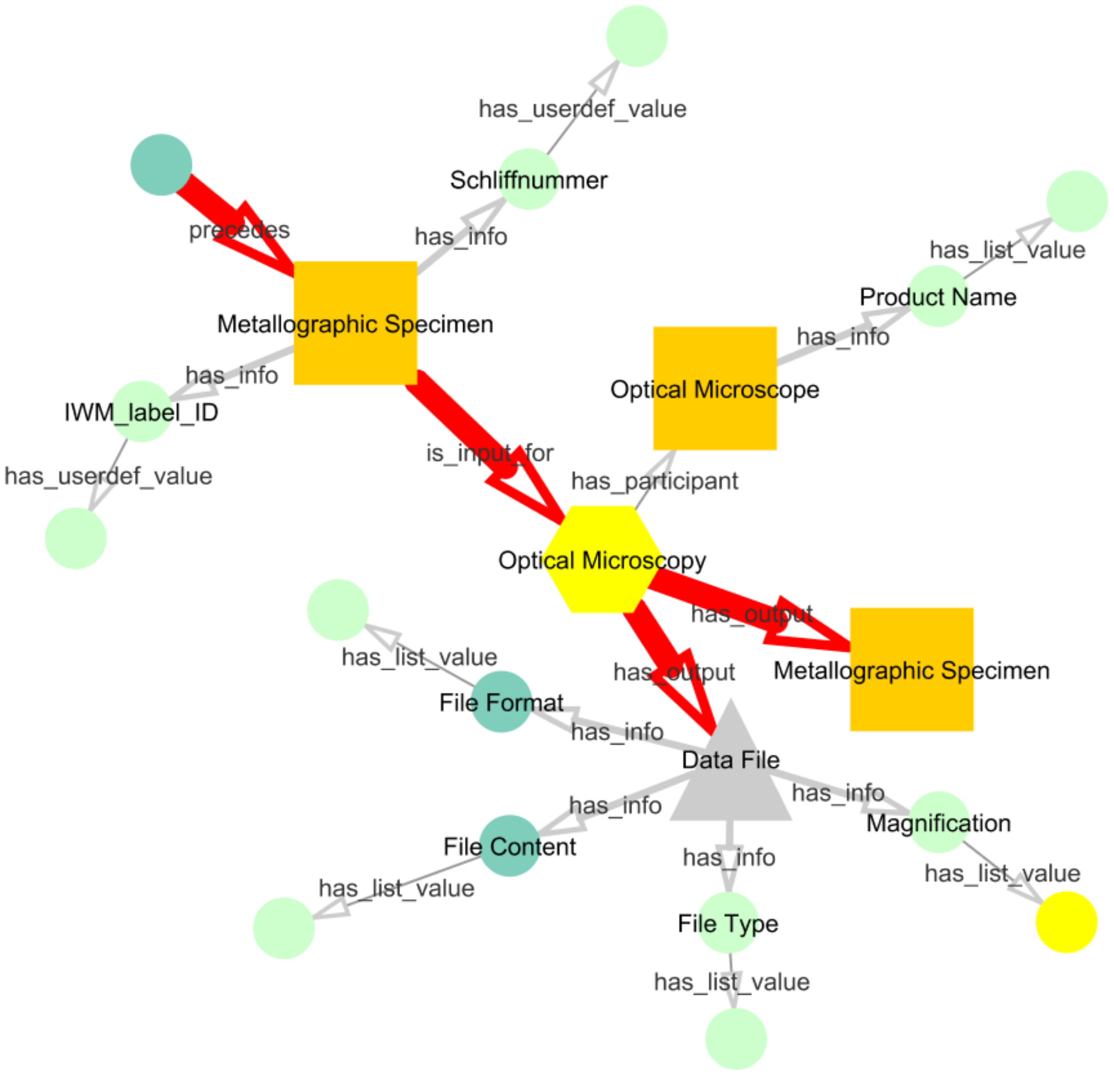
Sägen

Einbetten

Polieren

Ätzen

Mikrosko-
pieren

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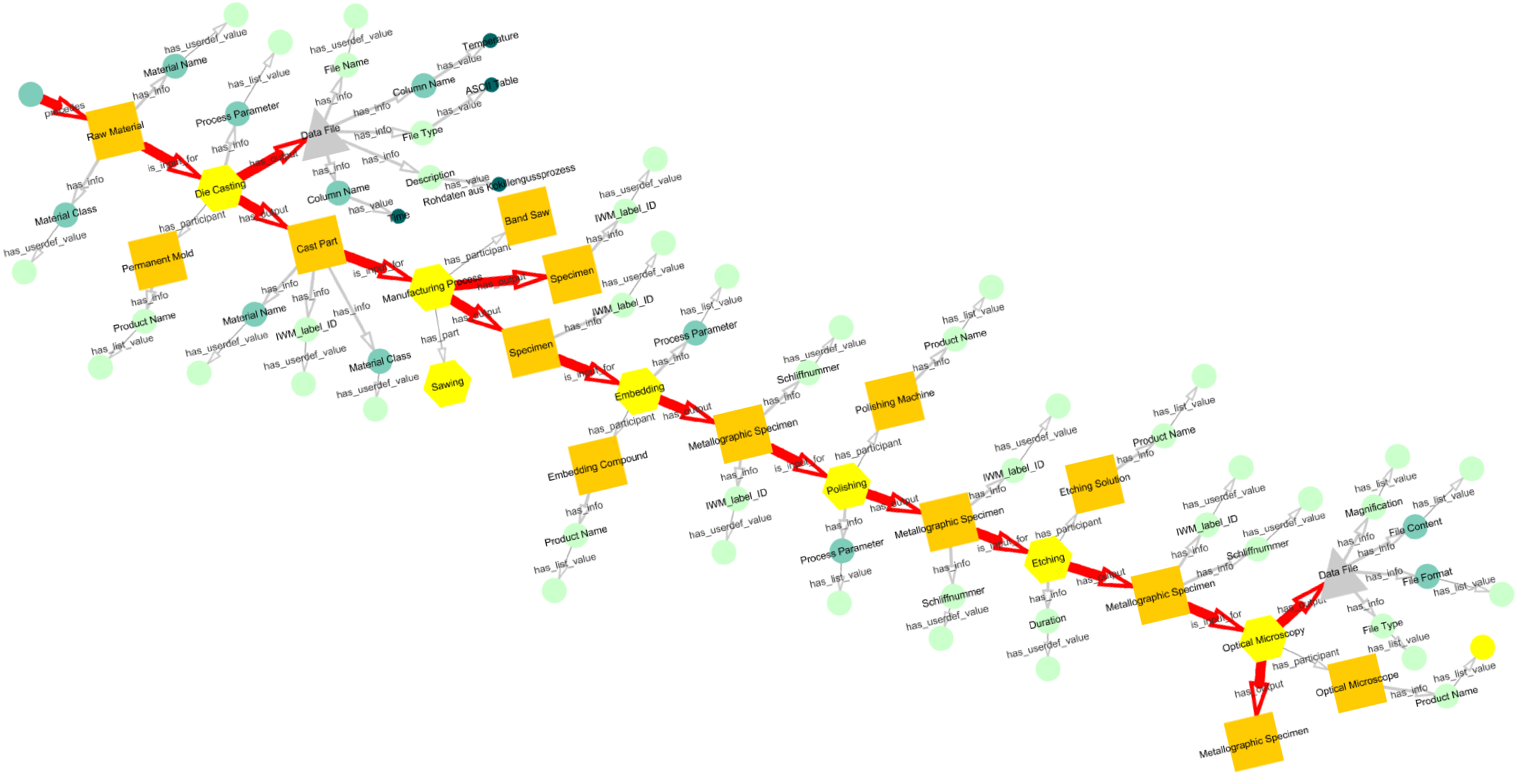
# Example work flow: Casting process – a glimpse of the workflow

- Guss-prozess
- Sägen
- Einbetten
- Polieren
- Ätzen
- Mikrosko-pieren







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(not yet EMO)

