July 19, 2021

Consortium NFDI-MatWerk

Participant-Project (PP) and Infrastructure-Use-Case (IUC) Overview

About this document

This document includes the complete list and descriptions of the Participant Projects and related Infrastructure-Use-Cases the consortium NFDI-MatWerk referred to within its proposal. For the NFDI-MatWerk proposal, refer to https://doi.org/10.5281/zenodo.5082837.

Methodically, the consortium proceeded by identifying so-called Participant Projects within its research community. Participant Projects represent the heterogeneity of this research domain in all its facets. They usually face diverse but recurring challenges in the context of research data management from a user or scientist's perspective. Such challenges, resulting from the PPs, were accumulated to shape the so-called Infrastructure-Use-Cases (IUCs). For this end, the consortium identified recurring technological user needs from the PPs and isolated them into individually necessary functionalities of the aimed research data management infrastructure for NFDI-MatWerk.

The consortium plans to reiterate this process as the project starts, to manage a continuous integration and feedback-loop from a strict user-centered perspective and thus ensure relevance of the developed solutions.

For more information on the consortium NFDI-MatWerk refer to www.nfdi-matwerk.de.

For questions about this method, refer to the contacts listed under www.nfdi-matwerk.de/kontakt/.

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PP01 From atoms to turbine blades (CRC/TRR 103)

Contact person: *Dr. habil. Thomas Hammerschmidt, Ruhr-University, Bochum*

URL: *www.sfb-transregio103.de*

<table>
<tr><td colspan="2">405-01 Metallurgical, Thermal and Thermomechanical Treatment of Materials
405-04 Mechanical Properties of Metallic Materials and their Microstructural Origins
406-03 Thermodynamics and Kinetics as well as Properties of Phases and Microstructure of Materials
406-04 Computer-Aided Design of Materials and Simulation of Materials Behaviour from Atomic to Microscopic Scale</td></tr>
<tr><td colspan="2">Material/Methodology: Ni-based and Co-based single-crystal superalloys, metallic complex solid solutions / experiments and simulations
Related Use Cases:
• IUC02: Framework for curation and distribution of reference datasets
• IUC09: Infrastructure interfaces with condensed matter physics (collaboration with FAIRmat)
• IUC14: Adaptive automated characterization pipelines and meta data schemas for high throughput experiments
• IUC17: Ontologies for defects in crystals</td></tr>
<tr><td>Contributions:
• own data from scale-bridging experimental characterization
• own data from scale-bridging modeling and simulation
• special-purpose data-structure solutions and
• special-purpose birth-certificates of samples
• 33% of technician</td><td>Engagement :
24 projects in CRC/TR103, 10 of them on ‘Machine-Learning and Material Informatics’</td></tr>
</table>

The CRC/TRR 103 “From Atoms to Turbine Blades - A Scientific Basis for a New Generation of Single Crystal Superalloys” is dedicated to the development of single-crystal superalloys that play a crucial role for the efficiency of gas turbines for aero engines and power plants. **Scale-bridging characterization and scale-bridging modeling** at the five involved institutions (RU Bochum, FAU Erlangen-Nürnberg, MPIE Düsseldorf, DLR Köln and FZ Jülich) generate a treasure of data on the evolution of the **superalloy microstructure** during processing and service and the resulting material properties. The CRC/TRR 103 just started its third funding phase and can contribute vast and comprehensive data for a narrowly focused material system as well as the expert knowledge in structuring and mining the heterogeneous data on superalloys.

PP02 Defect phases in structural materials (CRC 1394)

Contact person: *Prof. Dr. Sandra Korte-Kerzel, RWTH Aachen; Dr. Jörg Neugebauer, MPIE Düsseldorf*,

URL: *www.sfb1394.rwth-aachen.de*

<table>
<tr><td colspan="2">405-01 Metallurgical and Thermal Processes, Thermomechanical Treatment of Materials;
405-04 Mechanical Properties of Metallic Materials and their Microstructural Origins;
406-03 Thermodynamics and Kinetics as well as Properties of Phases and Microstructure of Materials
406-04 Computer-Aided Design of Materials and Simulation of Materials Behaviour from Atomic to Microscopic Scale</td></tr>
<tr><td colspan="2">Material/Methodology: Thermodynamic and Kinetics of Defects / Simulations and Experiments
Related Use Cases:
• IUC04: Model driven data space exploration
• IUC05: Digital infrastructure and workflows for labs
• IUC09: Infrastructure interfaces with condensed matter physics (collaboration with FAIRmat)</td></tr>
<tr><td>Contributions:
• Large data set (computation/experiment) on defect phases in Mg-alloys
• Materials-data infrastructure and support [1 full position]</td><td>Engagement :
15 project groups</td></tr>
</table>

In materials physics the **thermodynamic descriptions of crystalline phases** have enabled materials scientists and engineers to tailor and process alloys while obtaining the desired internal structure at the microscale. At the same time, improving control over **crystal defects** which govern the **material's strength**, **formability** and **corrosion resistance**, has led to the development of new alloying and processing concepts. The vision of this CRC1394 is to bridge the gap and combining both approaches into a **novel conceptual framework**. This PP therefore represents a fundamental direction in materials science. Further, it represents methods of combining atomic-scale data from experiment and simulation, as well as thermodynamics, mechanics and corrosion.

PP03 Method development for mechanical joinability in versatile process chains (CRC/TRR 285)

Contact person: *Prof. Dr.-Ing. Gerson Meschut, Dr.-Ing. Mathias Bobbert, Universität Paderborn*

URL: *www.trr285.de*

401-03 Joining and Separation Technology; **402-01** Engineering Design, Machine Elements, Product Development **402-02** Mechanics; **402-03** Lightweight Construction, Textile Technology; **405-04** Mechanical Properties of Metallic Materials and their Microstructural Origins;	
Material/Methodology: Joining processes and loaded joints (metals, FRP) / Experiments and Simulations **Related Use Cases:** • IUC01: Web-based demonstration and teaching framework for MSE research data infrastructure • IUC05: Digital infrastructure and workflows for labs	
Contributions: • Data sets for joint and material properties • Meta-data and ontology for joints and materials • Comparison with current data management system	**Engagement:** 16 groups

A growing number of material-geometry-combinations in all areas of product manufacturing requires not only a reliable prognosis of the joinability, but also in particular the versatility of mechanical joining processes. The vision of the CRC/TRR 285 is to ensure the mechanical joinability in versatile process chains. Using the example of mechanical joints, an interdisciplinary team of researchers is investigating methods for transformability in the three areas of material (joining suitability), design (joining safety) and production (joining possibility) as well as for reliable prognosis and design of the joinability. In the long term, a flexible, transferable and cross-industry design methodology will be available.

PP04 Magnetoelectric Sensors: From Composite Materials to Biomagnetic Diagnostics – Project A10 (CRC 1261)

Contact persons: *Prof. Dr.-Ing. Stephan Wulfinghoff, Thilo Paul-Stüve, Christian-Albrechts-Universität zu Kiel*
URL: http://www.sfb1261.de/index.php/en/

<table>
<tr><td colspan="2">406-01 Synthesis and Properties of Functional Materials
406-04 Computer-Aided Design of Materials and Simulation of Materials Behaviour from Atomic to Microscopic Scale</td></tr>
<tr><td colspan="2">Material/Methodology: Magnetoelectric composite materials; coupling of magnetic, electric and mechanical phenomena; Application to magnetoelectric sensors for medically relevant questions
Related Use Cases:
• IUC06: Integrating materials data from experiments and computation (ICME) into Industry 4.0 manufacturing paradigms
• IUC08: Interactive visual exploration for analyzing correlations in high dimensional materials data spaces
• IUC14: Adaptive automated characterization pipelines and meta data schemas for high throughput experiments</td></tr>
<tr><td>Contributions:
• Data Steward (University Computing Centre, 25% E13)
• Material data from different scales of a magnetoelectric sensor system
• Coordination of the project</td><td>Engagement :
Microstructure investigation for magnetoelectric sensors and conclusions on sensor behavior</td></tr>
</table>

The general topic of the Collaborative Research Centre CRC 1261 are magnetoelectric sensor approaches with high sensitivity at biomagnetic frequencies and their evaluation and utilization in medically relevant questions. The aim of project A10 – “Magnetic Noise of Magnetoelectric Sensors” is to comprehend and quantify the influence of geometrical and physical imperfections as well as the connected magnetic microstructure on the magnetic noise of ME sensors. Dedicated experimental methods are combined with high-resolved and adaptive micromagnetomechanical simulations. This participant project is important since it covers the important aspects “cooperation of materials science with medicine”, “CRC data handling”, and “multiphysical and multiscale data of functional materials”. The data steward will accompany the implementation and act as a linking point to central RDM services of Kiel University. The application for a second phase of the CRC is currently under review and granting is thus a necessary condition for a contribution to NFDI-MatWerk.

