

Ontology Modelling for Materials Science Experiments

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Abstract. Materials are either enabler or bottleneck for the vast majority of technological innovations. The digitization of materials and processes is mandatory to create live production environments which represent physical entities and their aggregations and thus allow to represent, share, and understand materials changes. However, a common standard formalization for materials knowledge in the form of taxonomies, ontologies, or knowledge graphs has not been achieved yet. This paper sketches the efforts in modelling an ontology prototype to describe Materials Science experiments. It describes what is expected from the ontology by introducing a use case where a process chain driven by the ontology enables the curation and understanding of experiments.

Keywords: Materials Science, Ontology Design, Data Curation

1 Introduction

The discipline Materials Science and Engineering (MSE) promises solutions to modern societal challenges, including climate change and resource scarcity. However, the complexity of the lifecycles of materials and their diversity poses several challenges in the management of materials' knowledge for a comprehensive sharing and understanding among various MSE disciplines.

Many experiments are conducted to study materials' behavior, which generates a variety of data, describing manufacturing process settings, material properties, material structures, and further MSE parameters. The sharing and interoperability of MSE findings are mainly achieved through the exchange of not standard and often not well-documented files [2]. They are often hardly processable and understandable by humans and machines, thus limiting the potential to support all stakeholders in their tasks. Therefore, modelling MSE data with formal semantics is crucial to consider a variety of MSE facets (e.g., multidisciplinary or spatial inhomogeneity) to provide a better understanding and support for the creation of new materials. A common and shared representation

for material knowledge in the form of taxonomies, ontologies, and knowledge graphs has not been achieved yet. Challenges arise in the representation of dynamic events that occur when materials change their state due to manufacturing processes [5]. In this paper, first insights about the semantics of MSE ontologies for material transformations that came up within the *Plattform MaterialDigital*⁶ project are presented; more specifically, the paper addresses the following research questions by discussing an ontology prototype:

- RQ1: How can ontologies represent and describe MSE process chains?
- RQ2: How can ontologies guarantee MSE data consistency?
- RQ3: How can ontologies support MSE experts to fully represent changes of material structures and material properties?

2 Related Work

Existing attempts try to represent top-level knowledge about materials properties and structures [1] with the objective to enable seamless data integration and sharing [6]. Recent ontologies are paving the road for the MSE data interoperability by providing a common ground to describe materials. For example, this challenge is currently being addressed by several communities including the European Materials Modelling Council⁷ (EMMC) which develops the European Materials & Modelling Ontology⁸ (EMMO) [3] an ontology developed to describe classical and quantum physics. It focuses on high-level properties of materials and manufacturing processes, and extensions to model specific use cases are required. A more recent effort in the MSE domain is given by the Materials Design Ontology (MDO) [2] which has the objective to make different outcomes generated by calculations interoperable. MDO introduces relations between materials' properties and materials' structures, but does not relate their transformations to process parameters. Hence, the description of materials manufacturing might result incomplete. Thus, the existing models can only ensure a limited formal description about material transformations, which is one of key aspect for new materials' generation. The proposed work aims to extend existing efforts, augmenting them with semantics to model material transformations.

3 Scenario and Vision

Imagine having a process chain. An object undergoes processes that transform the object's material structures and material properties (Figure 1). In this scenario, it is crucial to track how processes are performed and how objects change when describing material transformations. In detail, transformative processes (e.g., manufacturing processes) lead to changes in objects' status (i.e., material properties and material structures) according to their individual process parameters, thus creating new object entities as an output. Figure 2 shows a high-level

⁶ <https://materialdigital.de/>, accessed on June 10, 2021

⁷ <https://emmc.eu/>, accessed on June 10, 2021

⁸ <https://github.com/emmo-repo/EMMO>, accessed on June 10, 2021

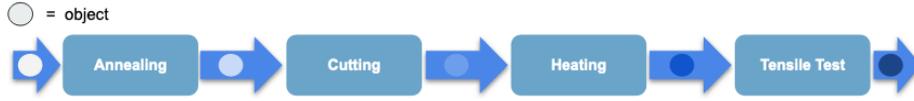


Fig. 1: A process chain with four processes.

sketch that represents the main top classes and object properties of the ontology under development. Every process comes with its own parameters that represent all the required variables. Processes that can transform material structures are represented by the class `pmd:ManufacturingProcess`, processes which perform analysis are represented by the class `pmd:AnalysisProcess`; however, they can still transform the object (e.g., a Tensile Test process), and therefore, they might also be transformative. Process parameters might have various effects on the materials and, therefore, the relations between processes to material structures are required. This can also be done at different granularity levels (e.g., nano, microscopic, mesoscopic, etc.) depending on the requirements of the application scenario. For example, the problem of locally heterogeneous materials in an object requires separating the object into a certain number of volumetric sub-areas made by the same material (`pmd:Material`), so called voxels (`pmd:Voxel`). Therefore, the voxel becomes the object of the ontology and describes the conditions of the material with its individually experienced process parameters. Object properties are defined to describe how `pmd:Process` modifies `pmd:MaterialStructure` affecting `pmd:MaterialProperty`, thus allowing machine and humans to understand what is performed in the experiment.

4 Practical Use of the Prototype Ontology

MSE ontologies will enable MSE scientists to curate, describe, share, and optimize experiments. An application example is given in Figure 3. There are 2 processes: c_0 and h_0 instances of `pmd:Cutting` and `pmd:Heating`, respectively.

