Using ELN Functionality of Kadi4Mat (KadiWeb) in a Materials Science Case Study of a User Facility

PRACTICE PAPER

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ABSTRACT

In this paper, we introduce our approach in using the web-based application Kadi4Mat (KadiWeb) as an electronic laboratory notebook (ELN) combined with an integrated instrument database to facilitate Findable - Accessible - Interoperable - Reusabe (FAIR) research data. Facing transmission electron microscopy (TEM), focused ion beam (FIB), atom probe tomography (APT), or scanning electron microscopy (SEM) tasks, including sample preparation challenges, we developed a strategy to document the complex processes in our user facility KNMF[i]. To create appropriate records in Kadi4Mat we are comprising one central record for the material/sample to be investigated, a record for the sample preparation, a record for the investigation/experiment, and a record for the data evaluation. Therefore, a set of appropriate templates for the categories 'sample preparation general,' 'sample preparation for TEM,' 'Focused Ion Beam and Scanning Electron Microscopy,' 'Transmission Electron Microscopy,' 'Atom Probe Tomography,' and 'Data Evaluation' was developed in 'atomistic units.' The templates can be combined easily and have been designed to be user-friendly, but at the same time requesting the relevant metadata in a structured and standardized way. The documentation process, including MaTeLiS-instrument database, is demonstrated in a use-case with several sample preparation steps and different investigation methods. The developed templates can be exported in JSON-format and might be used as models for other tasks.

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1. INTRODUCTION

The Karlsruhe Nano Micro Facility (KNMF[i]) is a user facility, offering currently 23 different dedicated state-of-the-art technologies in three different Labs (KNMFi-Team, 2023). Instrument time for the different technologies must be applied for on a proposal basis. The benefit of such a user facility is that the proposer can request several technologies to measure, structure, or investigate the material (sample, device under test), or to develop process chains. For materials characterization, it becomes critical to track the material and all the applied process steps (synthesis as well as sample preparation). This enables correlation of the obtained results locally, as well as with respect to the timeline, the process chain, or with respect to the various applied technologies. After successful experiments, the user must publish results, and the delivery of FAIR research data (Scheffler et al., 2022; Wilkinson et al., 2016), in combination with the publication, is becoming more and more relevant. Implementing electronic laboratory notebooks (ELN) in an academic research environment, therefore, becomes more and more important (Higgins, Nogiwa-Valdez, and Stevens, 2022). They may record the experiments, provide metadata, manage data, share data with collaborators, and also archive data.

A broad variety of ELNs can be found via the ELN-Finder (TU Darmstadt), while rules and instructions on how to implement an ELN are given by Vandendorpe et al. (2024). ELNs are usually developed in the respective academic research fields or on a commercial basis. Each system has its own strengths and weaknesses. The Helmholtz Center Hereon developed and uses 'Herbie' in the field of metallic biomaterials (Helmholtz-Zentrum Hereon). The Research Center Jülich developed and uses 'Pasta-ELN' (Brinckmann, 2023) for application in materials science. The ELN 'openBiS' was developed by the ETH Zürich (Barillari et al., 2015; ETH Zürich Scientific IT Services), with a focus on biology. A recent paper also showed its application potential in materials science (Plass et al., 2023). eLabFTW is a commercial, flexible solution provided by Deltablot (Capri, 2017a, Capri, 2017b). Kadi4Mat is a development of the KIT (Kadi4Mat-Team, 2023), also with a focus on materials science. For chemists, the ELN 'Chemotion' (Bräse, 2024; Tremouilhac et al., 2017) developed at KIT is very well suited as ELN and as a repository. As all the scientific domains are very different, there is no 'one-size-fits-all' solution for an ELN. All systems mentioned here are open source. The choice of which ELN is used depends on the budget (for commercial ELNs), its availability in the research institution, the respective IT support in the institution, the easy-to-use features (usually, the scientists applying a scientific method/technology are not the IT-experts and programmers), and on its discipline focus. Therefore, we are using the web-based Kadi4Mat in our materials research-related environment. For specific experimental cases, workflows have been developed using KadiStudio (Al-Salman et al., 2023).

Modern scientific high-end instruments like Transmission Electron Microscopes (TEMs), Focused Ion Beam systems (FIBs), Atom Probe systems (APT), or Scanning Electron Microscopes (SEMs) are fully computer-controlled nowadays. Quite often, the instruments are equipped with additional detectors like Energy Dispersive X-ray spectrometers for EDS in TEM or SEM, Electron Energy Loss Spectrometers for EELS in TEM, Electron Backscatter Diffraction Detectors for EBSD or t-EBSD in SEM, or direct electron detectors for imaging. These scientific instruments then produce huge amounts of digital data (as images or spectra, mostly in proprietary formats defined by the instrument vendors) from all detectors and cameras, also containing metadata. The metadata describes the scientific environment and the instrument parameters used for the specific image or spectrum. To access that data, metadata extraction tools have already been developed for FIB and SEM images (Joseph et al., 2021). This extracted data can directly be integrated into Kadi4Mat records reducing the workload of the scientists. A similar tool for extracting metadata of TEM-images is currently under development (Aversa et al., 2023).

Nevertheless, quite frequently, conventional sample preparation like cutting, grinding, etching, or polishing is needed before the investigation in TEM or SEM. The necessary steps are performed manually or semi-automatically, and the instruments used for these processes quite often do not deliver any metadata at all. In these cases, exact documentation of all steps and parameters is necessary to produce reliable data and results according to the FAIR-principles (Scheffler et al., 2022). Using an ELN will then also facilitate the researcher to publish FAIR data, as it is mandatory from August 2023 on (Bender, 2023) for scientists obtaining public funding, e.g., from the German Research Foundation (DFG).

In this paper, we present our approach of using Kadi4Mat, the Karlsruhe Data Infrastructure for Materials Science (Kadi4Mat-Team, 2023; Selzer, 2022), as a web-based application and its functionality as an ELN in the environment of the user facility KNMF*i*. We developed a series of templates related to TEM/FIB/SEM/APT investigations, data evaluation, and sample preparation tasks. The single elements can be considered as 'atomistic' process steps, enabling a flexible combination to generate records like in a workflow. The first step always addresses general information about the proposal, the funding, and the data storage path. The information about the material to be investigated and the relevant instrument-specific information during the experiment/investigation is added subsequently. Finally, with the help of a use case and a real, practical example, we will demonstrate the easy-to-use creation of records, record organization, and generation of so-called 'knowledge graphs' to visualize the cross-linking of the records.

