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 development to materials development
- Through Industry 4.0: Connecting materials information into the processing chain
- Higher safety, reliability, functionality and adaptivity to market changes
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.
McLean P Echlin*, William C Lenthe and Tresa M Pollock

The size of the representative volume element - RVE
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
Development of microstructure-property relation in lamellar cast iron

Digitizing microstructure

Finite Elemente Modell

digitizing

Calculation and Validation

M. Metzger, C. Schweizer et al.
Development of microstructure-property relation in lamellar cast iron

Digitizing microstructure
- Polieren
- Mikroskopieren
- Bildverarbeitung

Finite Elemente Modell
- ca. 2,5 Mio Elemente

Calculation and Validation
- Experiment
- Simulation
- Verfestigungsmodell
- XY-Dir
- Z-Dir

GJL-350

M. Metzger, C. Schweizer et al.
What will be necessary to connect materials knowledge to processing
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,
Adaptive materials processing is based on materials knowledge
Digitizing Materials within the Industry 4.0 Initiative

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,
Adaptive materials processing is based on materials knowledge
Digitizing Materials within the Industry 4.0 Initiative

The key performance indicators change!

*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,
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 future behavior
- Development of real time materials models through machine learning
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://github.com/emmo-repo)
Developing a structured data space (not yet EMO)
From single process steps towards a structured data space

Manufacturing process ➔ has_output ➔ specimen ➔ is_input_for ➔ tensile test ➔ has_output ➔ specimen ➔ is_input_for ➔ data file ➔ has_output ➔ analysis process ➔ has_output ➔ Young's modulus
data file:

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C. Schweizer, H. Oesterlin, E. Augenstei, A. Hashibon, V. Friedmann
How to structure knowledge and data? (not yet EMO)

Materials ontology implemented into knowledge graphs

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Materials ontology implemented into knowledge graphs

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Example work flow: Casting process
Example work flow: Casting process - sawing

C. Schweizer, H. Oesterlin, E. Augenstein, V. Friedmann, J. Preußner

(not yet EMO)
Example work flow: Casting process - embedding

Guss-prozess
Sägen
Einbetten
Polieren
Ätzen
Mikroskopieren

C. Schweizer, H. Oesterlin, E. Augenstein, V. Friedmann, J. Preußner

(not yet EMO)
Example work flow: Casting process - polishing
Example work flow: Casting process - etching
Example work flow: Casting process - microscopy
Example work flow: Casting process – a glimpse of the workflow

- Casting process
- Sawing
- Embedding
- Polishing
- Etching
- Microscope
HUB Digital@IWM

New structures are needed for the digital transformation

- Semantics and Ontology
- Structured Data
- Data Analysis
Are there initiatives which help us in the process?

European Materials Modeling Council (EMMC)
European Materials Characterization Council (EMCC)

Fraunhofer Materials Data Space
Fraunhofer Industrial Data Space

MaterialDigital@IWM
We can only master the challenges within the digital transformation together!