Digitization in Materials Science - Challenges in Multiscale Modeling of Oxygen-Free Production

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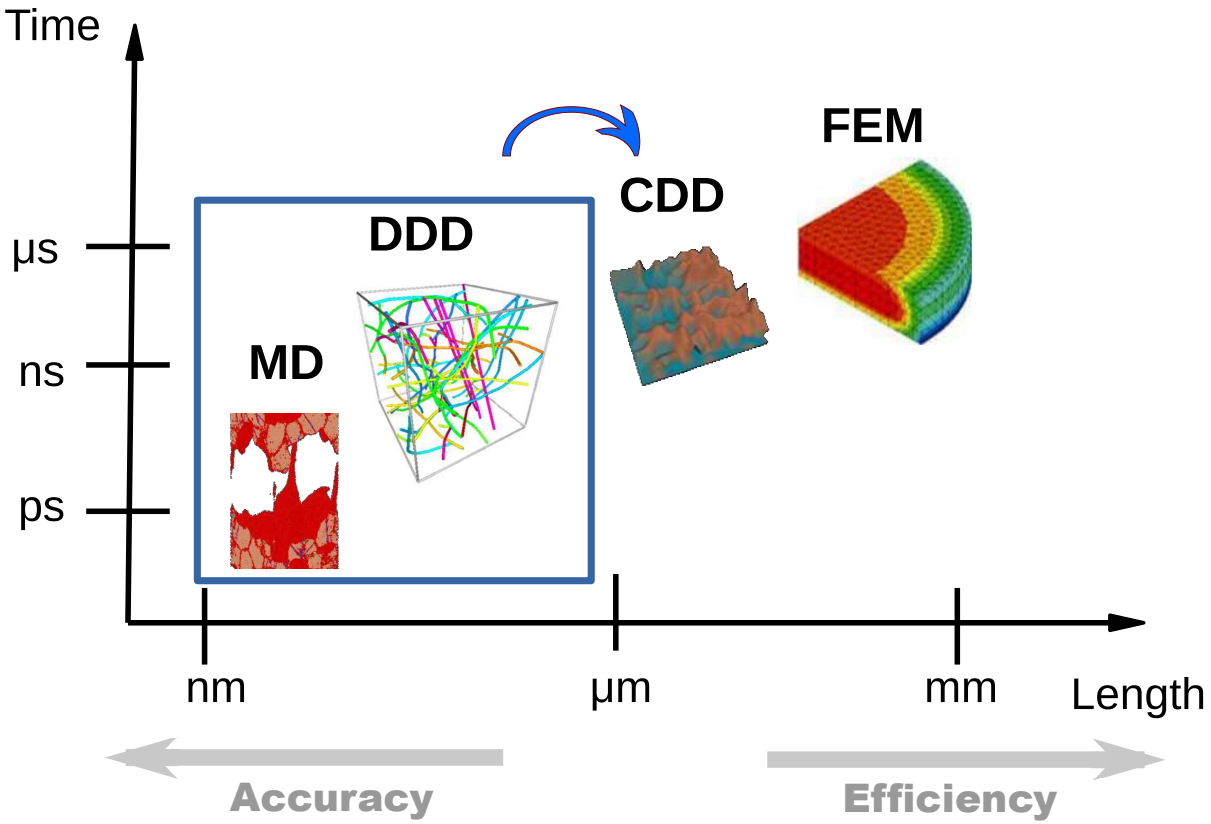
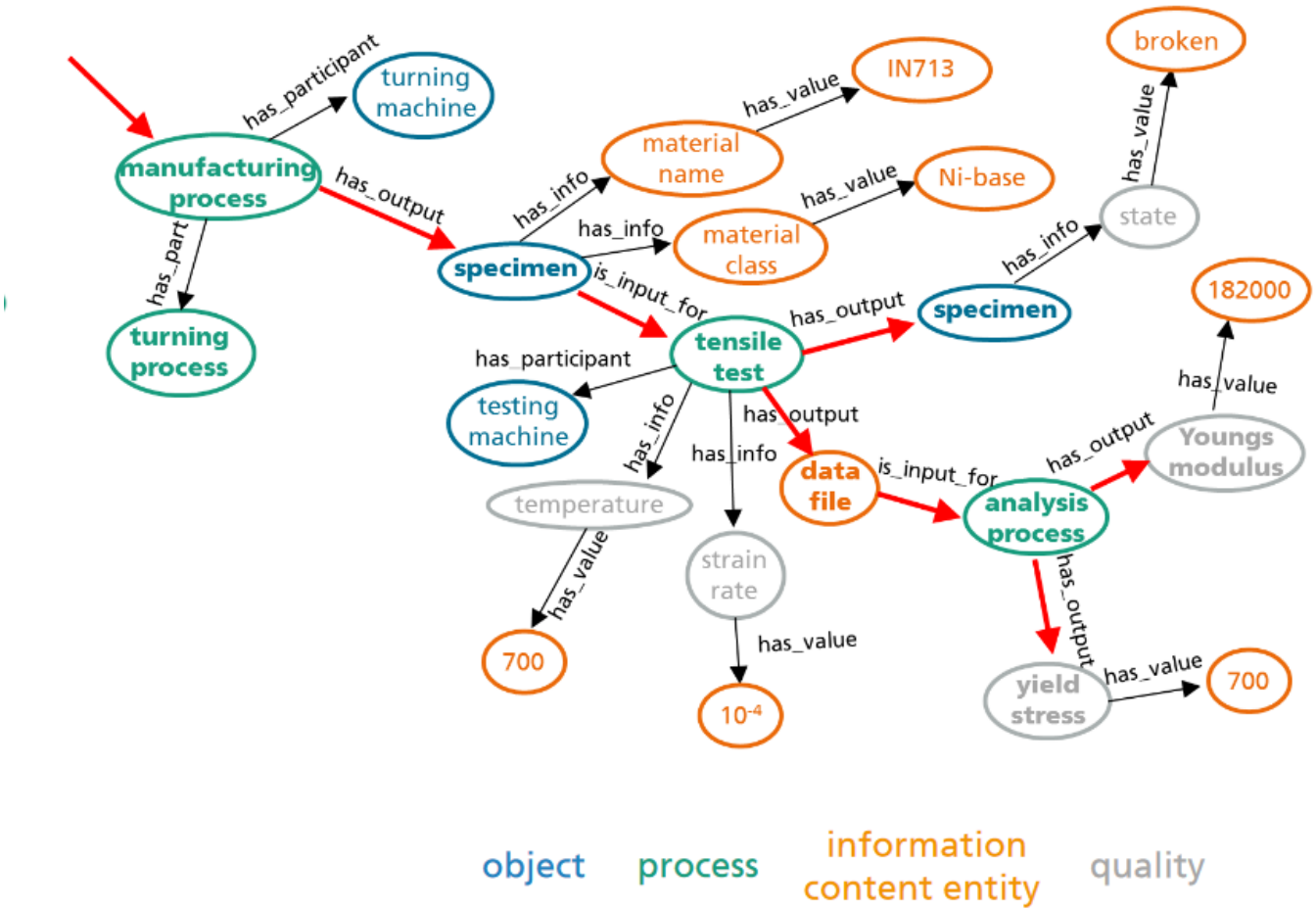
Content