PP05 HoMMage - Hysteresis Design of Magnetic Materials for Efficient Energy Conversion (CRC/TRR 270)

Contact person: *Prof. Dr. Karsten Durst, Technische Universität Darmstadt*
URL: *https://www.tu-darmstadt.de/sfb270/about_crc/index.en.jsp*

<table>
<tr><td colspan="2">406-01 Synthesis and Properties of Functional Materials
406-03 Thermodynamics and Kinetics as well as Properties of Phases and Microstructure of Materials
406-04 Computer-Aided Design of Materials and Simulation of Materials Behaviour from Atomic to Microscopic Scale</td></tr>
<tr><td colspan="2">Material/Methodology: Functional magnetic and magnetocaloric materials / Additive manufacturing, artificial intelligence
Related Use Cases:
• IUC04: Model driven data space exploration
• IUC06: Integrating materials data from experiments and computation (ICME) into Industry 4.0 manufacturing paradigms
• IUC08: Interactive visual exploration for analyzing correlations in high dimensional materials data spaces
• IUC12: Alignment of application- and higher-level ontologies</td></tr>
<tr><td>Contributions:
• Large data set on materials (computational and experimental)
• Materials data and infrastructure</td><td>Engagement :
20 groups</td></tr>
</table>

The Collaborative Research Centre/Transregio (CRC/TRR) 270 involves researchers from TU Darmstadt, Universität Duisburg-Essen, Max Planck Institut für Eisenforschung and Ernst Ruska-Centre for Microscopy and Spectroscopy with Electrons (ER-C) at Forschungszentrum Jülich. Their common goal is the development of new magnetic materials for efficient energy technologies. This requires to gain a detailed understanding of the structural, magnetic and electronic interactions within the material in order to adjust the local and global properties by new processing techniques to be developed like additive manufacturing and severe plastic deformation methods. Strong permanent magnets based on rare earth elements are a requirement for future mobility and sustainable electricity generation. The magnetocaloric effect causes a change of temperature of a material by the application of an external magnetic field. This principle will enable us to operate refrigerators and air-conditioning devices quietly, with low energy consumption and without the use of traditional refrigerants, themselves strong greenhouse gases. Within this CRC, they will develop new processing methods for innovative magnet materials. Material scientists, physicists, chemists and process engineers will work on magnetic materials by manipulating individual atoms but also by deforming massive samples. By linking the experimental and theoretical groups together in one centre they will be able to continuously cross-link their developments. Artificial intelligence, which accelerates materials discovery and the rapid identification of the most promising material combinations, will also be employed in HoMMage.

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

Contact person: *Jun. Prof. Dr. Nina Gunkelmann, Technische Universität Clausthal*

URL: *https://www.sfb1368.uni-hannover.de/nocache/de/forschung/arbeitsgruppen/modellbildung/*

<table>
<tr><td colspan="2">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)</td></tr>
<tr><td>Contributions:
• Atomistic and multiscale data
• Interfaces for Multiscale Simulations (20% W1 professor)</td><td>Engagement :
Working group modeling consisting of 13 projects</td></tr>
</table>

The influence of oxide layers on the physical properties of the bonding of composites will be investigated using multiscale simulations to understand different production processes. In particular, process conditions that lead to high-quality, metallurgically-bonded compounds are identified. The basic dependencies of the bond strength on oxygen concentration, temperature and oxide layer thickness will be investigated for interfaces. The hardness of the materials as an indicator for the quality of the joint will be determined experimentally by nanoindentation and compared with simulation values. By transferring the results to larger length and time scales, a cross-scale model for the fundamental understanding of the processes of joining technology is to be developed.

PP07 Processing uncertain microstructural data (EXC2075-PUMD)

Contact person: *Prof. Dr.-Ing. Felix Fritzen, University of Stuttgart*
URL: https://www.simtech.uni-stuttgart.de/exc/research/pn/pn3/pn3-1/

<table>
<tr><td colspan="2">402-02 Mechanics
405-05 Glass, Ceramics and Derived Composites
405-06 Polymeric and Biogenic Materials and Derived Composites
406-03 Thermodynamics and Kinetics as well as Properties of Phases and Microstructure of Materials
410-05 Applied Mechanics, Statics and Dynamics</td></tr>
<tr><td colspan="2">Material/Methodology: synthetic and experimental inclusion-matrix and porous microstructures / image-based homogenization and uncertainty prediction
Related Use Cases:
IUC03: Storage concepts for large hierarchical datasets
IUC06: Integrating materials data from experiments and computation (ICME) into Industry 4.0 manufacturing paradigms
IUC08: Interactive visual exploration for analyzing correlations in high dimensional materials data spaces
IUC16: Unified ontology for matrix-inclusion microstructure and composites</td></tr>
<tr><td>Contributions:
synthetic microstructure generators and microstructure data sets
doctoral researcher (50%)
support by the SimTech Data and Software Steward and the SimTech Research Software Engineer for RDM (up to 15%)
coordination with cooperating projects and experimentalists; methodological developments (10% professor/W3 position)</td><td>Engagement:
>14 EXC2075 projects
2 EXC2075 project networks
Fraunhofer ITWM collaboration
GAMM AG Data</td></tr>
</table>

Our research aims at the **image-based prediction of the material properties of stochastic microstructures**. Uncertain microstructure information is gathered from dedicated synthetic microstructures as well as from experimental measurements. Mechanical simulations feed in-silico databases for **data analysis** and processing in **machine learning** tools. These serve for the **automatic feature extraction** and for the development of dedicated **mechanical substitute models**. The inputs consist of 3D image data only. Linking the stochastic microstructure synthesis and experimental data is a key objective during this task, in EXC2075 Data-Integrated Simulation Science and in the GAMM AG Data in order to augment scarce real-world data.

PP08 Cluster of Excellence Living, Adaptive and Energy-autonomous Materials Systems (EXC 2193-livMatS)

Contact person: *Prof. Dr. Thomas Speck, Prof. Dr. Jürgen Rühe, Prof. Dr. Christoph Eberl, Albert-Ludwigs-Universität Freiburg*

URL: *https://www.livmats.uni-freiburg.de/en*

405-04 Mechanical properties of metallic materials and their microstructural origins **406** Materials Science **407-03** Microsystems **108** Philosophy **110-04** Social Psychology, Industrial and Organisational Psychology **202** Plant Sciences **321** Molecular Chemistry **322-01** Solid State and Surface Chemistry, Material Synthesis **327-02** Theoretical Chemistry. Molecules, Materials, Surfaces	
Material/Methodology: Polymers, functional materials, programmable materials / synthesis, additive manufacturing, simulations **Related Use Cases:** • IUC06: Integrating materials data from experiments and computation (ICME) into Industry 4.0 manufacturing paradigms • IUC12: Alignment of application- and higher-level ontologies • IUC13: Co-creation environment for experts	
Contributions: • Top-Level semantic schema bridging multiple disciplines in natural and engineering sciences. • Harmonized standards for interdisciplinary co-creation and documentation • Interdisciplinary research data infrastructure environment and data	**Engagement :** ~ 50PIs, 50PhDs, 3 Junior-Research-Groups 2 Fraunhofer Institutes Ecology Institute

In the Cluster of Excellence Living, Adaptive and Energy-autonomous Materials Systems (livMatS) the best of two worlds, the biological and the technological realm, are merged. While today's materials are largely static, in that their properties do not change with time, livMatS envisions materials systems that are autonomous from an external power supply and can respond to a changing environment by adapting their properties. Such systems, inspired by living nature, will harvest energy they need from the environment and will show complex adaptive behavior via interactions across all length scales, i.e. from the molecular to the macroscopic level. The material systems are produced by multi material manufacturing processes. Societal acceptance, the socio-economic impact as well as philosophical implications of livMatS will be scientifically scrutinized. In this sense, LivMats already offers a deep dive into interdisciplinary research and the resulting challenges and can offer its according progress in finding a common language to communicate between research domains in NFDI-MatWerk. Furthermore, the consideration of multi-stakeholder workflows involves relevant learnings in developing comprehensive harmonization in terms of interdisciplinary documentation methods as needed by NFDI-MatWerk.

PP09 DiWan - The Digital Transformation in Materials Testing: Necessary Actions for the Paradigm Change in Enterprises (BMBF)

Contact person: *Prof. Dr. Martina Zimmermann, Fraunhofer Institute for Materials and Beam Technology*

URL: https://www.digitales-laborbuch.de/

405-04 Mechanical Properties of Metallic Materials and their Microstructural Origins **407-05 Human Factors, Ergonomics, Human-Machine Systems** **409-06 Information Systems, Process and Knowledge Management**	
Material/Methodology: various materials / digital lab book, workflow management in the lab, knowledge system **Related Infrastructure Use Cases:** • IUC01: Web-based demonstration and teaching framework for MSE research data infrastructure • IUC05: Digital infrastructure and workflows for labs • IUC06: Integrating materials data from experiments and computation (ICME) into Industry 4.0 manufacturing paradigms	
Contributions: • workflows for metallographic analysis, domain-specific ELN, interface definition for testing machines, taxonomy for metallographic analysis	**Engagement :** 7 Partners

Within the research project DiWan (within the framework of the BMBF-call “Zukunft der Arbeit”) a digital expert-/assistance system will be developed consisting of an electronic lab book, a digital job and workflow management and a material and knowledge database. The project focuses on the digital transformation of skilled workers rather than academic staff within the MSE community. The DiWanconsortium consists of participants from research institutes, industry and experts from the fields machine learning and work psychology. The digital assistance / expert system developed within DiWanshall be compatible with the DME of the NFDI-MatWerk. Focus group of DiWanwill be skilled workers, hence educational material has to be developed and shall be integrated within and mirrored by the activities within NFDI-MatWerk. Experimental workflows for metallographic preparation routines including metadata will be defined and structured within the knowledge system of DiWan, an exchange and evaluation of the approach shall be discussed with the domain competence “experimental workflow” of NFDI-MatWerk.