2. DESCRIPTION OF THE SCIENTIFIC ENVIRONMENT: TEM, APT AND FIB IN THE USER FACILITY KNMF*i*

The technologies 'Transmission Electron Microscopy,' 'Atom Probe Tomography,' and 'Focused Ion Beam' are part of the 'Laboratory for Microscopy and Spectroscopy' of KNMF*i*. TEM and FIB technologies are integrated into the 'Advanced Electron Microscopy in Materials Research' research unit (Kübel, 2023). We operate two transmission electron microscopes (ThermoFisher Themis300, ThermoFisher ThemisZ) with several TEM-sample holders available, three Dual Beam/Focused Ion Beam Systems (FEI Strata 400, Zeiss Auriga 60, Tescan Solaris X), and a sample preparation laboratory. Many different users operate our instruments, use our labs, or hand over the samples to us. Additionally, there is also intense interaction and collaboration with other KNMF*i* technologies, like Atom Probe Tomography (APT), nano Computer Tomography (nanoCT), or Photo Electron Spectroscopy (XPS).

In the 'Laboratory for Microscopy and Spectroscopy,' scientists and technicians work on a variety of projects. They mainly obtain samples from researchers stemming from different materials science and engineering disciplines, from different institutions and Helmholtz programs, and have different scientific questions to be answered. Documentation of the synthesis steps is beyond the scope of KNMF*i* and this paper. Examples for the variety of materials and scientific questions in the user-facility are high-entropy alloys (Dollmann et al., 2022; Taheriniya et al., 2023), metals (Kashiwar, Hahn, and Kübel, 2021; Hong et al., 2022), metallic glasses (Kang et al., 2023), catalysts (Prates Da Costa et al., 2023), battery materials (Wang et al., 2023; Pantenburg et al., 2023), (Ikram et al., 2019; Kroll et al., 2021) solid-state electrolytes (Ding et al., 2022), fuel cells (Léon, Schlabach, and Villanova, 2023), magnetic materials (Molinari et al., 2022), hybrid materials (Krüger et al., 2018), hydrogen storage materials (Jin et al., 2022), porous materials (Reinhardt et al., 2020), interfaces (Eusterholz et al., 2023), or biological materials (Barthlott et al., 2020). In an ideal case, the materials/samples to be investigated or prepared for investigation are well described and labeled, so that material/sample tracking is easily feasible. In reality, scientists often obtain samples just unimaginatively labeled like 'sample1,' 'sample2,' and so on, combined with only a little information about the material. This shows the necessity of implementing an electronic laboratory notebook strategy in the TEM, APT, and FIB labs of KNMF*i*.

Since the beginning of 2023, KNMF*i* requires the usage/implementation of an ELN for each technology. The ELN is supposed to be used to document experiments in a record, describe the used experimental method or equipment, store raw data, connect experimental results with the instrument used, and provide metadata. Furthermore, collaboration between different technologies of KNMF*i* (beyond TEM, APT, and FIB described in this paper), technology experts of the user facility, and collaboration partners from other institutions should be easily realizable. Taking into account the reasons mentioned in the introduction, Kadi4Mat (Brandt et al., 2021; Kadi4Mat-Team, 2023) as web based application (KadiWeb), running at the KIT+ instance, is the ELN of choice. This instance is also accessible to many external institutions collaborating with KIT (e.g., TU Darmstadt, RWTH Aachen, diverse Helmholtz Centers, diverse Max-Planck-Institutes, TU Munich, Marburg University, Nürnberg-Erlangen University, Ulm University, DLR, Fraunhofer Society, and many more). Upon request, users not belonging to one of these institutions can also obtain access.

Figure 1 exemplarily shows a constructed complex research scenario, which would be a typical scenario in the scope of battery materials synthesis and investigation. In this example, it also becomes apparent why sample names such as 'sample1' and 'sample2' are insufficiently unique. In such a research scenario, different technology experts/persons are involved.

For example, researcher A is synthesizing a high-entropy oxide material (HEO, named 'master batch') for use as an electrode material in batteries. This master batch material may be investigated as a starting or reference material using different technologies available at the user facility, like nano Computer Tomography (nanoCT), Scanning Electron Microscopy (SEM), and Electron Backscatter Diffraction (EBSD), X-Ray Diffraction (XRD), or X-Ray Photoelectron Spectroscopy (XPS), or Transmission Electron Microscopy (TEM). The samples for TEM-investigations in this example are prepared by FIB. All the experiments produce research data and metadata.

Researcher B uses the master batch material to assemble several battery cells. Here, further components like carbon binder, separator material, electrolyte type, incl. additives, counter electrode material, or battery housing type, and glove box conditions come into play. All steps and parameters have to be documented as accurately as possible. The cells may now be tested, e.g., by cyclic voltammetry, by impedance spectroscopy, or with respect to their electrochemical cycling performance, using different testing conditions. These investigations yield a large amount of data.

After electrochemical testing, the cells are disassembled in a glove box. The electrode material is separated from the current collector, rinsed, retrieved, and again analyzed by using the several methods mentioned before. With these experiments, structural or chemical changes can be identified, and the degradation behavior is examined. Therefore, it is important to know which testing step yields which cycled electrode material.

This virtual experimental setup shows the need for exact documentation for all steps and investigations and the need for sample tracking in all states. This can easily be realized when all involved researcher document and share their information in a common ELN. Only if all steps are documented precisely can all obtained data be correlated and used as FAIR data for scientific publication.

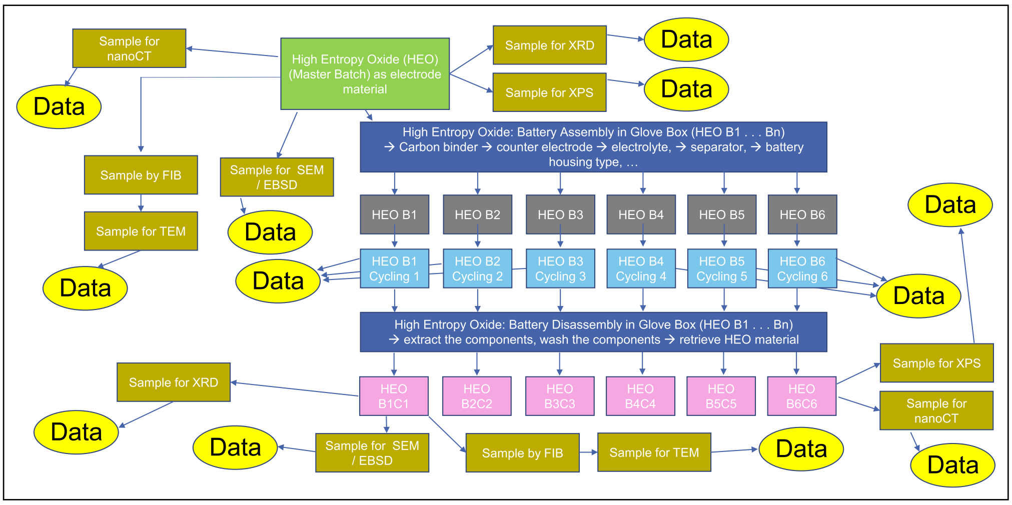

Figure 1 A virtual complex experimental setup for a typical materials characterization task in the field of battery research.

