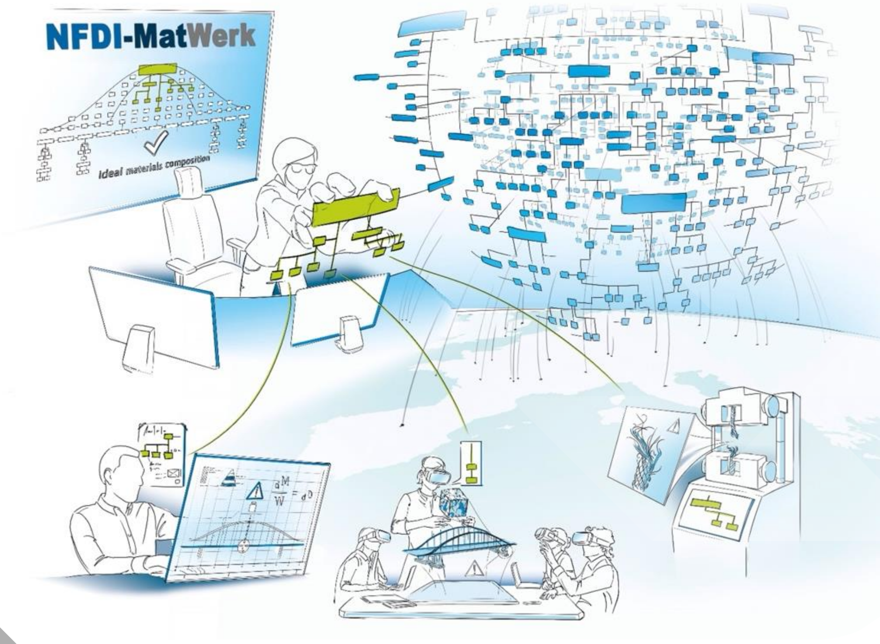

NFDI-MatWerk Progress Report

Part 1

September 30, 2024

www.nfdi-matwerk.de

NFDI MatWerk

Table of Contents

B-1 Progress Report Part 1, <u>for publication</u>

1 General Information

- Name of the consortium in English and German:
  DE: Nationale Forschungsdateninfrastruktur für Materialwissenschaft & Werkstofftechnik
  EN: National Research Data Infrastructure for Materials Science & Engineering

- Research domains or research methods addressed by the consortium
  - 4.31 – Materials Engineering
  - 4.32 – Materials Science
  - 4.12-02 – Mechanics
  - 4.12-03 – Lightweight Constructions
  - 4.51-03 – Construction Material Sciences, Chemistry, Building Physics

  according to the DFG review board classification system.[1]

- URL of the consortium website and repositories used for publishing output

Website of the consortium:	https://nfdi-matwerk.de/
NFDI-MatWerk Zenodo Community:	https://zenodo.org/communities/nfdi-matwerk/

Further output is published on various institutional repositories, available via the individual tools and services on the solutions area of the consortium website.

2 Summary

NFDI-MatWerk supports the Materials Science and Engineering (MSE) community in its effort to theoretically and experimentally characterize materials, to study their processing and manufacturing. The ultimate goal of MSE is to design materials with optimized properties and to maximize reusability at their end-of-life. In this context, one major challenge particular to MSE data is their inherent interdisciplinary and multiscale character. This is caused by the strongly heterogeneous microstructures present in virtually all materials, ranging from crystal defects at

[1] DFG Classification of Subject Areas and Review Boards (2024-2028): https://www.dfg.de/resource/blob/331950/85717c3edb9ea8bd453d5110849865d3/fachsystematik-2024-2028-en-data.pdf

the atomistic level, through microscale secondary phases up to macroscale pores. Furthermore, any process applied to a sample may change the material's microstructure and, thereby, its complete mechanical and a substantial fraction of its functional performance.

Due to the vast number of different experimental, computational and analytical methods to reveal these dependencies, essentially every lab used to develop its own data tools and services. This rapid but previously uncoordinated development had hampered the digital transformation in MSE as well as the implementation of the FAIR principles. With the start of NFDI-MatWerk, we have steered the development of this infrastructure into a community-driven process. Based on the analysis of data usage profiles of many Participant Projects from different sub-disciplines we have identified the most relevant scientific scenarios within MSE. The resulting Infrastructure Use Cases (IUC) formed the backbone of NFDI-MatWerk, as they continuously guided and challenged the development of our infrastructure.

At the same time, these IUCs have resulted into a large number of success stories of the NFDI-MatWerk strategy. For example, the team of the IUC02 has developed a structured approach for collecting all required information on a creep experiment in such a way that it can serve as a reference dataset. The IUC04 has identified a way how experimental and computed data of defect phases can be jointly analysed by exploiting electronic lab notebooks. The IUC09 has demonstrated how software solutions of different communities can be made interoperable within a common workflow environment. And IUC17 is about the development of semantic representations describing crystalline structures and crystalline defects (such as point defects, line defects, area and volume defects) incl. their temporal evolution and about an assessment of these descriptions regarding their applicability for different types of simulations, experiments, and microscopy. All these examples have been designed in a way that can straight-forwardly be adapted to different scientific scenarios, which ensures their relevance for the MSE community.