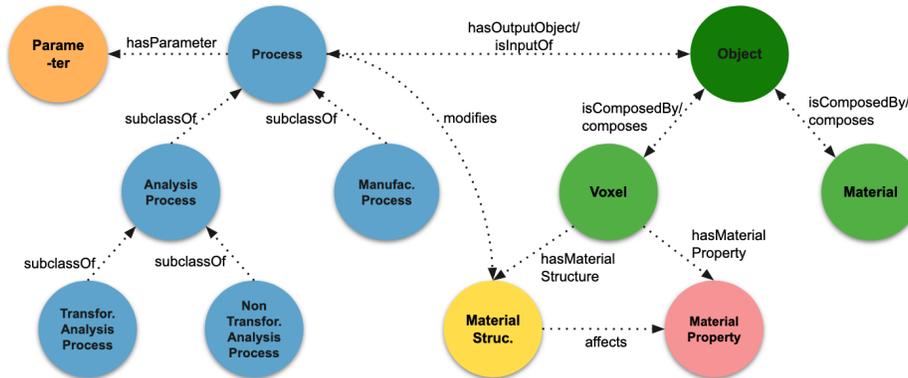


Fig. 2: Visualization of the main elements that constitute the ontology.

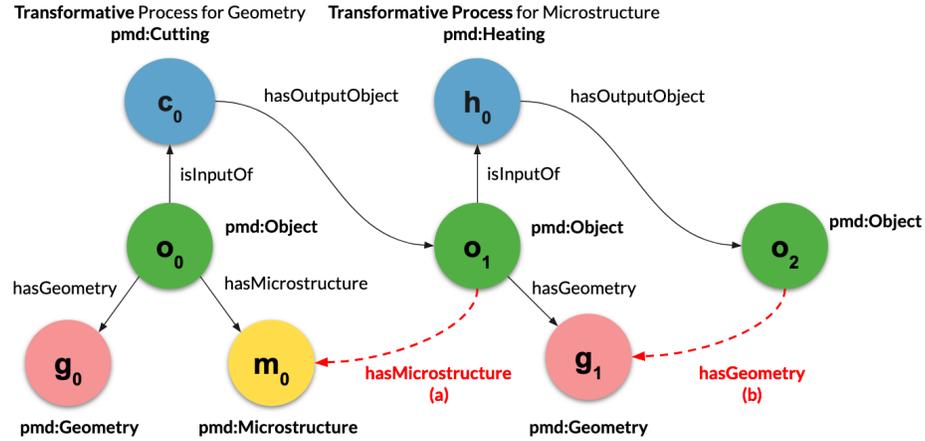


Fig. 3: Material structures and properties preservation in a process-chain.

There are 3 `pmd:Object` namely o_0, o_1, o_2 ; o_1 is originated from o_0 and o_2 is originated from o_1 . o_0 has a `pmd:Geometry` g_0 and a `pmd:Microstructure` m_0 . In the example, `pmd:Cutting` class represents cutting processes that are transformative for the geometry, `pmd:Heating` processes that are transformative for the microstructure. When o_0 undergoes c_0 , it is transformed in o_1 ; since c_0 does not transform the microstructure, it is preserved in o_1 (edge *a*). However, o_1 will have a different geometry i.e., g_1 . When o_1 undergoes h_0 , it is transformed in o_2 . In this case, the geometry is not transformed and, therefore, o_2 has the same geometry of o_1 i.e., g_1 (edge *b*). Thus, the preservation of material structures and material properties can be defined by means of description logics and Semantic Web Rule Language (SWRL) rules, which enable automatic reasoning on experimental data, e.g., to find inconsistencies. For example, an object with a different microstructure after a cutting process raises an inconsistency. At the same time, this semantics helps to create connections between objects involved in a process chain, thus enabling reasoning on the process-object relations (e.g., an object after a cutting process preserves its microstructure). The reader can find the prototype ontology as well as the SWRL rules used by this practical application in GitHub⁹.

5 Insights from the proposed prototype

The presented prototype provides a modelling philosophy to describe process chains. Furthermore, it shows how Materials Science semantics can be injected into a formal model to represent material transformations. The prototype addresses the RQs by providing the following insights.

RQ1. The ontology prototype includes the first efforts to represent core elements (`pmd:Process`, `pmd:Object`, `pmd:MaterialStructure`, `pmd:MaterialProperty`,

⁹ <https://github.com/ISE-FIZKarlsruhe/pmd-onto-poster>

etc.) and their relationships that a MSE ontology must represent in order to describe MSE process chains.

RQ2. The semantics within the model shows how data consistency can be obtained. More specifically, this is shown by propagating material structures and material properties through SWRL rules. If a user injects erroneous data (e.g., a different microstructure for an object after a cutting process), the reasoner is able to spot the introduced error.

RQ3. The prototype ontology provides the semantics to reason on experiments, and links objects to material structures and material properties that are not directly generated by the experiment itself, and thus supports MSE experts in fully representing and understanding material transformations.

6 Conclusions and Outlook

This paper introduces the vision to model process chains and MSE experiments through an ontology with the long term goal of studying material transformations. It provides three RQs that are driving the research and shows an ontology prototype. Perspectively, the data modelled by specific use case ontologies will enable the curation and preservation of data as well as the possibility to interpret various outcomes. These ontologies are being developed within the *Platform MaterialDigital*. They will enable a substantial step towards the provision of findable, accessible, interoperable, and reusable [4] MSE data.

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