PP10 Integrated engineering of continuous-discontinuous long fiber reinforced polymer structures (IRTG 2078)

Contact person: *Prof. Dr.-Ing. Thomas Böhlke, Karlsruhe Institut für Technologie.*

URL: *http://www.grk2078.kit.edu*

402-01 Engineering Design, Machine Elements, Product Development **402-02** Mechanics **402-03** Lightweight Construction, Textile Technology **403-03** Mechanical Process Engineering **406-03** Thermodynamics and Kinetics as well as Properties of Phases and Microstructure of Materials **410-05** Applied Mechanics, Statics and Dynamics	
Material/Methodology: Long fiber reinforced polymers (thermoset and thermoplastic materials) **/** Real process chain is modeled and optimized by digital twin which is based on multi-scale characterization and simulation **Related Use Cases:** • IUC01: Web-based demonstration and teaching framework for MSE research data infrastructure • IUC06: Integrating materials data from experiments and computation (ICME) into Industry 4.0 manufacturing paradigms • IUC08: Interactive visual exploration for analyzing correlations in high dimensional materials data spaces • IUC15: Method- and scale-bridging workflows and data structures for tomography • IUC16: Unified ontology for matrix-inclusion microstructure and composites	
Contributions: • Thermo-mechanical and multi-scale (micro, meso, macro) data (25% scientist) • Materials model ontology (5% W3 professor)	**Engagement :** 14 doctoral projects at 8 institutes (6 KIT and 2 Fraunhofer institutes)

This International Research Training Group (IRTG) 2078 provides a fully integrated engineering approach (processing, characterization, simulation, design) to continuous-discontinuous fiber reinforced polymers by combining the real process with the virtual counterpart (digital twin) in an integrated framework. The PP provides for a complex manufacturing process thermo-mechanical material and process data. Along the process chain, macroscopic and scale-bridging models are deployed. The virtual process is based on a material database and a model ontology.

PP11 ERC Starting Grant MuDiLingo: Ontology Design for Dislocations (ERC MuDiLingo)

Contact person: *Prof. Dr. Stefan Sandfeld, Technische Universität Freiberg*

URL: *https://tu-freiberg.de/fakult4/imfd/mimm/erc-projekt-mudilingo*

<table>
<tr><td colspan="2">406-04 Computer-Aided Design of Materials and Simulation of Materials Behaviour from Atomic to Microscopic Scale</td></tr>
<tr><td colspan="2">Material/Methodology: single and polycrystalline materials including superalloys, HEAs / Molekulardynamik (MD), Discrete Dislocation Dynamics (DDD), TEM
Related Use Cases:
• IUC01: Web-based demonstration and teaching framework for MSE research data infrastructure
• IUC07: Beyond 3D: Tools for spatiotemporal microstructure studies
• IUC12: Alignment of application- and higher-level ontologies
• IUC17: Ontologies for defects in crystals</td></tr>
<tr><td>Contributions:
• own data
• support by a PostDoc (25% FTE)</td><td>Engagement :
a group of 6 PhD students and PostDocs</td></tr>
</table>

Dislocations are particularly important defects in MSE as they are responsible for plastic deformation in metals. Controlling the evolution of dislocations allows tailoring material behaviors on multiple length scales. This PP is based on the ERC Starting Grant project “MuDiLingo – A Multiscale Dislocation Language for Data-Driven Materials Science”. Here, formal ontologies shall be designed together with TA-OMS: Dislocations are/can be treated as one-dimensional mathematical lines; they exist as defects in a crystal structure. “Local rules” are responsible for a specific type of topology change of such dislocation networks. Together with boundary conditions and additional governing equations that define physical relationships this use-case develops an idealized conceptualization for which a formal ontology as an explicit specification will be created. The ontology shall be extended towards idealized representations of other defects such as, e.g., grain boundaries or point defects.

PP12 Data Science in MSE education, qualification and life-long learning (EUSMAT)

Contact person: *Prof. Frank Mücklich, Saarland University; Prof. Stefan Sandfeld, TU Freiberg; Prof. Alexander Hartmaier, RUB Bochum*

URL: *https://www.eusmat.net/*

<table>
<tr><td colspan="2">406-04 Computer-Aided Design of Materials and Simulation of Materials Behaviour from Atomic to Microscopic Scale</td></tr>
<tr><td colspan="2">Material/Methodology: Independent of a specific material/methodology. Supports teaching with a focus on using data science methods in MSE.
Related Infrastructure Use Cases:
• IUC01: Web-based demonstration and teaching framework for MSE research data infrastructure
• IUC13: Co-creation environment for experts</td></tr>
<tr><td>Contributions:
• Network of EUSMAT (European School of Materials), Saarland University
• Expertise in organization of international study and exchange programs in MSE
• Expertise in intercultural communication with focus on science and education
• Experience in implementation of transversal skills in study programs
• Staff hours by EUSMAT office located at Saarland University, Germany</td><td>Engagement :
3 University chairs, 1 group leader at DFKI.</td></tr>
</table>

Making the digital transformation in MSE part of education and qualification is central for sustainable dissemination of concepts developed by NFDI-Matwerk. Specialised modules (e.g. lectures, seminars, etc.) will be developed together with experts in data science and informatics, in order to provide students with the proper tools for future developments in the field (part of the new transversal skill module). Special attention will be paid to implementation of FAIR criteria and psychology of change management. The educational foundation of this project is given by the European School of Materials (EUSMAT), situated at Saarland University. EUSMAT is coordinating and developing international study and exchange programs in MSE from Bachelor to PhD level since 2008. It has repeatedly received funding from the European Commission and relies on an international network comprised of universities in Spain, France, Sweden, Italy and Austria.

PP13 Tomography and Microstructure-based Modelling (Tomography)

Contact person: *Prof. Frank Mücklich, Prof. Stefan Diebels, Prof. Hans-Georg Herrmann, Saarland University*

<table>
<tr><td colspan="2">405-04 Mechanical Properties of Metallic Materials and their Microstructural Origins
406-03 Thermodynamics and Kinetics as well as Properties of Phases and Microstructure of Materials
406-04 Computer-Aided Design of Materials and Simulation of Materials Behaviour from Atomic to Microscopic Scale</td></tr>
<tr><td colspan="2">Material/Methodology: Mainly metallic materials, e.g. steels, aluminium alloys, Ti-6-4 / Atom Probe Tomography, nano-CT, FIB/SEM Tomography, Metallographic Serial Sectioning, Mechanical FE Simulation, Material Modeling.
Related Use Cases:
IUC03: Storage concepts for large hierarchical datasets
IUC05: Digital infrastructure and workflows for labs
IUC07: Beyond 3D: Tools for spatiotemporal microstructure studies
IUC15: Method- and scale-bridging workflows and data structures for tomography</td></tr>
<tr><td>Contributions:
Instrument hours (FIB/SEM, nano-CT, Atom Probe)
Tomographic data from own samples
Scientist hours for test of developed infrastructure tools
IT support for installation of developed infrastructure tools</td><td>Engagement :
3 chairs at Saarland University</td></tr>
</table>

Tomographic methods on different scales are essential tools in materials research. Each method spans a characteristic area in the resolution-volume-space from atoms to millimeters. However, the resulting data are isolated from each other in terms of compatibility and description. This project therefore aims at demonstrating how scale-bridging tomographic data of a sample and derived mechanical simulations can be combined and made accessible in the sense of NFDI and FAIR criteria. This involves identifying relevant data by the community, development of an ontology to properly describe the different techniques, development of software tools to gather generated data and derived results and to integrate this into the shared materials knowledge fabric. Finally, a workflow for the transfer of tomography data to related multi-scale simulations will be established. Relevance for the MSE community is given by the broad range of methods covered and incorporation of national expert committees.