3. BASIC ELEMENTS OF KADI4MAT

3.1 RECORDS

The basic component in Kadi4Mat is the 'record'. It may be datasets on individual samples, on processing steps, on experiments, on measurements, or on program codes. The record consists of general metadata describing the record itself and additional so-called 'extra' metadata. The metadata are arranged by key/value pairs. These key/value pairs contain descriptive and specific metadata of the record. The following key/value pairs are available:

- String (text value)
- Integer (plus optional unit)

- Float (plus optional unit)
- Boolean (true or false)
- Date (date and time)
- Dictionary (can be used to combine multiple metadata entries under a single key)
- List (similar as dictionary, but values in the list have no key)

With these basic key/value pairs, it is very easy to create meaningful records. They can be structured uniformly for comparable scientific procedures. Additionally, research data (e.g., images, spectra, documents, drawings) or other data can be uploaded into the record. Tags and a label 'record type' can be added to each record to make filtering easier. The records can be linked, e.g., with an instrument record from the instrument database or with the material record, and grouped into collections. The records obtain a timestamp and a persistent ID, respectively. Permissions, defining the roles to access the record, can be set. Records can be exported in JSON, RDF (Turtle), PDF, QR-Code, or RO-Crate format. Each record obtains a time stamp and persistent ID to make it unique.

Records may have 'private' status (noticeable by a 🔒). In these cases, the record creator can give individual rights and group rights for access. If no rights are given, the record is only visible to the creator. Consequently, access to such entries will be lost when the creator leaves the institution, or the Kadi4Mat account of the creator changes. On the other hand, records may have 'public' status (noticeable by a 🔓). This means that everyone using the same Kadi4Mat instance has a 'read'-permission for the record. Nevertheless, a dedicated rights management is necessary to allow collaborators to edit, link, or manage records.

3.2 TEMPLATES

When records of the same structure for identical processes have to be created, it is meaningful to use templates. They are blueprints to represent similar metadata of repeating structures as key/value pairs. They are specifically designed for each intended purpose (device of the same category, experiment, protocol, dataset), requesting the relevant metadata in a structured and standardized way. In the case of the technologies TEM/FIB/APT/sample preparation, the MSLE ontology (Jalali et al., 2023), materials science vocabulary (Medina-Smith et al., 2021), and classical materialography vocabulary (Petzow, 1999) were used. Each template obtains a time stamp and persistent ID to make it unique.

There are two types of templates: the 'Record-Template' and the 'Extra-Template. The record template is to create a record and contains the record's own metadata plus an entity of generic 'extra' metadata, linked collections, and permissions. 'Extra-Templates' contain only generic metadata and can be loaded into a record or a template to extend the generic metadata field. Our templates contain mainly mandatory elements (values where an entry is mandatory) but also recommended elements (values where an entry is recommended but not necessary).

Templates may also have the status 'private' or 'public'. Here, the same rules for access management apply as for records.

3.3. COLLECTIONS, GROUPS, AND ROLE MANAGEMENT

Collections are simple and logical groupings of multiple records (e.g., instruments of a lab, results/datasets of experiments in a specific project, sample-related results). Sub-collections can be defined (e.g., a collection for a project, sub-collections for the individual materials, records assigned to the respective sub-collection). This facilitates collaborative working on a project. Additionally, a record can also be assigned to multiple collections.

Groups are lists of users (members), which can be defined according to their needs (e.g., group members, members of a specific research project, and administrators for instruments). Role management can be handled very easily in groups. Instead of giving access rights to records or collections to individual persons, access rights can be defined for a group (e.g., administrative rights for a limited group of persons). By adding or removing persons to or from the group, access rights are automatically updated.

The functionality of collections, groups, and role management will be explained in detail in the use case example.

4. THE MaTeLiS INSTRUMENT DATABASE

The KIT Center Materials in Technical and Life Sciences (MaTeLiS) integrates KIT research groups from the natural sciences, engineering, and life sciences, which share a common interest in material research and in the development of new materials. The ‘MaTeLiS’ Materials Device Pool (MaTeLiS-Team, 2023) is a searchable database of scientific instruments established in the data infrastructure Kadi4Mat. Within Kadi4Mat, each instrument is registered as a record with detailed information about the application area, system/instrument specification, and access possibilities. The records are classified according to their methods based on the MSLE-Ontology (Jalali et al., 2023). The sample preparation lab equipment for the steps like grinding, polishing, ion-polishing, etching, or ultramicrotomy is labeled as ‘lab-equipment’. The allocation is based on the classification of instruments and metallographic processes into ‘device types’ according to traditional metallographic preparation techniques described by Petzow (1999). The aim is to set up a KIT-wide searchable database of the preparation and analysis devices available in materials science and to make existing expert knowledge accessible.

Although this database is only accessible KIT-internally, the idea of having such a database integrated into an ELN structure might be of general interest. The database currently includes large-scale instruments and lab equipment for sample preparation with respect to the analysis/characterization of materials, and it is constantly extended. High-end instruments like TEMs, FIBs, or SEMs are labeled as ‘devices.’

The registered devices/instruments are fully described with metadata, and each instrument obtains a ‘persistent identifier’ to make it unique. Each record defines a unique instrument, as the serial number of the instrument is part of the metadata. The equipment registered in the Kadi4Mat Database provides a digital twin of the lab (Griem et al., 2022). Currently, the database is still under construction.

Figure 2 shows two knowledge graphs of two different device classes from the MaTeLiS database. Level 1 represents the basic level of the device class; level 2 shows more linked entries, partially even with linked experimental records.

An example of ‘devices’ from the MaTeLiS-Database is shown in Figure 3.