Multiscale character

Processes on different length scales: highly heterogeneous microstructures ranging from crystal defects at the atomistic level up to macroscale pores; any process changes the microstructure



Path dependence of microstructure evolution



[C. Schweizer, H. Oesterlin, E. Augenstein, A. Hashibon, V. Friedmann, Simple bfo based materials testing workflow (2017)]

Challenges

- Different communities
- Language, ontologies and metadata
- Institutionalization
- Socialization and culture of data sharing
- Heterogeneity of data sets
- Handling large data streams
- Maintenance and usability of digital infrastructures

Conclusion

- For simulations in material sciences a combination of different methods on different scales is needed.
- This requires a precise control of the processes and the data flow using workflows, which represent all process information.

Challenges in Multiscale Modeling

Integration in NFDI-MatWerk

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Sustainable research data management according to FAIR principles (Findable, Accessible, Interoperable, Reusable),
Community-Integration via Participant Projects,
`www.nfdi-matwerk.de/participant-projects`

PP06 Working group modeling of oxygen-free production (CRC 1368)

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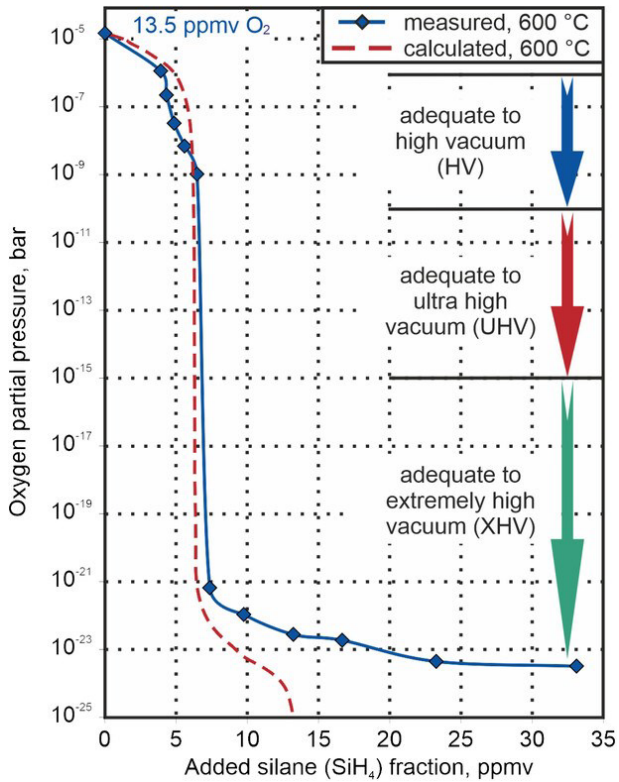
406-04 Materials Science
Material/Methodology: Composites between pure aluminum and iron and later alloys / MD simulations to study atomic interactions at interfaces, transfer to the continuum scale by multiscale simulations **Related Use Cases:** • IUC07: Beyond 3D: Tools for spatiotemporal microstructure studies • IUC10: Interoperability of workflow systems (in collaboration with NFDI4Ing)

Contributions:	**Engagement :**
• Atomistic and multiscale data • Interfaces for Multiscale Simulations (20% W1 professor)	Working group modeling consisting of 13 projects

