Towards Digitizing Physical Entities in Materials Science

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Abstract. Materials are either enabler or bottleneck for the vast majority of technological innovations e.g., fighting climate change or resource scarcity. Efforts for digitizing materials and processes have recently become mainstream. However, open challenges in the digitization of Materials Science and Engineering (MSE) involve the multidisciplinarity of the field, the nonlinear multi-scale structure-properties relations, and the spatial inhomogeneity of the material in a component. For addressing these challenges the scientific community has recently been mobilized to create material digital representations and models which are able to describe materials changes (e.g., physical), and at the same time allow to reconstruct all structural levels of the materials. A common standard formalization for materials knowledge in the form of taxonomies, ontologies or knowledge graphs has not yet been achieved. This paper sketches the process-structure-property dependencies for a simplified use-case of tensile testing and the evaluation of the mechanical properties of elements from a cast component. It describes first steps towards designing a domain ontology and the ontology design challenges posed by the domain of Materials Science.

Keywords: Materials Science, Ontology Design, Data Integration

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 materials' life cycles and their diversity pose a challenge in the field of MSE. Aims, such as accelerated materials development, flexible production as well as efficient component use in future applications will require a change in how we manage knowledge about materials.

Many experiments are conducted to study materials' behavior, generating a huge amount of data that describes the variation of their properties throughout

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specific processing chains. For example, a heat treatment can be described as a sequence of the sub-processes annealing, quenching and aging. Each of these sub-processes has an effect on the material's inner structure and thus its properties, which can be described on different granularity levels:

- The *continuum* level, which includes the entire geometry consisting of a specific material,
- the *mesoscopic* level, including multiple grains,
- the *microscopic* level, looking at single grains,
- the *nano* level, involving individual features like dislocations,
- and the *atomistic* level, referring to the atomic structure of the constitutional matter.

Modelling this data with formal semantics is still an open challenge within the field of MSE. In datail, one must consider numerous facets such as multi-disciplinarity or spatial inhomogeneity, which make it difficult to come up with standardized models. In addition, challenges arise in the representation of dynamic events that occur when materials change their state due to manufacturing processes. Existing models usually include analytical equations, numerical models or are implemented into data driven material models. However, efforts which have been undertaken to introduce digital representations are typically non-standard, and often rely on single implementations, which are difficult to maintain and reuse over time. More precisely, a common standard representation for material knowledge in the form of taxonomies, knowledge graphs, or in well defined and formal data structures has not been achieved yet. Currently, the literature provides MSE knowledge exclusively without a defined and clear structure, and thus takes a certain human effort for its employment within modern technological infrastructures. Resulting information given by plain text is hardly processable by machines since it is not stored in a structured way and presents issues related to the ambiguity of the natural language. In a world with ever growing masses of knowledge, a standardized way for its explicit representation is hence highly necessary.

Representing knowledge by means of formal symbolic representations (e.g. ontologies) allows structured digitized information, which may be made available for queries by experts, enabling the sharing and reuse of knowledge about material transformations within manufacturing processes. For example, a query can be a request of material information at any desired position of the component linked to process parameters including the entire workflow and covering all available material properties. The basic purpose of a formal representation in MSE is therefore to provide comprehensive material data at varying positions of a component and link this data to the process history, which the material has experienced at this particular position. Perspectively, the resulting comprehensive data querying provides a chance to feed increasingly more sophisticated statistical applications, such as machine-learning, for deriving completely novel scientific insights [7].

In this paper, we introduce our first efforts within the project Platform MaterialDigital[5] (PMD). We aim to design and implement an ontology for MSE, which regards processes and their effects on different materials granularity levels in order to model and make structured data about materials and experimental results through semantic technologies available. More precisely, in this work, our goal is to model the semantics behind a specific use case of the multidimensional interaction between material-changing processes and material properties. Furthermore, this paper reports the experience between ontology and MSE experts to even learn how to jointly enable the creation of such a formalized structure in the most effective and appropriate way.

To sum up, the contribution of this paper is twofold:

- We describe our methodology to model the workflow of the manufacturing process of a component and the subsequent specimen extraction for a tensile test by semantic technologies.
- We discuss open issues and possible solutions for modelling materials and processes with ontologies.

This paper is structured as follows: Section 2 gives an overview of existing efforts towards a unified ontological description for the MSE discipline. Section 3 continues by thoroughly describing the aimed use case that we consider for developing an application ontology. Section 4 describes the modelling constraints and system boundaries of this use case for representing the regarded MSE characteristics. Section 5 closes and points to our future work.