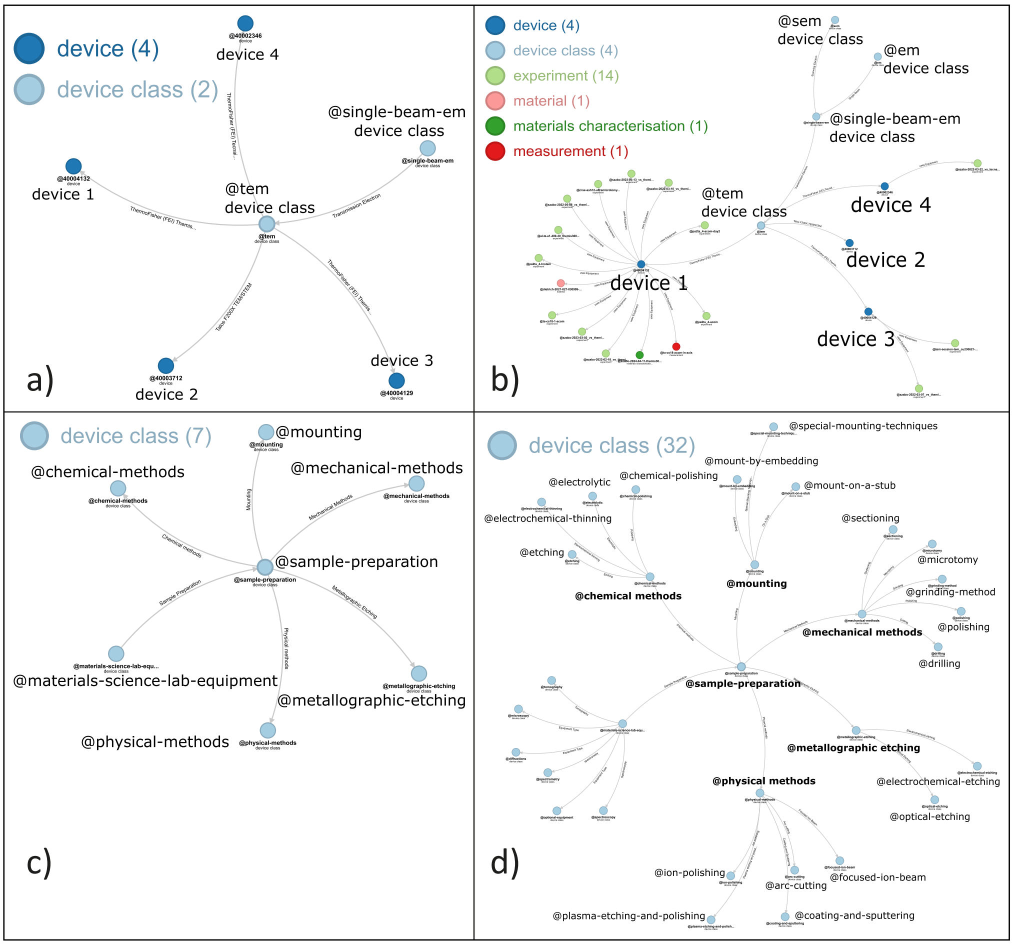

Figure 2 Knowledge graphs of the MaTeLiS Database. **a)** Device class ‘TEM,’ level 1, showing 4 devices in this category; **b)** Device class ‘TEM,’ level 2, linking the instruments to experiments; **c)** Device class ‘Sample preparation,’ level 1, showing the basic classification; **d)** Device class ‘Sample preparation,’ level 2, showing the links to several further sub-classes.

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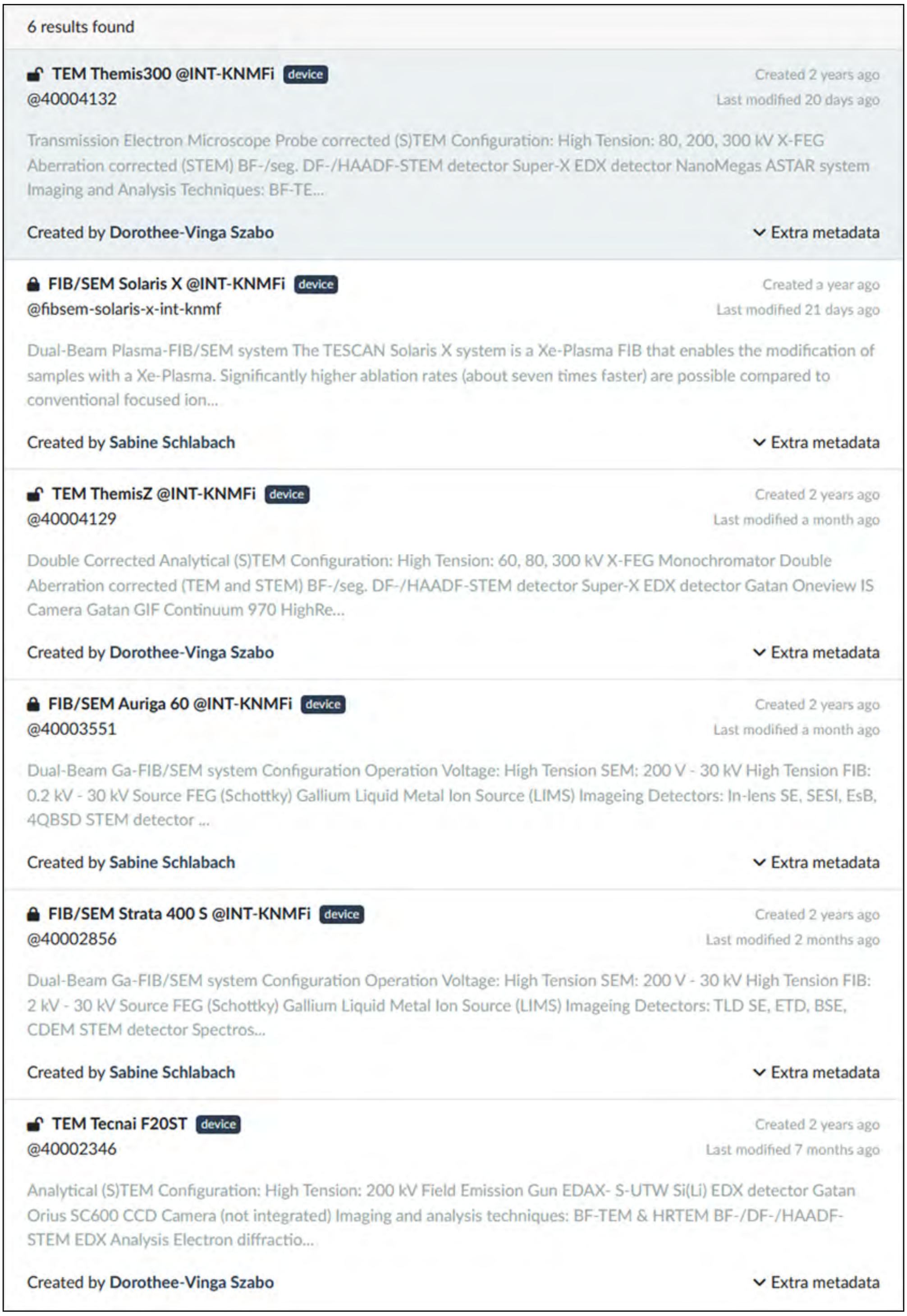

Figure 3 List of devices (Transmission Electron Microscopes, and Focused Ion Beam/SEMs) in the MaTeLiS database.