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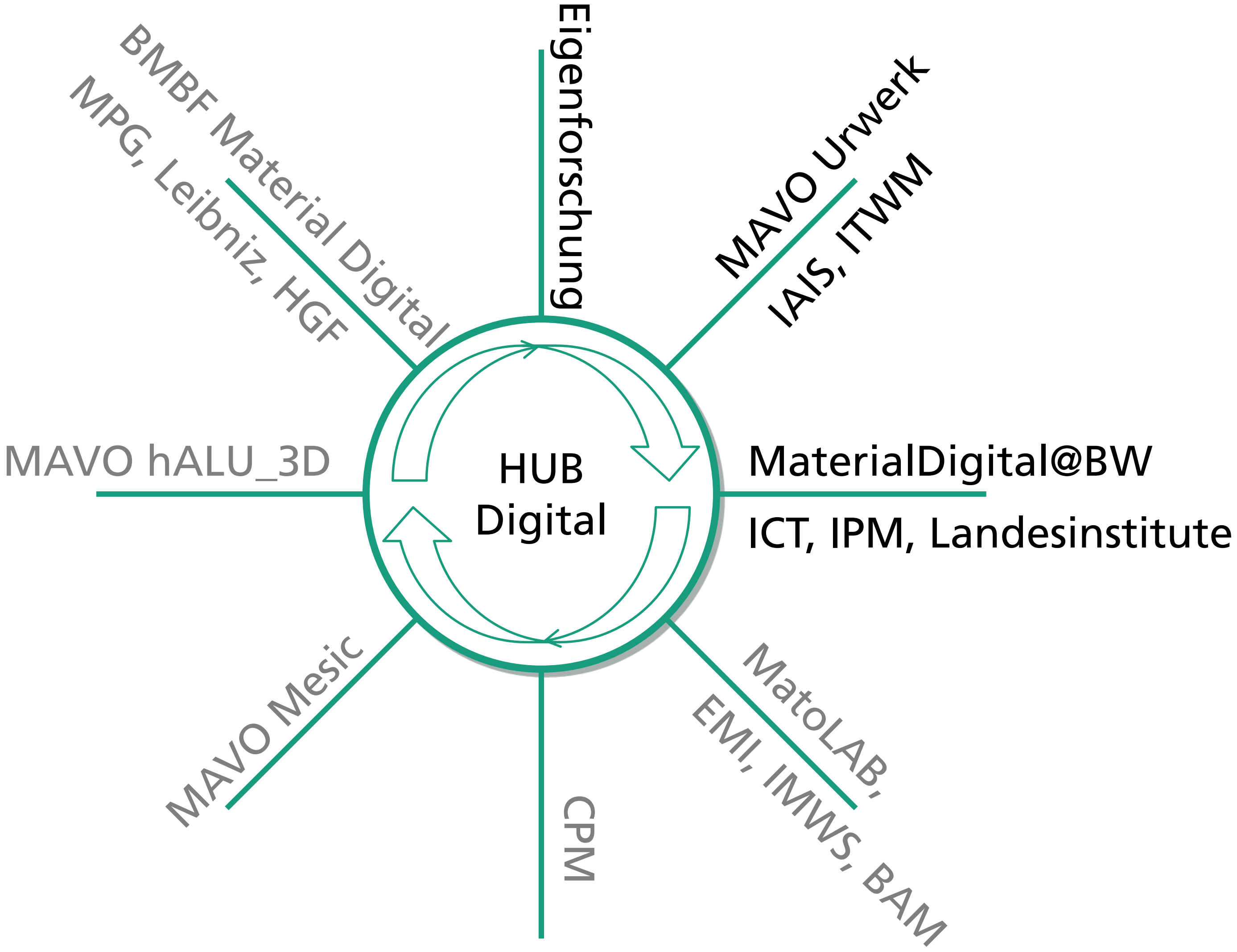
# HUB Digital@IWM

New structures are needed for the digital transformation

Semantics and Ontology

Structured Data

Data Analysis







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# Are there initiatives which help us in the process?

Baden-Württemberg
WIRTSCHAFTSMINISTERIUM

Bundesministerium für Bildung und Forschung

Bundesministerium für Wirtschaft und Energie

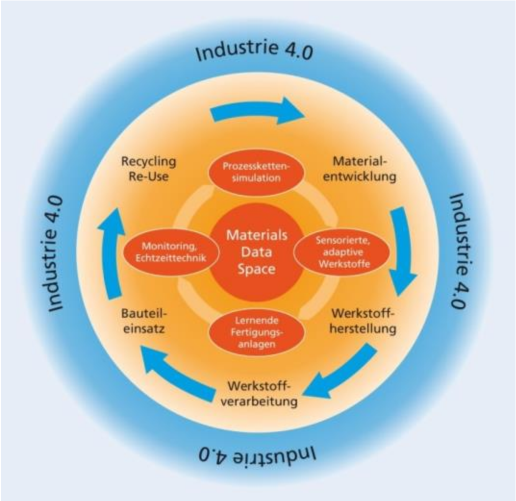
DFG

NFDI

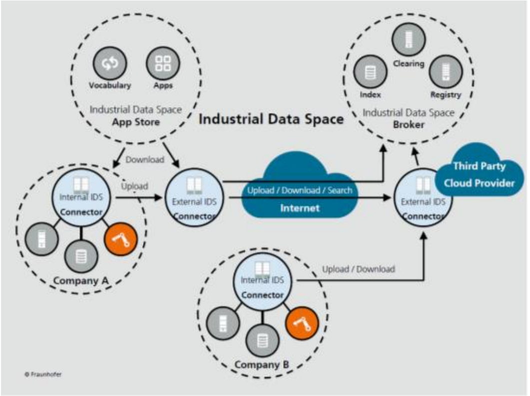
**European Materials Modeling Council** EMMC
**European Materials Characterization Council** EMCC

EMMC


Fraunhofer Materials Data Space




Fraunhofer Industrial Data Space




DGM

VDI


intern

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We can only master the challenges
within the digital transformation together!