PP14 Interdisciplinary Centre of Advanced Materials Simulation – Micromechancial modelling (ICAMS)

Contact person: *Prof. Dr. Alexander Hartmaier, Ruhr-Universität Bochum; Dr. Franz Roters, Dr. Jaber Rezael Mianroodi, Max-Planck-Institut für Eisenforschung Düsseldorf*

URL: *http://www.icams.de*

<table>
<tr><td colspan="2">406-04 Computer-Aided Design of Materials and Simulation of Materials Behaviour from Atomic to Microscopic Scale
405-04 Mechanical Properties of Metallic Materials and their Microstructural Origins
406-03 Thermodynamics and Kinetics as well as Properties of Phases and Microstructure of Materials</td></tr>
<tr><td colspan="2">Material/Methodology: Micromechanical and scalebridging modeling of plastic deformation, fracture and fatigue of structural materials
Related Use Cases:
• IUC07: Beyond 3D: Tools for spatiotemporal microstructure studies
• IUC08: Interactive visual exploration for analyzing correlations in high dimensional materials data spaces
• IUC10: Interoperability of workflow systems (in collaboration with NFDI4Ing)</td></tr>
<tr><td>Contributions:
• Toolbox to predict macroscopic mechanical properties of materials (microstructure generation, crystal plasticity models, numerical solvers)
• Data repository for mechanical properties of various microstructures</td><td>Engagement :
3 departments with 9 groups, Advanced Study group at MPI für Eisenforschung</td></tr>
</table>

ICAMS focuses on the development and application of a new generation of **simulation tools** for multi-scale materials modelling with the aim of reducing development cost and time for new materials. Within the approach taken by ICAMS, the **different length scales** that are relevant for materials are bridged. The MPI für Eisenforschung is associated with ICAMS, contributing in particular simulation tools on crystal plasticity within a finite-strain continuum mechanical framework. In sum, a powerful toolbox based on **micromechanical modelling** and **microstructure-property relationships** and a data repository obtained from its application can be contributed to NFDI-MatWerk. In this way, a community interaction on the requirements for repositories with mechanical data can be stimulated.

PP15 Working Group “Metadata in Nanoindentation and Micromechanics” (NanoData)

Contact person: *Prof. Dr. Ruth Schwaiger, FZ Jülich GmbH; Prof. Dr. Erica Lilleodden, Helmholtz Zentrum Geesthacht; Prof. Dr. Karsten Durst, TU Darmstadt*

URL: *https://www.fz-juelich.de/iek/iek-2/DE/Forschung/Metadaten_in_der_Nanoindentation_und_Mikromechanik/Metadaten_node.html*

<table>
<tr><td colspan="2">405-04 Mechanical Properties of Metallic Materials and their Microstructural Origins
406-04 Computer-Aided Design of Materials and Simulation of Materials Behaviour from Atomic to Microscopic Scale</td></tr>
<tr><td colspan="2">Material/Methodology: Nanoindentation raw data and analysis / Experiments
Related Use Cases:
• IUC05: Digital infrastructure and workflows for labs
• IUC08: Interactive visual exploration for analyzing correlations in high dimensional materials data spaces</td></tr>
<tr><td>Contributions:
• Nanoindentation data sets based on different hardware
• Provision of data, including material descriptions, meta-data, calibration files
• Identification of needed analyses, results desired, e.g., hardness, modulus
• Provision of governing equations</td><td>Engagement :
Three scientific research groups</td></tr>
</table>

The Working Group “Metadata in Nanoindentation and Micromechanics” focuses on the **development and application of different micro/nanomechanical testing methods** to study the structure-property relationships of metals, ceramics, and polymers. Nanoindentation has proven particularly powerful for exploring mechanical behaviors at small-length scales and is widely employed in the materials science community as well as in industry. It is highly versatile and can be applied to all materials classes allowing the extraction of, e.g., elastic, plastic, and fracture properties. Even standard nanoindentation experiments are already “high-throughput“, and even more so the novel high-speed nanoindentation techniques yielding thousands of indents within a few minutes. In this working group we combine the expertise of researchers working with **different instrumentation and data formats,** and aim at defining **unified data- and analysis frameworks** for nanoindentation and other micromechanical (in-situ) testing methods.

PP16 Profile Area Advanced Materials Engineering TU Kaiserslautern (TUK-AME)

Contact person: *Prof. Dr.-Ing. Tilmann Beck; Prof. Dr. Heike Leitte, TU Kaiserslautern*

URL: *https://www.uni-kl.de/en/ame/*

<table>
<tr><td colspan="2">405-04 Mechanical Behaviour of Construction Materials
409-05 Interactive and Intelligent Systems, Image and Language Processing, Computer Graphics and Visualisation</td></tr>
<tr><td colspan="2">Material/Methodology: Metallic alloys / Analysis of mechanical as well as physical properties and microstructure / Development of interactive visual data exploration and topological data analysis tools
Related Use Cases:
IUC05: Digital infrastructure and workflows for labs
IUC08: Interactive visual exploration for analyzing correlations in high dimensional materials data spaces</td></tr>
<tr><td>Contributions:
Data on microstructure features and mechanical properties
Input on uniform format for experimental data including metadata
Interactive visual data exploration and topological data analysis tools</td><td>Engagement:
15 Professors with their working groups involved in AME</td></tr>
</table>

AME is an interdisciplinary collaboration of **materials research**, production and process engineering and **computer science**. **Institute of Material Science and Engineering (WKK)** focuses on experimental investigations of microstructure and mechanical properties of metallic alloys. For a **comprehensive microstructure characterization** on different length scales MOKE, SEM, SEM-FIB and XRD as well as **mechanical testing** like cyclic micro-indentation and fatigue experiments as well as characterization of **physical properties** are realized within CRC926 “Morphology of Components Surfaces” and CRC/TRR176 “SPIN+X”. **Institute of Visual Information Analysis (VIA)** is focused on machine-learning-based interactive data analytics and works together with engineering and physics within IRTG 2057, Forschungsbau LPME and a Carl-Zeiss Perspective Project. Together, both institutes will contribute in NFDI-MatWerk by works on **digital transformation of experimental data and expertise** in a **stable and robust infrastructure** for breadth use.

PP17 Leibniz-Institut für Werkstofforientierte Technologien (IWT)

Contact person: *Dr. Matthias Steinbacher, IWT Bremen*

URL: http://www.iwt-bremen.de

<table>
<tr><td colspan="2">403 Verfahrenstechnik, Technische Chemie
405 Werkstofftechnik
406 Materialwissenschaft</td></tr>
<tr><td colspan="2">Material/Methodology: highly stressed metallic structural materials / material, process and production engineering
Related Use Cases:
• IUC07: Beyond 3D: Tools for spatiotemporal microstructure studies
• IUC10: Interoperability of workflow systems (in collaboration with NFDI4Ing)
• IUC11: Development of coupled ontologies and workflows for thermochemical treatments</td></tr>
<tr><td>Contributions:
• Instrument hours (dilatometry, technical heat treatment furnaces)
• Heat treatment data from own equipment and furnaces
• Scientist hours (20% of FTE)</td><td>Engagement :
4 departments, 6 groups in department of Materials Science</td></tr>
</table>

The Leibniz Institute for Materials Engineering (IWT) conducts research on highly stressed metallic structural materials. The department of heat treatment within the main department of material science is focused on tailoring micro structures by thermochemical and thermal heat treatment methods. To engage and facilitate the future transfer of heat treatment knowledge as a key technology for micro structure design in structural materials to the community the development of an ontology for heat treatment processes is aimed for. This involves identifying relevant data, a proper description of the relevant processes, tailoring of software tools to gather and condense data and the derived results to integrate them into the shared materials knowledge database.

PP18 Bundesanstalt für Materialforschung und -prüfung (BAM)

Contact person: *Prof. Dr. Birgit Skrotzki*

URL: *www.bam.de/Navigation/EN/About-us/Organisation/Organisation-Chart/President/Department-5/Division-52/division52.html*

<table>
<tr><td colspan="2">405-01 Metallurgical, Thermal and Thermomechanical Treatment of Materials;
405-04 Mechanical Properties of Metallic Materials and their Microstructural Origins
406-03 Thermodynamics and Kinetics as well as Properties of Phases and Microstructure of Materials</td></tr>
<tr><td colspan="2">Material/Methodology: High-Temperature metal alloys / Mechanical testing, Continuum Simulations
Related Use Cases:
• IUC02: Framework for curation and distribution of reference datasets
• IUC17: Ontologies for defects in crystals</td></tr>
<tr><td>Contributions:
• Researcher (50%)
• Datasets determined by accredited testing laboratory</td><td>Engagement :
3 Departments
(about 400 people)</td></tr>
</table>

The Bundesanstalt für Materialforschung und -prüfung (BAM) is a scientific and technical Federal Institute. It performs tests for academic and industrial partners, conducts research, advises regulation agencies and participates in standards committees and contributes to the development of test standards. Its mission to provide reference materials and processes has been recently extended to include reference data sets. The department of Materials Engineering has extensive expertise in characterizing and modeling the mechanical behavior of materials using certified equipment. Single crystalline nickel-based superalloys are one of the classes of materials that have been particularly well studied and for which in IUC02 a framework for the provision of reference material data sets will be developed.