5. USE CASE EXAMPLE

5.1. METHODOLOGY FOR THE DEVELOPMENT OF TEMPLATES FOR THE TEM AND FIB LAB AT KNMF[i]

The idea behind the templates for the different steps in the TEM/FIB/SEM/or sample preparation environment is to create workflows by dividing the processes into 'atomistic units' of the steps (Brandt et al., 2021; Griem et al., 2022) and combining those steps in manifold ways. Additionally, the use of templates makes it possible to specify terms for recording metadata. This means that they are well-defined from the outset and easier to search later on. Regarding FAIR principles, this is of importance. The templates were created using the seven different key/value pairs described in section 3.1., and without programming knowledge. Only the understanding of the technology is needed to divide the processes into smaller steps.

The templates were structured as follows:

1. ‘Sample Questionnaire’ ‘record’ template

   This is the template to create a record of the type ‘Material’ or ‘Sample’ as a starting point for subsequent investigations, as in the TEM, FIB, and APT lab, we handle different materials/samples. Basic information about the proposal number, physical properties, and hazards of the material, storing conditions of the material/sample, and the planned investigations is requested from the proposer/user/material provider. In this record template, group rules for visibility of the records and administrative access have been predefined to ensure accessibility even when coworkers are leaving the group or the related institution. When a ‘Material’ or ‘Sample’ record has been created from this template, the Kadi4Mat-link of this record can be exported as QR-code. This QR-code can be printed, together with descriptive text, on a durable label, which is then used to mark the sample box.

2. Institutional relevant ‘record’ template header, to be used as starting point

   The record of every experimental process step starts with the very generic ‘record’ template, named ‘KNMFi-header.’ This is the starting template for the subsequent documentation for all sample preparation/experiments/measurements/or data evaluation steps. It contains the basic elements/metadata for our user facility (like proposal number, technology used, general funding information, and researcher). This metadata is important to be able to find records belonging to one project or one proposal. Also, in this template, group rules for visibility of the records and administrative access have been preset. This template must be combined with technology-specific ‘Extra’ templates. Figure 4 shows the general structure of this ‘KNMFi-header’ template. The upper part contains the general metadata of the record itself. A title and an identifier have to be given, and the record type (e.g., ‘Sample,’ ‘Material,’ ‘Experiment,’ ‘Data Evaluation’ or others) should be selected in the drop-down menu. A description of the record can be added. The lower part contains the fields with the specific metadata of the record. The experiment-specific ‘Extra Templates’ are inserted at the end of the template (+ Add extra ➔ select a template).

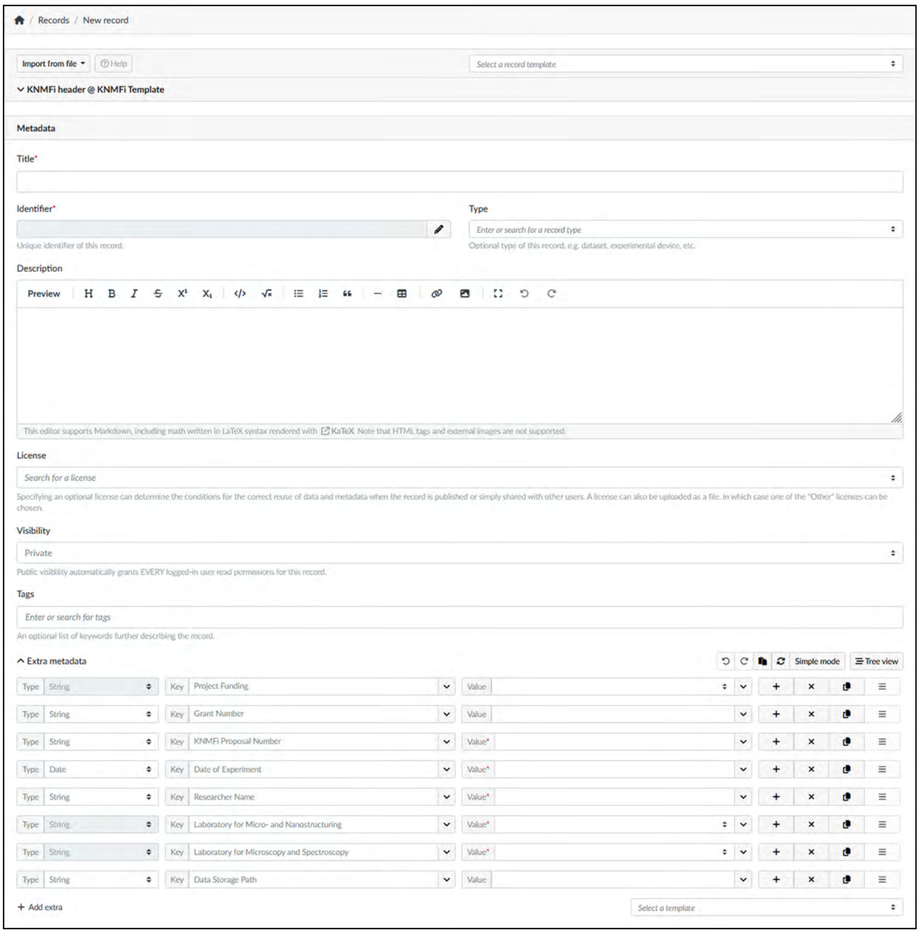

Figure 4 Details of the starting ‘KNMFi-Header’-Template when applied to create a record. The fields marked with a red ‘*’are mandatory fields.

3. Notional fragmentation of each technology/characterization method/sample preparation/data analysis step

For creating templates related to our experiments/investigations in the lab, all necessary process steps were analyzed (see Figure 5) and grouped into the categories 'Sample Preparation' with diverse sub-steps, 'Sample Investigation' with diverse investigation methods belonging to the respective technology, and finally 'Data Evaluation' with relevant sub-steps.