Five Task Areas (TA) have been implemented to bring these developments into a broader context and to advance the five most important objectives of NFDI-MatWerk: (i) to integrate and include all stakeholders with our Community Interaction strategy (TA-CI); (ii) to provide a Materials Data Infrastructure (TA-MDI); (iii) to easily share Workflows and Software Developments in processing environments (TA-WSD); (iv) to provide and integrate a unified Ontology in Materials Science (TA-OMS) and to allow for a community-driven Strategy Development (TA-SD). As a result of this work, the main overarching achievements in NFDI-MatWerk have been in the following fields:

i) We have designed an NFDI-MatWerk infrastructure architecture (exemplary for NFDI) that combines all services developed in the TAs.

ii) We have achieved a seamless integration of the FAIR Digital Object concept, which will support the findability, sharing and reusability of data and computing resources.

iii) We have developed a consortia-overarching ontology (MWO), including relevant tools and services.

iv) We have established an integrated development for computational workflows, which ensures FAIR solutions for research software.

v) “The ELN Consortium” has been founded together with NFDI4Ing, NFDI4Chem and other international research data experts, which aims at improving the data exchange and interoperability between the different electronic lab notebooks (ELNs). For example, we actively contribute to the standardization of a common “ELN File Format”.

vi) A user-driven agile infrastructure development process has been established, allowing the community to participate in the effort (e.g., as expert, developer or Product Owner).

The biggest challenge for the next years of NFDI-MatWerk will be the roll-out of these solutions such that the individual scientist of the MSE community can see the added value for his/her daily research in the lab. To this end, the different services and task areas still need to be better interlinked, making them intrinsic part of an overarching strategy of NFDI-MatWerk.

3 Composition of the consortium

- Applicant institution

Applicant institution	Location	Duration
Fraunhofer-Gesellschaft zur Förderung der angewandten Forschung e.V.	Hansastraße 27 c 80686 München	10/2021 - today

- Spokesperson

Spokesperson	Institution, location	Duration
Prof. Dr. Christoph Eberl Deputy Director Fraunhofer Institute for Mechanics of Materials (IWM) https://orcid.org/0000-0001-9449-9583	Fraunhofer-Gesellschaft zur Förderung der angewandten Forschung e.V., Fraunhofer IWM, Wöhlerstraße 11, 79108 Freiburg	10/2021 - today

- Co-applicant institutions

Co-applicant institutions	Location	Duration
Deutsches Forschungszentrum für Künstliche Intelligenz (**DFKI**)	Stuhlsatzenhausweg 3 66123 Saarbrücken	10/2021 - today
FIZ Karlsruhe – Leibniz-Institut für Informationsinfrastruktur GmbH	Hermann-von-Helmholtz-Platz 1 76344 Eggenstein-Leopoldshafen	10/2021 - today
Forschungszentrum Jülich GmbH (**FZJ**)	Wilhelm-Johnen-Straße 52428 Jülich	10/2021 - today
Friedrich-Alexander-Universität Erlangen-Nürnberg (**FAU**)	Schloßplatz 4 91054 Erlangen	10/2021 - today
Karlsruher Institut für Technologie (**KIT**)	Kaiserstraße 12, 76131 Karlsruhe	10/2021 - today
Max-Planck-Institut für Nachhaltige Materialien GmbH (**MPI SusMat**) (formerly: Max-Planck-Institut für Eisenforschung GmbH, MPIE)	Max-Planck-Straße 1 40237 Düsseldorf	10/2021 - today
RWTH Aachen	RWTH Aachen University Templergraben 55, 52062 Aachen	10/2021 - today
Technische Universität Bergakademie Freiberg (TUBAF)	Akademiestraße 6, 09599 Freiberg	Left before project start
Universität des Saarlandes (**UdS**)	Campus, 66123 Saarbrücken	10/2021 - today

- Co-spokespersons

Co-spokespersons	Institution, location	TA(s)	Duration
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Prof. Dr. Matthias S. Müller https://orcid.org/0000-0003-2545-5258	**RWTH** Templergraben 55 52062 Aachen	Materials Data Infrastructure	10/2021 - today
Prof. Dr. Harald Sack https://orcid.org/0000-	**FIZ Karlsruhe** Hermann-von-Helmholtz-	Ontologies for Materials Science	10/2021 - today

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Prof. Dr. Martina Zimmermann https://orcid.org/0000-0001-5498-1340	**Fraunhofer IWS** Winterbergstraße 28, 01277 Dresden	Community Interaction	10/2021 - today

- Participants

Participating institutions	Location	Duration
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