PP19 Physikalisch-Technische-Bundesanstalt - Persistent Identifiers (PTB)

Contact person: *Dr. Joachim Meier*

URL: *https://www.ptb.de/*

<table>
<tr><td colspan="2">307 Condensed Matter Physics
308 Optics, Quantum Optics and Physics of Atoms, Molecules and Plasmas
309 Particles, Nuclei and Fields
310 Statistical Physics, Soft Matter, Biological Physics, Nonlinear Dynamics
311 Astrophysics and Astronomy</td></tr>
<tr><td colspan="2">Material/Methodology: n/a / physical standardization in metrology
Related Use Cases:
• IUC02: Framework for curation and distribution of reference datasets
• IUC12: Alignment of application- and higher-level ontologies</td></tr>
<tr><td>Contributions:
• Expertise in standardization; liasing with other relevant consortia on cross-cutting topics concerning metadata harmonization, data quality assurance, and PIDs services for ontologies, as input to DME.</td><td>Engagement :
international network on standardization and metadata harmonization in metrology</td></tr>
</table>

The definition and elaboration of harmonized standards marks an essential ingredient to the NFDI goal of making data interoperable. This need for harmonization among NFDI consortia but also with the outside world is reflected in the importance of cross-cutting topics for the NFDI process. The PTB is planning to contribute its expertise in the development of fundamental, internationally recognized standards to NFDI-MatWerk as well as other relevant NFDI consortia. We are going to provide expertise and liaise with relevant parties in the following critical areas, building on our experience:

1. Fundamental, internationally harmonized data and metadata standards
2. Fundamental quality assessment of research data and algorithms
3. Basic infrastructure for persistent identifiers for 1.) and 2.)

PP20 Mat-o-Lab - Materials-open-Laboratory

Contact person: *Prof. Manfred Füting, Dr. Thomas Hanke*

URL: *https://www.fraunhofer-materials-data-space.de*

<table>
<tr><td colspan="2">405-01 Metallurgical, Thermal and Thermomechanical Treatment of Materials
405-02 Materials in Sintering Processes and Generative Manufacturing Processes
405-03 Coating and Surface Technology
405-04 Mechanical Properties of Metallic Materials and their Microstructural Origins
405-05 Glass, Ceramics and Derived Composites
405-06 Polymeric and Biogenic Materials and Derived Composites
406-04 Computer-Aided Design of Materials and Simulation of Materials Behaviour from Atomic to Microscopic Scale</td></tr>
<tr><td colspan="2">Material/Methodology: Al-alloys, fiber-composites / Fraunhofer Materials Ontology Stack for Methods and Processes
Related Use Cases:
• IUC11: Development of coupled ontologies and workflows for thermochemical treatments
• IUC12: Alignment of application- and higher-level ontologies
• IUC13: Co-creation environment for experts</td></tr>
<tr><td>Contributions:
• Joined community platform of Fraunhofer MATERIALS and BAM
• Fraunhofer MATERIALS ontology stack spanning manufacturing processes and research methods
• Co-working space for domain experts on purpose including their own methods</td><td>Engagement:
Experts of Fraunhofer MATERIALS (18 Fraunhofer Institutes) and BAM</td></tr>
</table>

The Materials-Open-Lab as a joined venture between Fraunhofer Alliance MATERIALS and Bundesanstalt für Materialforschung und -prüfung (BAM) aims to digitalize research results and research workflows by building a strong data foundation side by side with an open source ontology stack spanning from manufacturing processes to research methods and workflows. The project aims for a comprehensive data ecosystem that is designed to participate in the NFDI but is also industry 4.0 ready and still ensures data sovereignty of all participants. Mat-o-Lab with its close community ties to one of the biggest Fraunhofer Alliances aims to enable domain experts to integrate their data and methods and also participate in the creation of an ontology stack semantically connecting the whole data economy. The cooperation with BAM ensures this aims by the aspects of standardization and regularity and includes best practice examples and valid high-quality data.

IUC01 Web-based demonstration and teaching framework for MSE research data infrastructure

PP03 CRC/TRR 285, PP09 DIWAN, PP10 IRTG2078, PP11 ERC MuDiLingo, PP12 EUSMAT

Main Task Area: TA-CI **Other related Task Areas:** TA-MDI, TA-WSD **Possible connections within NFDI:** NFDI4Ing, FAIRmat
Material/Data: Teaching **Main Success Scenario:** Students can experience the the full functionality of the DME and learn to use workflows with pre-existing datasets and ontologies. **Added value for the MatWerk community:** teaching personnel can tailor the demo framework as well as datasets and workflows to match their study courses.
Main requirements: • Support for the development of academic teaching materials (TA-CI) • DME (TA-MDI) • Validated and well-documented workflows (TA-CI) **Cross-Sectional Requirements: -**

New developments in digitalization and data science needs to be transferred to the new generation of scientists and professionals. Therefore, it is necessary to incorporate these concepts already during their university studies and life-long learning. The IUC aims to provide the necessary materials related demonstration and teaching infrastructure.

EUSMAT will provide its international study programmes, like the Erasmus Mundus Master AMASE, and its network of international partners for implementing the designed modules for all academic levels, taking in account also intercultural aspects. In addition to that, the PP participant universities will be at the forefront of implementation and testing. Evaluations will be conducted after the training activities in order to identify potential ways of improvement. The modules will be made available for the MSE community for being implemented in other study programmes.

IUC02 Framework for curation and distribution of reference datasets

PP01 CRC/TRR 103, PP18 BAM, PP19 PTB

Main Task Area: TA-MDI **Other related Task Areas:** TA-CI, TA-WSD, TA-OMS **Possible connections within NFDI:** NFDI4Ing
Material/Data: Single crystal Ni-based superalloys / Creep data **Main Success Scenario:** Users can find and access single crystal Ni-based superalloy reference data sets with full information about uncertainties regarding the data, material, production and measurement process to validate own measurements and models. **Added value for the MatWerk community:** General framework for the definition, selection, curation and distribution of reference data sets, best practice example.
Main requirements: • Steered community process (definition of criteria for reference data) • Data governance (usage analytics for reference data) • MDE backend (data registration, PID, authenticity of reference data) • Metadata store (search and discover of data and interrelationships) • Incentivation mechanisms • Legal aspects (licenses) **Cross-Sectional Requirements:**

The aim of this IUC is to develop a **framework for reference material data sets** using creep properties of single crystal Ni-based superalloy as example. Such reference data sets are necessary for (i) evaluating and validating experimental/modeling methods and their uncertainties, (ii) assessing the performance of analysis, modelling and simulation tools by use of standardized processes and (iii) providing **comprehensive material descriptions** (e.g., meta-data schemas and ontologies). **Community-driven processes** will be established for the **definition, identification** and **curation** of **reference material data sets**, including **metadata, raw data** and **processed data,** and **quality assessment routines**. Reference data set will contain detailed meta-data and context concerning **materials history**, **data collection** (e.g., testing and measurement equipment, calibration status/certificate) and the **related** specific **uncertainty/error** (measurement, model, simulation). Existing data on Ni-base superalloys from PP18 BAM and PP01 SFB/TR103 will be used, where superalloys have been well characterized using a broad spectrum of characterization methods and in-depth data is available.

IUC03 Storage concepts for large hierarchical datasets

PP07 EXC 2075-PUMD, PP13 Tomography

Main Task Area: TA-MDI **Other related Task Areas:** TA-WSD, TA-Strategy **Possible connections within NFDI:** NFDI4Ing, FAIRmat
Material/Data: (mainly) metallic materials/tomographic data and related simulations with focus on large datasets **Main Success Scenario:** Large amounts data from various, scale-bridging tomography methods of a given sample as well as simulations can be fused, specific volume elements can be accessed at different scales. **Added value for the MatWerk community:** An exemplary implementation of a storage concept for large fused and linked datasets which is accessible through the DME and a web-based interface.
Main requirements: • Digital Materials Environment (DME) Backend (MDI) • Materials Data Infrastructure Support (MDI) • Connection of workflows and ontologies (WSD) **Cross-Sectional Requirements:** -

Tomographic data from different techniques (e.g. Atom Probe Tomography, FIB/EBSD serial sectioning) and related simulations need to be stored in the DME in accordance with the underlying ontology for materials tomography and with reference coordinate systems that allow for the fusion of the datasets. A particular challenge here is the large amount of data that needs to be integrated and accessed, testing the performance and scalability of the DME.

IUC04 Model driven data space exploration

PP02 CRC 1394, PP05 CRC/TRR 270

Mainly related to Task Areas: TA-WSD **Other related Task Areas:** TA-OMS **Possible connections within NFDI:** NFDI4Ing, FAIRmat
Material/Data: Mg-Al-Ca alloys / Thermodynamic and structural data of defects **Main Success Scenario:** User can automatically generate defect phase diagrams that can be used to predict the performance of materials **Added value for the MatWerk community:** General framework of model-driven thermodynamic databases that combine computation and experiment
Main requirements: • Workflows combining theoretical and experimental structural data of defects • Adaptive databases for high dimensional data structures containing sparse data • Visualization (of thermodynamic dataspace from microstructure, chemical or mechanical perspective) • Multiscale simulation (of multiphysics data) • Electronic lab book (for defect data), **Cross-Sectional Requirements:**

Since defect phase diagrams are a novel concept in materials science, only a limited amount of thermo-chemo-structural data is currently available. They need to attributed to certain defect types, defect characters and defect states. The main purpose of the IUC is to ensure a model-driven (guided probing) collection of the relevant experimental and computational data to construct these diagrams and their post-processing according to newly established simulation protocols. The construction and visualization of the diagrams should reflect the multidisciplinary perspective on these diagrams (i.e., the perspective of atomic configurations, chemical potentials, and of materials properties).