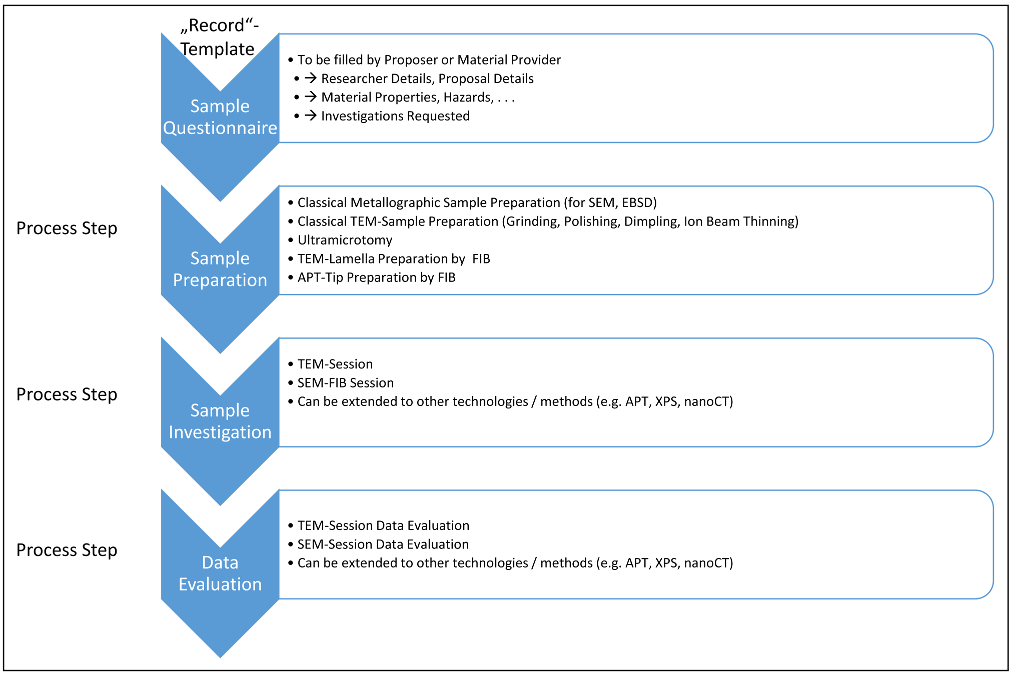

Figure 5 Overview of general process steps for a complete TEM/FIB/SEM-investigation. This corresponds to the first step of the notional fragmentation.

4. Division of process steps into technology-specific smaller units of the technology steps

The main parameters of each step, respectively sub-step, have been translated into key/value pairs to create the respective 'Extra-Templates.' The workflow is shown schematically in Figures 6 and 7.

   a. Creation of a 'master' template with general technology-specific information for each technology or main process step

The experiment-specific 'Extra' Master-Template has to be added, where the basics of the experiment are retrieved (e.g., which instrument is used, which holder is used, which acceleration voltage is used in case of TEM or FIB).

   b. Creation of 'sub-templates' for the technology-specific sub-methods

Special experiments such as element analysis, special crystallographic experiments, tomography, or *in-situ* experiments can be added with the appropriate 'Extra' Sub-Templates. As each investigation is very individual with respect to the working steps, the 'atomistic' units of the steps allow a versatile and individual combination of the single steps. With this practice, a sort of flexible workflow can be established.

5. Combination of the appropriate templates to create a record

For the documentation of the whole experimental process, one starts with the KNMFi-Header 'Record' template, inserts the technology-specific 'Master' Extra template, followed by the experiment-specific 'Sub' Extra-templates.

Files can be uploaded once a record is created.

6. Linking the records with the devices/lab equipment records from the MaTeLiS database and with the sample questionnaire record

In this documentation step, records can be linked (e.g., instruments used with the 'experiment'-record, or 'experiment' record with the 'data-evaluation' record, or 'experiment'-record with the 'material' or 'sample'-record). Then, sample tracking is possible, and even very complex connections can be visualized by using the knowledge graphs.

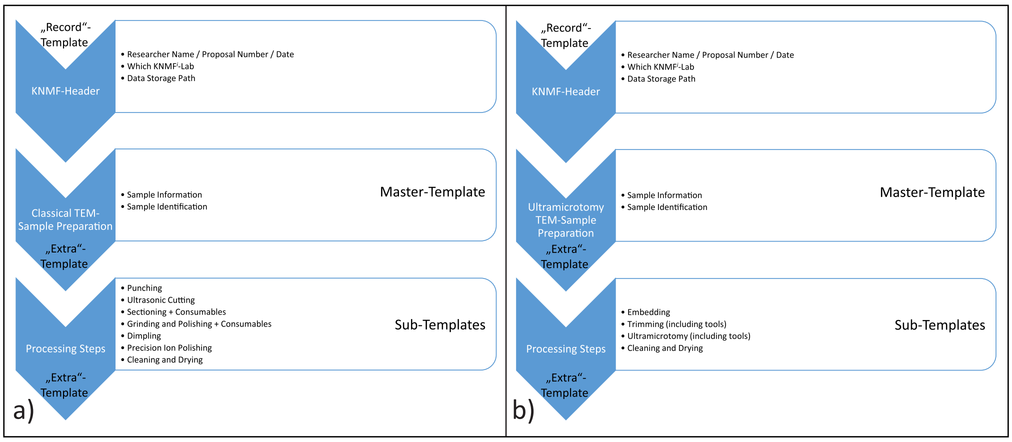

Figure 6 Workflow for classical TEM-sample preparation **(a)**, and TEM-sample preparation by ultramicrotomy **(b)**. The steps are the basis for the developed templates and correspond to the further division into sub-steps.

Especially for the manual processes of classical TEM-sample or metallographic sample preparation, flexible but reliable documentation is important. Most of the instruments (like the saws, the polishing and grinding instruments) are 'manually'-controlled, meaning that they generate no metadata. Some process steps (like 'Sectioning' or 'Grinding') are used as well as in classical TEM-sample preparation as well as in metallographic sample preparation. In addition, 'Cleaning and Drying' is a process that will be used for several process steps in classical sample preparation or ultramicrotomy, e.g., after any mechanical treatment. Therefore, a template used for this process step will only exist once and can be integrated easily at any place where needed. Figure 6 shows exemplary workflows for classical TEM-sample preparation (a) and ultramicrotomy preparation (b). For the documentation of a FIB or TEM session, the procedure is analogous. One starts with the KNMFi-Header 'Record' template, adds SEM/FIB or TEM-session Master 'Extra' template, and integrates the specific Sub-Templates of the experiments done. This is shown schematically in Figure 7.