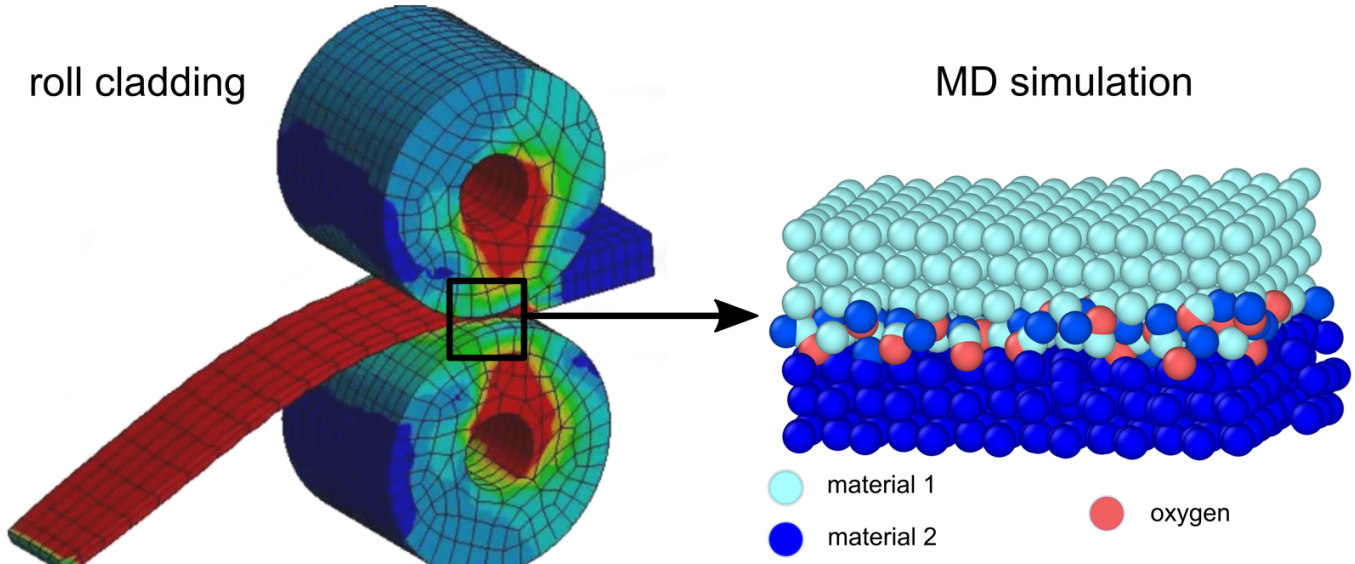
CRC 1368, Oxygen-free production

- Significant contribution in saving resources, saving energy and realizing new processes
- O_2 is a disruptive factor in almost all main manufacturing groups as forming, joining and coating



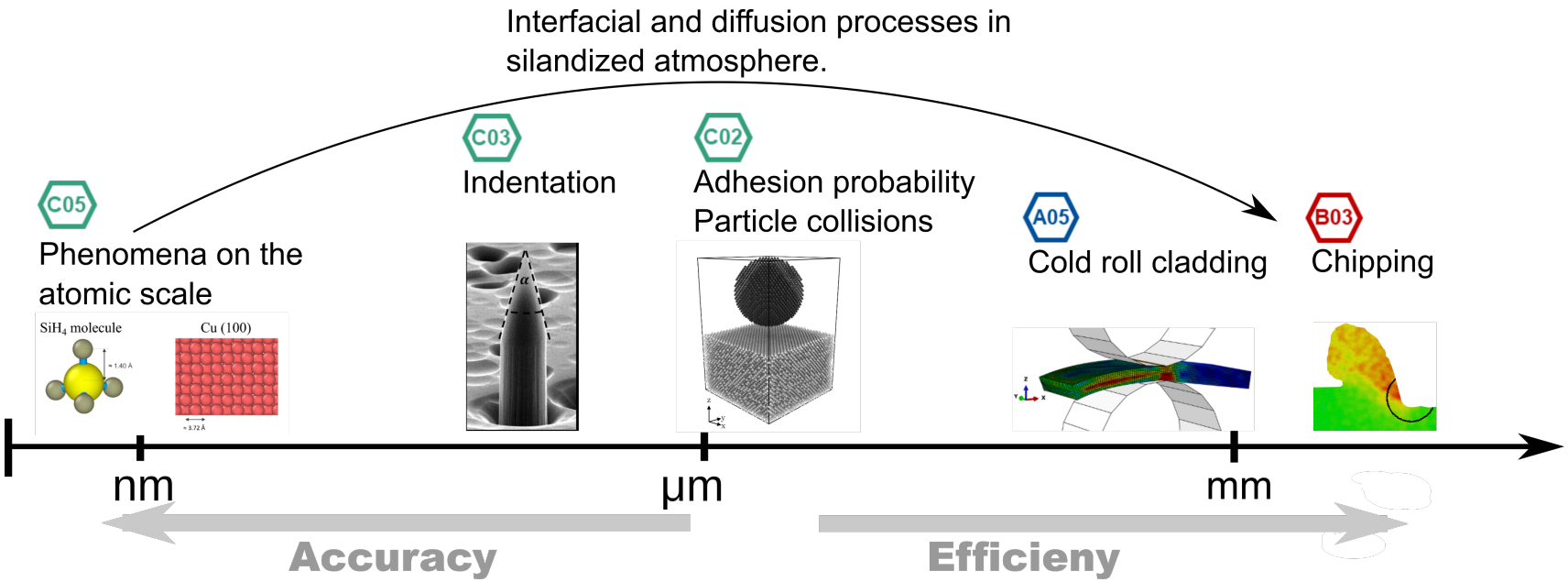
CRC 1368, Subproject C05

- Investigation of the influence of the oxide layers on the physical properties of the bonding of the joining partners in the contact zone with atomistic simulations.
- Macro-scale physico-chemical processes are reduced to interactions between atoms and molecules