IUC05 Digital infrastructure and workflows for labs

PP02 CRC 1394, PP03 CRC/TRR 285, PP09 DIWAN, PP13 Tomography, PP15 NanoData, PP16 TUK-AME

Main Task Area: TA-WSD **Other related Task Areas:** TA-MDI **Possible connections within NFDI:** NFDI4Chem
Material/Data: Mechanial characterization workflows - nanoindentation data-sets in form of load, displacement, time, possibly extended to dynamic response (load and displacement amplitude, phase shift), temperature; meta-data associated with instrument specifications and calibration files, specimen geometry, material description (possibly based on material/microstructure ontology) **Main Success Scenario:** (i) a data base and workflow for nanoindentation-based testing and analysis is established for appropriate comparison and/or re-evaluation of data, (ii) electronic lab-books and procedures to handle the synthesis of materials and history of samples implemented, (iii) the data be made accessible to the materials community. **Added value for the MatWerk community:** The implementation can be used by the community as example for many characterization lab workflows and the integration of equipment. It will allow (i) old data sets to be readily re-analyzed with updated algorithms from new knowledge, with access to complete data sets (raw and meta-data previously not of interest), (ii) comparison of data across different groups, instruments, testing protocols, (iii) allow robust statistical analyses, (iv) contribute to updatable material data base
Main requirements: • Exemplary machine interface implementations • Storage of data, meta data, based on a materials ontology • Automated analysis workflows • Flexible data labeling system (can be updated, changed) for sorting of data sets, allowing appropriate comparisons of data **Cross-Sectional Requirements:** Electronic Lab Books with NFDI4Chem

Results of mechanical tests are often presented as evaluated material properties, such as yield stress or elongation to failure. However, the raw data of the machine and the continuously recorded “raw data”, i.e. load, displacement and time data, are typically not part of the presentation. The IUC shall provide a tool for storing and evaluation of raw mechanical test data while maintaining typically “hidden” information of the mechanical testing setup. Data analysis frameworks according to standards as well as new methods should be considered.

- Instrument artifact identification via statistically robust comparison of data sets on standard samples using different instrumentation
- Establish mechanical response catalog for a given sample and link to material structure ontology IUC and correlation IUC for new knowledge on structure-property relations
- Extending nanoindentation data evaluation to other test sample geometries (flat surface, pillar compression, beam bending, different tip geometries)

Nanoindentation data from different indentation systems will be stored in a systematic way, allowing the consistent analysis of the data according to established models and new methods.

IUC06 Integrating materials data from experiments and computation (ICME) into Industry 4.0 manufacturing paradigms

PP04 CRC 1261, PP05 CRC/TRR 270, PP07 EXC 2075-UMD, PP08 EXC 2193-livMatS, PP09 DIWAN, PP10 IRTG 2078

Main Task Area: TA-WSD **Other related Task Areas:** TA-MDI, TA-OMS **Possible connections within NFDI:** NFDI4Ing
Material/Data: Polymeric matrix material reinforced with glass and carbon fibers / Computed tomography data, thermo-physical properties on different scales (e.g. stiffness, heat capacity), process data (e.g. molding pressure or temperature), product design data (e.g. part, bead, ribs geometry) **Main Success Scenario:** Users can integrate materials data into digital representations of process and manufacturing chains and make the data accessible for the community. **Added value for the MatWerk community**: An infrastructural framework coupling and materials data and industry-relevant manufacturing processes with their model representations (digital twins).
Main requirements: • Data storage infrastructure and DME platform for data from different levels of the process chain • Workflows combining physical and synthetic data on different levels of the process chain **Cross-Sectional Requirements:** • Industry 4.0 Standards and Interfaces (NFDI4Ing) • Cross-discipline ontology-matching (NFDI4Ing)

This IUC provides a framework for the integration of materials data into I4.0 manufacturing data infrastructures. This will be implemented as a physical **process chain** of two polymer systems (sheet molding compounds (**SMC**), long fiber reinforced thermoplastics (**LFT**)). The materials data will be integrated in a **material database infrastructure**. The simulation models are part of a model hierarchy which will be further developed/integrated into a materials model ontology. Based on the model ontology the compatibility of simulation models and material data can be examined and analyzed. Model ontologies are a prerequisite for **ontology based knowledge systems** and will be made available for the class of long fiber reinforced polymers.

IUC07 Beyond 3D: Tools for tracking spatiotemporal microstructure evolution

PP06 CRC 1368, PP11 ERC MuDiLingo, PP13 Tomography, PP14 ICAMS, PP17 IWT

Main Task Area:TA-WSD **Other related Task Areas:** TA-OMS, TA-CI **Possible connections within NFDI:** NFDI4Ing, FAIRmat
Material/Data: Spatiotemporal point, triangle cloud/mesh, and tensorial field data from computer simulations of microstructure evolution at the microscopic and atomic scale **Main Success Scenario:** The user can characterize the geometry (and topology) of the crystal defects and describe their motion and interaction in time by flexibly exchanging spatiotemporal data from representative-volume-element (RVE) models, dislocation dynamics codes and force-field/MD codes. **Added value for the MatWerk community:** A computational geometry description for crystal defects (point, line, and surface patches) is connected with a corresponding ontology. This enables users to identify crystal defects agnostic of a specific implementation in a simulation code, enables a seamless encoding between the atomic and the microscopic/macroscopic scales and provides access to the study of the time evolution of defects.
Main requirements: • Workflows to store/extract e.g. atomic positions, atom types, material point data (continuum, voxel data) including metadata and contextualization • Workflows to execute existing modeling tools for microstructure evolution (plasticity, recrystallization, grain growth, precipitation, dislocation dynamics, and force-field codes) • Workflows how to use existent MatWerk post-processing tools including metadata and contextualization • Development of ontology for defects • Tools for 3D visualization • Integration in institutional education **Cross-Sectional Requirements:** Workflow description

Spatiotemporal microstructure data are the key results of continuum full-field and atomic-scale computer simulations, as well as cutting-edge diffraction microscopy experiments. Typically represented as voxel, point, line, or finite-element meshes, these data **cover a variety of materials information**, such as the **spatial distribution** of crystal defects and their embedding into **three-dimensional field quantities** like temperature, mechanical stress and strain, or concentration fields of chemical species. Especially when many such time-dependent snapshots are taken, the volume and acquisition velocity can quickly become impractical to work with (GB, TB, or even larger). In addition, the large variety of computer codes within the MSE community, limits interoperability and repurposeability when **hand-shaking between different microstructure characterization tools**. Here, we aim for infrastructure work that describes crystal defects and their motion embedded in fields across different length and time scales in a **code-agnostic representation** that can complement existent code-specific outputs. Proof-of-concept workflows are developed, which exemplify how such description and ontology connection can be exported from existent MSE simulation tools, covering continuum-scale crystal plasticity, RX, GG, precipitation, dislocation dynamics, and atomistics.

IUC08 Interactive visual exploration for analyzing correlations in high dimensional materials data spaces

PP04 CRC 1261, PP05 CRC/TRR 270, PP07 EXC 2075-PUMD, PP10 IRTG 2078,
PP14 ICAMS, PP15 NanoData, PP16 TUK - AME

Main Task Area: TA-WSD **Other related Task Areas:** TA-OMS **Possible connections within NFDI:** NFDI4Ing, NFDI4Chem and DataPlant
Material/Data: Metallic alloys / microstructural features and mechanical as well as physical properties **Main Success Scenario:** Users can identify and validate correlations for highly complex, sparse materials data sets and can predict materials properties based on microstructural features. **Added value for the MatWerk community:** Development interactive data and topology analysis tools based on a materials knowledge management system. This will be used to support and validate the materials ontology developed within the NFDI4-MatWerk.
Main requirements: • Uniform (Meta)data formats to enable a utilization of heterogenous data obtained at different test devices • Metadata scheme to ensure comparable information for different test methods • Standardized units to facilitate data transformation • Electronic lab book for uniform data documentation and management • Integration of measurement devices to simplify utilization of different test devices • Visualization tools for interactive correlation analysis **Cross-Sectional Requirements:** • Curation software, Collaboration on Interoperability with DataPlant

The **mechanical properties** obtained with a **variety of testing methods** (e.g. tensile and fatigue testing, (cyclic) indentation, etc.), **microstructural features** (e.g. grain size, phase contents, etc.) and **physical properties**(e.g. electrical conductivity, magnetic permeability, etc.) provide **huge opportunities for exploring correlations. Interactive visual data exploration** and**topological data analysis** are promising to find and evaluate correlations within materials datasets. The major **challenges** for data analysis are the **lack of standardization** on the data input, the lack of helpful guidelines for applying existing data analysis/visualization packages, and the **complex nature of the data** that is commonly not directly supported by these libraries. To **address these challenges**, the following support is required: (i) **Standard data formats** have to be defined and described by an **ontology**and the transformation from arbitrary data to this format has to be elaborated. (ii) **Correlation analysis** techniques need to be **revisited** and **systematized** along. (iii) **Best practices** need to be **defined** and **tested** as well as augmented with novel analysis techniques.