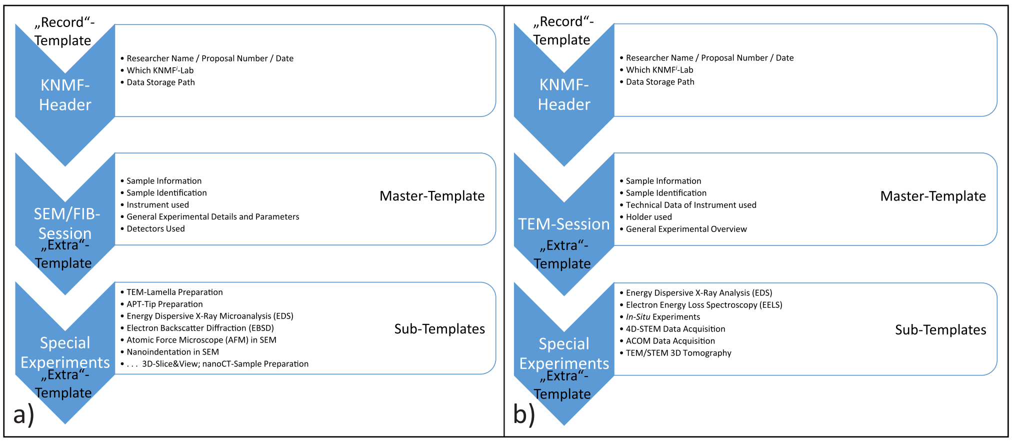

Figure 7 Workflow for an SEM/FIB session **(a)** and a TEM session **(b)**. The steps are the basis for the developed templates and correspond to the further division into sub-steps.

Templates for metallographic sample preparation, light microscopy, SEM or EBSD investigations or APT- investigations, and data evaluation are structured in a similar fashion. The created records can then be linked together (instrument used-material-experiment-data evaluation) to generate knowledge graphs of the whole experiment chain. It is also possible to upload data files to the records.

With this concept, it is easy to integrate 'Extra'-Templates for other technologies (like nanoCT or XPS) or to create a 'Record'-Template similar to 'KNMFi-Header' to the needs of other research structures. The templates can be exported into JSON-format and thus made available to other scientists and institutions. Those institutions running Kadi4Mat on another instance can easily import and then modify our templates.

5.2. PRACTICAL EXAMPLE

This practical example demonstrates how the developed templates described prior are used in a DFG-funded project for documentation of the experimental steps and sample tracking. The collaboration partner synthesizes the starting material, which is then handed over to the scientist, and characterizes the materials using various KNMF[i]-technologies. For each material handed over, a 'sample' record is created. From the main sample, sub-samples for SEM and EBSD measurements are prepared by the scientist using mechanical and physical methods. APT-tips and TEM-lamellae are prepared for detailed analysis from selected regions using FIB. These preparation steps are documented in records of the type 'sample preparation'. The final samples are then characterized by SEM/EBSD, APT, and also by TEM. These investigations are documented in records of the type 'experiment.' The created records are structured in a main collection and child collections, as shown in Figure 8.

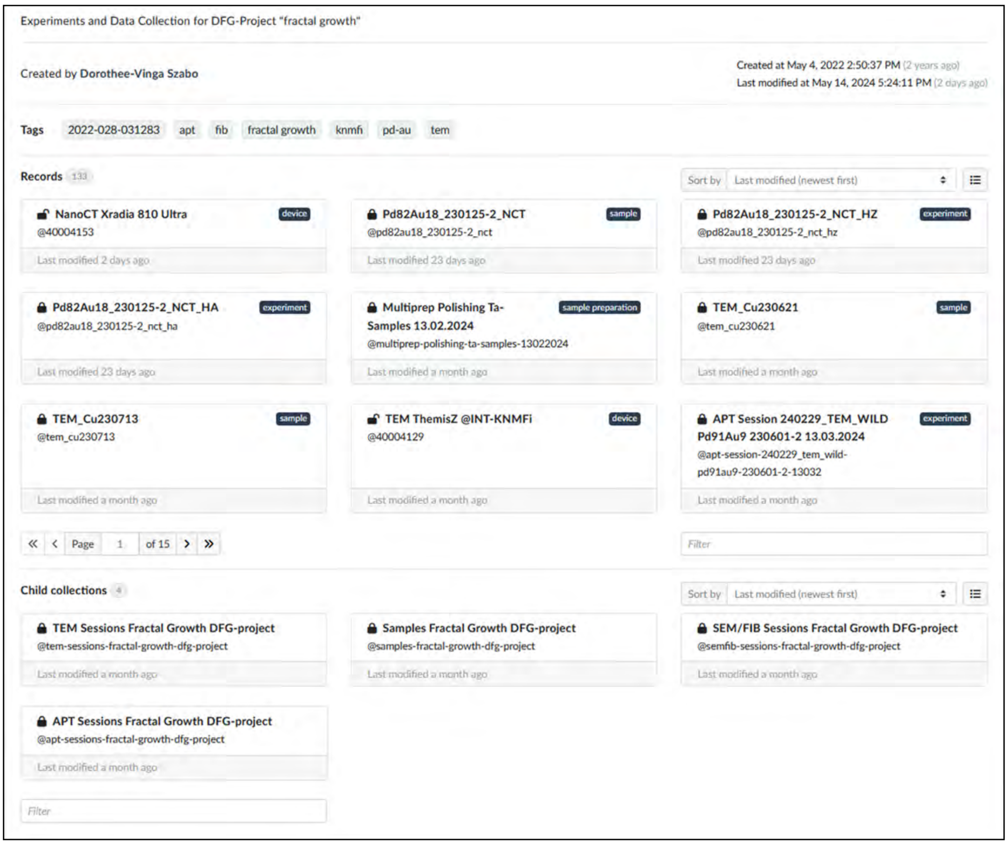

Figure 8 Records and child collections in the DFG-project collection described.

A group of persons (collaboration partners) involved in the project was created. Within this group, individual templates, records, and also collections are shared. The group creator automatically obtains an 'Admin' role. The group creator can manage the members of the group and their rights with respect to the group. In this example, the status of the collections is set to 'private', and access to the collaborators is granted via role manag ement.