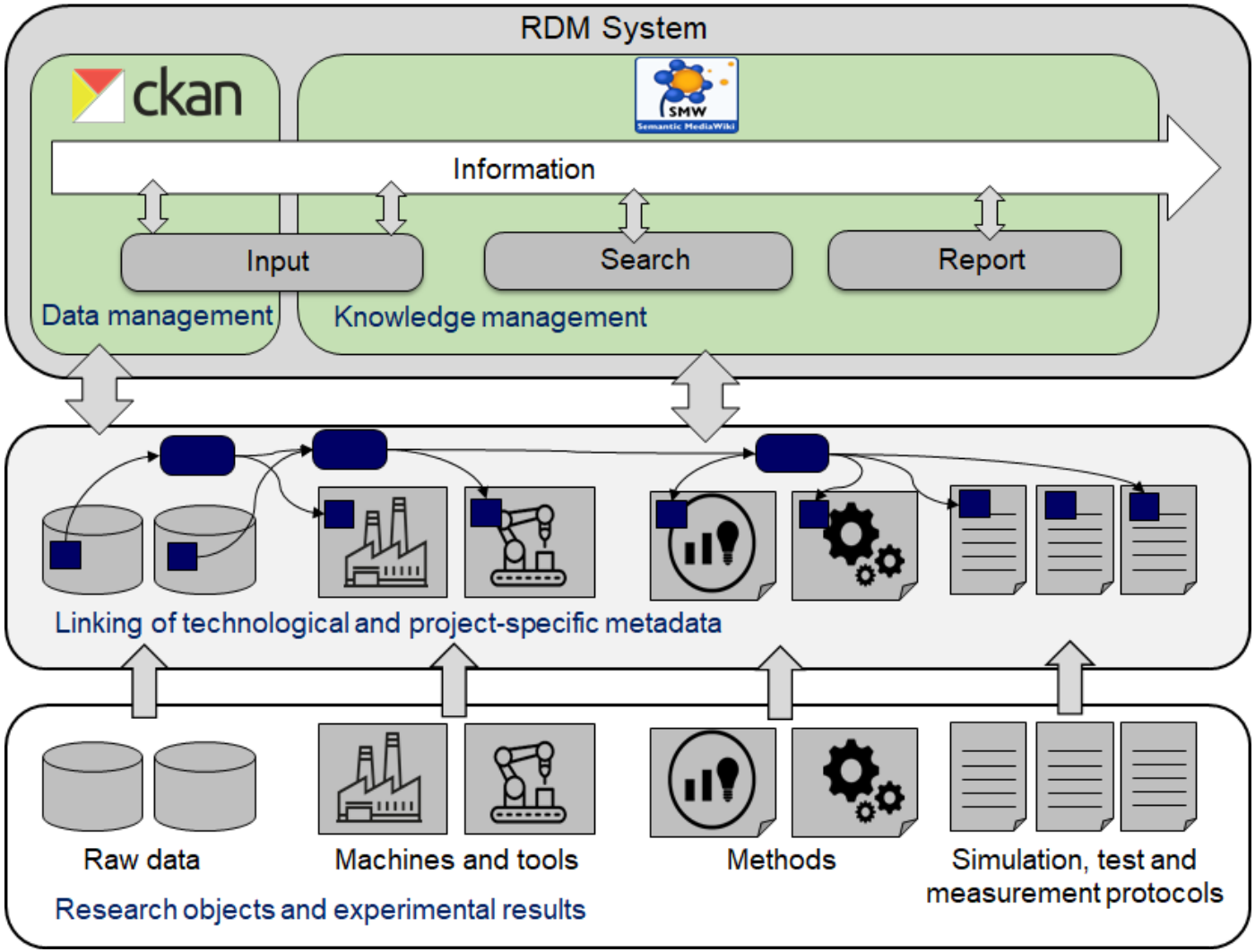


Multiscale model

- Goal: fundamental understanding of the processes in production engineering excluding oxygen
- Different modeling approaches are combined across scales



Concept for research data management



Conclusion

- Oxygen-free production techniques can lead to high-quality, metallurgically-bonded compounds.
- By mapping and transferring the outcomes, a cross-scale model for the fundamental comprehension of joining technology processes will be developed.