IUC09 Infrastructure interfaces with condensed matter physics (collaboration with FAIRmat)

PP01 CRC/TR103, PP02 CRC 1394

Main Task Area: TA-WSD **Other related Task Areas:** TA-OMS
Possible connections within NFDI: FAIRmat

Material/Data: Atom Probe Tomography (APT) for metallic alloys

Main Success Scenario: Through the physical modeling of the measurement process, users get more precise information and a deeper understanding of their experimental results, in particular to distinguish defect states in the microstructure.

Added value for the MatWerk community: Workflows are designed in coordination with FAIRmat such that the exchange of data, metadata, ontologies, and concepts for data curation between two NFDI consortia is ensured without a loss of information. In this way, both consortia can mutually benefit from ongoing improvements in the infrastructure for condensed-matter physics (FAIRmat) and the interpretation of microstructure data (NFDI-MatWerk).

Main requirements:

- Workflows how to process measured data (e.g. detector hit positions, time-of-flight per ion) into atomic position and atom types (chemical species) including all metadata with contextualization (e.g. sample preparation, electric field) (FAIRmat)
- Close interaction with device software via open-source parsers and converters
- Machine learning/statistical analysis of APT atomic data to detect and interpret defect structures
- Interface between formats and queries of (meta)data in FAIRmat and NFDI-MatWerk
- Ontology matching between both communities
- Workflow combining experimental data, image processing and theoretical models / properties of defects in microstructured materials (NFDI-MatWerk)

Cross-Sectional Requirements: Data format and ontology standards

The interface to **FAIRmat** is most relevant for NFDI-MatWerk, since condensed-matter physics is the basic science perspective on solid-state phenomena. The resulting consequence for the infrastructure is explored in this IUC. FAIRmat focuses their effort on fundamental chemo-physical effects. In the case of atom probe tomography (APT), for example, the **correlation** of details of the electric field and the electronic density in the sample needs to be analyzed and exploited in order to predict the emission of atoms from steps at the surface. Such predictions are the key to arrive at more accurate and precise predictions of the ion launch and trajectories; and thereby are a route to improve current methods for backing out atomic positions. In contrast, NFDI-MatWerk addresses the **relevance of the microstructure** for engineering materials and their applications. Therefore, the focus of NFDI-MatWerk is on the correlation of **atomic positions** and defect states as a function of the chemical potential and the sample history (processing, heat treatment). For both perspectives, several gigabyte of data needs to be handled and needs to be evaluated with machine learning approaches.

IUC10 Interoperability of workflow systems (collaboration with NFDI4Ing)

PP06 CRC 1368, PP14 ICAMS, PP17 IWT

Main Task Area: TA-WSD **Other related Task Areas:** TA-OMS, TA-CI **Possible connections within NFDI:** NFDI4Ing
Material/Data: Multiscale simulation of microstructure formation **Main Success Scenario:** The user will be able to connect the tools and concepts employed by different communities to complete simulation protocols. Therewith, a multi-scale simulation of microstructures in materials becomes accessible, which connects, e.g. atomistic and phase field simulations. **Added value for the MatWerk community:** The purpose of the IUC is to demonstrate the transfer of simulation protocols from one workflow system to another one. This gives the MatWerk community the chance of accessing tools designed for the needs of the whole engineering community captured in NFDI4Ing.
Main requirements: • Integrated development environment that allows flexible adaptations • Special workflow formats for multiscale materials simulations • Ontology development at the interface of different communities • Data formats for materials data infrastructure **Cross-Sectional Requirements:** • Workflow-Ontology interaction

Within **engineering sciences**, **NFDI4Ing** received a funding admission to implement common interfaces between the different disciplines of engineering sciences. Within their archetype **Ellen** the exchange of information between heterogeneous disciplines is addressed, with a focus on diverse data sources. In the present IUC, we extend this concept to the **exchange of workflows**. More specifically, an integrated development environment for the specific needs of NFDI-MatWerk is developed within measure WSD-4. At the same time NFDI4Ing uses the workflow system KaDI4Mat within the **community cluster**"Materials Science and Engineering" for simulations as well as tracking samples (in archetype **CADEN**). Ensuring the interoperability between both systems, optimally **connects NFDI-MatWerk to the whole framework of engineering science**. Within this IUC the advantages will be prototypically demonstrated for the multiscale simulation of hierarchical microstructures. Here, the interoperability of workflows will be used to connect atomistic simulations (NFDI-MatWerk) with continuums simulations of microstructure formation during solidification (NFDI4Ing).

Exemplary Case Studies

Multiscale simulations form a central challenge in materials science that needs to be taken care of by workflow systems. It requires the connection of various distinct data types (atomistic vs. continuum, wave functions vs. field equations and representative volume elements). As a consequence, also computer codes of different communities need to be connected. Within the TA-WSD these challenges are addressed in measure WSD-5. Nevertheless, the developments strongly depend on the requirements and support of the MSE community. For example, the cross-scale model for the processes of joining technology, which is developed in PP06 (Nina Gunkelmann), will be used to benchmark the workflow system. At the same time, the connection to other NFDI communities is highly relevant for this purpose. The way this can work is demonstrated in the IUC09 for condensed-matter physics and in IUC14 for the engineering sciences.

IUC11 Development of coupled ontologies and workflows for thermochemical treatments

PP17 IWT, PP20 Mat-o-Lab

Main Task Area: TA-OMS **Other related Task Areas:** TA-WSD **Possible connections within NFDI:** NFDI4Ing
Material/Data: high strength structural materials / time-temperature-transformation relations to microstructures **Main Success Scenario:** Users can utilize a knowledge graph populated by process and material data to predict microstructures and their alteration by thermochemical heat treatments. Using a graph based experimental data structure enables a FAIR datastorage to allow for a new level of reproducibility and comparability of experimental results from different experimental setups and groups. **Added value for the MatWerk community:** Concepts for the combined ontologies will be developed, combining thermo-chemical processing and materials transformation. General framework for heat treatment representation and resulting erroneous and intended experimental impact on materials microstructure.
Main requirements: • Ontology for representation of heat treatment courses and transformation in structural materials • Workflow management systems that can be adapted during use (e.g., primary data acquisition, assertion augmentation, heterogeneous post-processing) • Tools for automated data assembly • Data augmentation and condensation for advanced data handling **Cross-Sectional Requirements:** Data standards with NFDI4Ing

In structural materials the microstructure formation is triggered using specific thermo- or thermos-chemical heat treatment cycles. The final microstructure derived from a heat treatment is a result of subsequent and parallel transformations which mostly are transient and/or temperature driven. In this IUC, a **research data management framework** for experimental data with domain-specific semantics is to be designed. Semantic structured data processed in the framework is **based on experimental data** from different transformation characterizing schemes. Workflows for experimental procedure and data acquisition to data representation will be developed. A **ontological representation** encompassing both **heat treatment courses and material transformation** is designed in order to provide a common and unified description. Moreover, scalability from lab size experimental data derived from, e.g., dilatometry and technical furnace equipment is represented.

Exemplary Case Studies

Dilatometry data derived for common high strength structural materials, such as steels, will be assessed using corresponding descriptive data stored in the ontology. Additionally, a tool for condensing large datasets derived from dilatometry will be developed -- based on mathematical representations of the transformations occurring during heat treatment by Johnson-Mehl-Avrami and Koistinen-Marburger equation. Condensing data via parametrization will provide significantly reduced data sets and a direct representation of the measured data to be used in common FE-solver based mesoscopic materials simulation.

IUC12 Alignment of application- and higher-level ontologies

PP05 CRC/TRR 270, PP08 EXC 2193-livMatS, PP11 ERC MuDiLingo, PP19 PTB,

PP20 Mat-o-lab

Main Task Area: TA-OMS **Other related Task Areas**: TA-SD **Possible connections within NFDI:** all consortia, in particular NFDI4Ing, FAIRmat, NFDI4Chem
Material/Data: Other ontologies, e.g. EMMO, ontologies from NIST **Main Success Scenario:** Users are able to easily connect application and higher level ontologies with general ontologies. **Added value for the MatWerk community:** Consistently interface with all neighboring communities and benefit from their expertise.
Main requirements: • Existing application domain or general ontologies • Basis ontology advisory • Ontology development support • Software Interfaces for ontology alignment **Cross-Sectional Requirements:** Generally necessary ontology frameworks, formalized units, interfaces, ontology visualization

This IUC is mainly dedicated to all aspects touching upon the question how to create the connection between **domain and application ontologies with general ontologies**. Such **"ontology matching"** is crucial for enabling the interoperability between different (sub-)domains and therefore important for linking different sub-domains within NFDI-MatWerk. Furthermore, it is one of the prerequisites for creating a well-connected "network" of ontologies across different NFDI consortia. One of the main challenges is the dynamic alignment of ontologies that are constantly changing and developing. The "data" required for this IUC are the existing application domain or general ontologies.