The records are linked with the respective instruments/devices/lab equipment records from the MaTeLiS database and with the 'Material' or 'Sample' record. Thus, this is quite a complex research scenario, where different technologies and methods play a role, and where it is important not to lose an overview of samples/experiments/data and their interrelation. An example of interlinked records is shown in Figure 9. The knowledge graph is the visualization of the very complex relations that exist between the 133 records of the project. It can easily be seen, that

- one single 'sample' was not used yet for any experiment (single dot, no links to other dots),
- a few samples have only been used for a low number of experiments (only a few links),
- that four devices are used as experimental equipment
- that two lab-equipment instruments are mainly used for sample preparation
- that the focused ion beam device is used for many experiments

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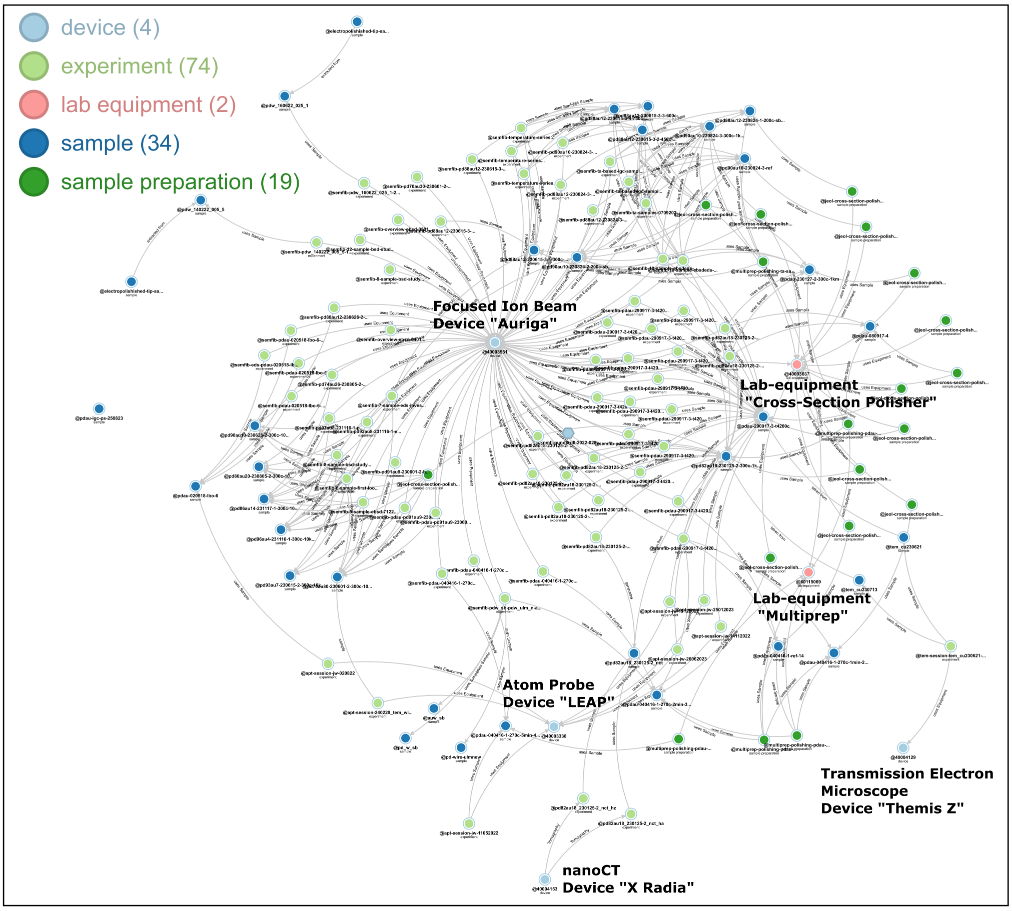

Figure 9 Knowledge-graph of record links created in Kadi4Mat for the collection discussed in this paper. Light-blue spots represent the used devices (TEM, FIB, APT, nanoCT), the light-red spots represent the used lab equipment, the dark blue spots represent the registered samples, dark-green spots are related to sample preparation, and the light-green spots represent the records of performed experiments.

6. CONCLUSIONS AND OUTLOOK

In this paper, we showed a use case for the application of Kadi4Mat (KadiWeb) as ELN in a user-facility environment. The processes for the experimental steps in transmission electron microscopy (TEM), atom probe tomography (APT), and focused ion beam (FIB), including traditional sample preparation steps in a metallographic lab, were analyzed and translated into key-value pairs to create the respective templates. This is easily feasible without programming knowledge.

The MaTeLiS instrument database in Kadi4Mat is a useful tool that enables to find instruments in our institution and to link the used instruments to an experiment.

In an application-related practical example, we showed the way how the developed Kadi4Mat templates can be used for the documentation of experimental procedures in the TEM, APT, and FIB environment and how the MaTeLiS instrument database is integrated into Kadi4Mat. Experimental data can easily be added to the records. This enables FAIR data publication.

The developed strategy can be extended to other KNMF[i]-technologies. The templates are general for their specific subject and can easily be adapted to be used in a broader scientific community for general materials science characterization issues in other scientific institutions. This is also a step towards open science.

With our templates, a basis has been created so that a transition to KadiStudio (the desktop-based software version of Kadi4Mat, which allows the formulation and execution of workflows) should also be easily feasible in the future. Research value is expected in the long run, as research data will be documented in a structured and FAIR way. Our approach may serve as a model for other researchers on how to apply an ELN.

Our practical experience shows that there are still open issues e.g., the interaction with other ELNs. In addition, a deep understanding of which parameters are relevant for reliable documentation of an experimental process, especially manual processes, is important. Therefore, optimization and completion of workflows are still in progress. It is also very important to think about how to structure and organize records and how to link the records together, not just produce records.

In the future, a direct connection of the high-end instruments to an ELN with direct transfer of instrument metadata is desirable. This would reduce the workload of scientists and also increase the acceptance of ELNs.

DATA ACCESSIBILITY STATEMENT

The templates developed in the framework of this study and the original images are available under https://doi.org/10.5281/zenodo.11234285.

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COMPETING INTERESTS

The authors have no competing interests to declare.

AUTHORS CONTRIBUTIONS

SSch: Template strategy and development, conceptualization of the paper, manuscript writing, review, and editing.

JW: Template development, data curation, manuscript writing, review, and editing.

OP: MaTeLiS database development, manuscript writing, review, and editing.

MS: Kadi4Mat development, manuscript writing, review, and editing.

DVS: Template strategy and development, conceptualization of the paper, manuscript writing, original draft preparation, review, and editing.

No AI tools were used in the writing of this text or the generation of graphics used with it.

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