Besides a number of PPs, a close interaction with NFDI4Ing is planned in particular with regards to their base services Measure S-3 "Metadata and terminology services".

IUC13 Co-creation environment for experts

PP08 EXC 2193-livMatS, PP12 EUSMAT, PP20 Mat-o-Lab

Main Task Area: TA-OMS **Other related Task Areas:** TA-WSD **Possible connections within NFDI:** -
Material/Data: This depends on the selected expert scenarios, currently, including Mat-o-Lab's Use Cases on Steel, Copper and fiber-composites **Main Success Scenario:** MSE-domain experts and interdisciplinary contributors from informatics and information science can jointly work on digitizing scientific workflows and develop their semantic representations. **Added value for the MatWerk community:** Known and teachable processes for transforming expert domain knowledge into formalized structures as well as the resulting formalized workflows themselves
Main requirements: • Basis Ontology advisory • Ontology development support • Multi-scale bridging ontologies • Software Interfaces for accessing workflow data semantically • Implementation of DME for applying the representation **Cross-Sectional Requirements:** Generally necessary Ontology frameworks, including tools for building knowledge graphs for non-experts, formalized units, interfaces, ontology visualization

This Infrastructure Use Case expresses the demand to extract implicit process and theory knowledge from experts to represent their domain-specific expertise in a formalized manner. Although this procedure depends on exemplary material systems to conduct this process, its theory is detached from concrete data.

The IUC requires ways of formalizing such expert knowledge by applying schemas based on other model contexts, to develop didactic frameworks that allow the structured formalization of the needed information and to have a working infrastructure at one's disposal to implement and query the formalized knowledge expression.

The IUC works with dedicated PPs that tackle the challenge of formalization from an interdisciplinary, exemplary and collaborative point of view. In doing so, it vastly supports NFDI-MatWerk's targets in the context of the FAIR-principles, since structured expert knowledge leads to standards, which then leads to interoperability.

IUC14 Adaptive automated characterization pipelines and meta data schemas for high throughput experiments

PP01 CRC/TR 103

Main Task Area: TA-OMS **Other related Task Areas:** TA-MDI, TA-WSD **Possible connections within NFDI:** FAIRmat, NFDI4Chem
Material/Data: Combinatorial thin films synthesis and automatized X-ray diffraction data analysis **Main Success Scenario:** A toolkit for the automated handling of all meta data during sample characterization is set up. This allows for a high-throughput analysis of structural data for materials design and materials discovery **Added value for the MatWerk community:** Data management for automated experimental characterization techniques; Concepts and software solutions for a continuous adaptation of data management workflows in conjunction with a developing meta data schema;
Main requirements: • Standardized formats for data and metadata • Flexible storage of large amount of data obtained in high-throughput measurements • Workflow management systems that can be adapted during use • Combination of automated experimental characterization and automated data analysis • Device software and electronic lab books **Cross-Sectional Requirements:**

In this IUC a research data management for highly **diverse experimental data** is developed and established in order to match the special requirements of automated experimental characterization setups. The desired solution should **continuously adapt data management workflows**. Starting with a relatively limited meta data schema, a **continuous adaption over the period of use** is foreseen to develop more and more data procedures into dedicated data management workflows. By continuous adaptation and integration of **analysis workflows and metadata schemes**, the amount and the quality of the meta data improves. A prototype system for such a setup has been developed by the PP01 and will be integrated in the materials data infrastructure of NFDI-MatWerk.

IUC15 Method- and scale-bridging workflows and data structures for tomography

PP10 IRTG 2078, PP13 Tomography

Main Task Area: TA-OMS **Other related Task Areas:** TA-CI, TA-WSD **Possible connections within NFDI:** NFDI4Ing, FAIRmat
Material/Data: Tomographic data and related mechanical simulations of mainly metallic materials **Main Success Scenario:** A description of scale- and method-bridging ontology and workflows has been developed which allows to connect tomographic (meta-)data and related mechanical simulations from a given sample**.** **Added value for the MatWerk community:** A general framework for workflows and metadata of materials tomographies and related microstructure features is supplied.
Main requirements: • Ontology development support (TA-OMS) • Multiscale-bridging ontologies (TA-OMS) • Support from professional societies to identify relevant data by involvement of expert committees (TA-CI) • Metadata Store (TA-MDI) • Graphical programming language (TA-WSD) **Cross-Sectional Requirements:** Common data standards and formats (FAIRMat, NFDI4Ing)

Materials tomography methods and resulting data vary strongly depending on the method used, the experimental approach and the workflow for post-processing, i.e. creating a reconstructed volume from the raw data for further analysis and mechanical simulations. Currently, there is no established protocol which would allow to conduct all necessary steps in a well-defined manner. The resulting data from different methods are therefore not interconnected and workflows are intransparent. An ontology for materials tomography data on different scales and related mechanical simulations needs to be developed in order to solve this issue. The ontology, which will be developed with the help of expert societies, will provide a framework of relevant (meta-)data and workflows that need to be recorded in order to provide a meaningful and transparent description of the way from data acquisition to reconstructed volume and further analysis.

IUC16 Unified ontology for matrix-inclusion microstructure and composites

PP07 EXC 2075-PUMD, PP10 IRTG 2078

Main Task Area: TA-OMS **Other related Task Areas:** TA-MDI, TA-WSD **Possible connections within NFDI:** MaRDI, NFDI4Ing
Material/Data: various materials with matrix-inclusion morphology (containing, e.g., particles, fibers, whiskers) / microstructure data from experiments, simulations and abstract models **Main Success Scenario:** users from different disciplines can query matrix-inclusion morphology information from various sources of data; the main application is the exploitation of the microstructural data in simulations, surrogate modeling and in connecting experimental evidence with models **Added value for the MatWerk community:** The ontology can be used in many applications, both for existing data and newly captured data sets and can be generalized to other materials.
Main requirements: • basis ontology • metadata schema • ontology development support • multiscale-bridging ontologies **Cross-Sectional Requirements:**

Matrix-inclusion materials constitute a material class of major practical significance and generality (e. g., particle/whisker/fiber reinforcement; porous materials and foams). The **unified description of such materials** will accept discrete data sources (e.g. X-ray CT), probabilistic models (e. g. Boolean models) as well as parameterized microstructure synthetization. **Universal ontologies** will allow **interoperability** of these fundamentally different data types for the description of matrix-inclusion materials. Thereby, **different communities** will be brought together, connecting experimental material scientists with mathematicians and engineers. The universal description will enable the discovery and exploration of relevant data at reduced overhead. Through a dedicated intellectual property management, the community will be appealed to publish data. Having an extensible base ontology will enable future developments with backwards compatibility. The community can then focus on linking the microstructure information with complex physical data and dedicated thermo-chemo-mechanical material models by limiting overhead for data generation, data gathering and implementing data access.

Exemplary Case Studies (TA-OMS)

The Task Area Ontologies will directly benefit from the base ontology for matrix-inclusion materials, which cover a wide range of relevant real-world materials such as particle and fiber reinforced composites. Porous materials are contained when identifying one phase with the pore space. The rich availability of data sets for this material class leverages the usability within the community. Further, the compatibility of the ontology with many existing datasets will enable simple to manage queries. In view of possible interactions with other NFDI consortia, the proposed ontology is tailored to serve material-specific demands in the abstract methodologies opted for within MaRDI (measure 2.4; TA4 Cooperation with other disciplines).

IUC17 Ontologies for defects in crystals

PP01 CRC/TRR 103, PP11 ERC MuDiLingo, PP18 BAM

Main Task Area: TA-OMS **Other related Task Areas:** TA-WSD, TA-CI **Possible connections within NFDI:** NFDI4Ing
Material/Data: Single- and polycrystalline materials/metals including superalloys and HEAs / Simulation data as well as postprocessed microscopy data **Main Success Scenario:** Users can describe the defect structure with a defined vocabulary and quantitative mathematical representation that is comparable between experiments and transferable to simulations **Added value for the MatWerk community:** A consistent and standardized description of crystalline structures and defects that can easily be extended and adjusted
Main requirements: • Metadata store • Software tools for creating and visualizing ontologies **Cross-Sectional Requirements:** Common data standards, generally necessary Ontology frameworks, formalized units, interfaces, ontology visualization

This IUC will test if a certain class of **metadata and ontologies describing crystalline structures and crystalline defects**(such as point defects, line defects, area and volume defects) and their temporal evolution are **well designed and applicable for different types of simulations, experiments and microscopy**. A representation of such defects and structures is at the heart of many studies or investigations conducted MatWerk. Therefore, it is important that such an ontology works well for all relevant fields and methods, even if many other more complex properties and relations strongly differ across different PPs or other applications. For this, specialized ontologies are needed, which, however, still should contain the basic ontology for crystallography and crystalline defects. Furthermore, this IUCT benefits from a close relation with IUC12 for ensuring/testing **if the crystalline ontology can be aligned other, existing ontologies**for crystallographic structures.