2 Related Work

In the last years, there have been already attempts on the development of ontologies, taxonomies and metadata schemata for the Materials Science field. For example, authors in [4] have developed the MatONTO ontology aiming at representing materials, properties, structures, and processes stages involved in materials engineering. MatONTO is developed upon DOLCE [6] a top ontology enabling its reusability and cross-domain integration. Moreover, it leverages some of the already existing domain ontologies [8] by extending it and combining its concepts into a common semantic framework. In [9] the authors developed MatOWL ontology based on the MatML schema to enable a seamless data integration and sharing. In [2], the authors developed the Materials Ontology (MatOnt) specific to material representation including the material and manufacturing processes. The Tata Consultancy Services[6] developed the Premap ontology [3] in order to support the designing of manufacturing processes, and identification of optimal design of parameters to ensure satisfaction of products specifications. However, these efforts do not always comply with the scope of an ontology which entails the adoption of standardized rules and logics, formalisms, common conceptualization and strong classification and typing, posing a challenge in terms

[5] https://www.material-digital.de/

[6] https://www.tcs.com/

of interoperability. This issue is currently being addressed by several communities including the European Materials Modelling Council[7] (EMMC) and the Research Data Alliance[8] (RDA), which are making efforts towards a common standardization in Materials Science. In particular, EMMC has developed the European Materials & Modelling Ontology [9] (EMMO) that provides a common semantic framework for describing materials, models and data with the possibility of extension and adaptation to any other domain of interest. However, the current version of EMMO focuses on high level properties of materials and manufacturing processes, and novel ontologies or extensions to model specific use cases are required. In particular, EMMO is not well suited to be employed to query information systems in order to retrieve material information about properties in relation to specific manufacturing processes parameters. It's underlying topdown design approach based on the Basic Formal Ontology (BFO) as an upper ontology impedes query efficiency [1]. Therefore, in this introductory work we present our bottom-up approach describing which are the challenges in representing low level properties of materials and their changes when materials undergo manufacturing processes.

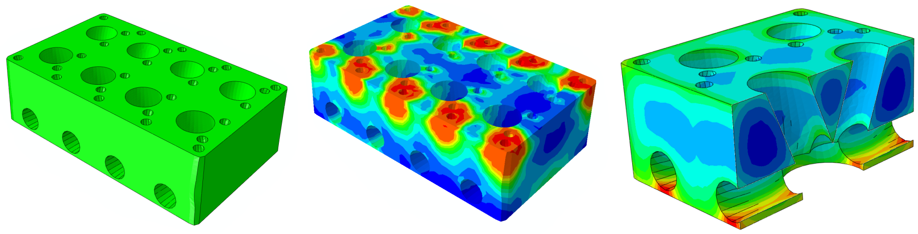
3 Use Case Scenario

Our considered use case covers a chain of material-relevant processes starting from a casted wrought material via the heat treatment up to a tensile test conducted at a specimen extracted from a ready-to-use cylinder head of a car engine. The component's material is assumed to be the hardenable aluminum alloy AlSi7Mg (EN AC-42000).

Figure 1(a) shows the facilitated model of the considered 4-cylinder double overhead camshaft engine. The cylinder head is mounted on top of the engine block and contains the intake and exhaust valves, which act as a sealing cap to the cylinder during the combustion cycle. At the top of the cylinder head, two camshafts are mounted which manage the timing of the valves. The camshafts are not displayed, but their forces are modelled to the respective boreholes of the camshaft mount. Accordingly, the maximum in-service stresses occur at so called hotspots, which are located in the area near the camshaft mount and the boreholes of the mounting bolts of the cylinder head to the engine block. They are derived by a basic finite element simulation (see Figure 1(b)). Generally, a tensile test is aiming to gather the material's mechanical properties at these hotspots to allow for an accurate fatigue assessment of the component.

In some cases it may be difficult or impossible to access the material properties at these hotspots due to the geometric requirements of the standard tensile test specimen. Therefore, the mechanical properties can be derived by interpolation or extrapolation of testing results at different positions of the component. Due to the variation of locally experienced process parameters throughout the

[7] `https://emmc.info/`
[8] `https://www.rd-alliance.org/`
[9] `https://github.com/emmo-repo/EMMO`



(a) (b) (c)

Fig. 1. (a) Schematic model of a cylinder head of a common DOHC car engine. (b) Simulated in-service stresses of the cylinder head model. (c) Exemplarily, temperature field in the cross section of the cylinder head model during the heat treatment process.

component, the respective material properties are assumed to be heterogeneous. Exemplarily, Figure 1(c) shows the temperature field of the component during the heat treatment process, as indicated by the rainbow spectrum. The locally experienced temperature history of the material diverges significantly not only from the nominal temperature of the oven but also of the average temperature of the component, which therefore leads to locally individual material properties. This example illustrates the complexity of a comprehensive description of process parameters and the according challenge of data gathering and distinction.

Tensile tests are a frequent and well understood materials testing and characterization method. A specimen of defined material and standardized geometry is elongated up to its rupture. The history of the reaction force and the elongation during the tensile test are the basis for the resulting stress-strain curve. The stress-strain curve, as shown exemplarily in Figure 2, gives access to relevant information about the material's mechanical properties such as its Young's modulus, yield strength or ultimate tensile strength, which are important for component manufacturers and designers of any industrial background. When interpreting the mechanical properties determined by the tensile test, previous workflow steps of the component's lifetime must be considered. Variations within the component's manufacturing process lead to varying material properties.

Overview of considered process and system boundaries: For the cylinder head's manufacturing, we consider the material to be in a post-casted state and disregard any variations in commodity sourcing, which may also have an influence on the materials properties . The specimen's workflow involves the following processes (semantic concepts to be included in the ontology are exemplarily given in cursive):

- *Heat treatment* of the component is supposed to optimize the material's *structure* and thus its *properties* (for example to increase the *tensile strength* by *precipitation hardening*). A heat treatment consists of further sub-processes:
  - *solution annealing*, alloying elements are dissolved at high temperature.

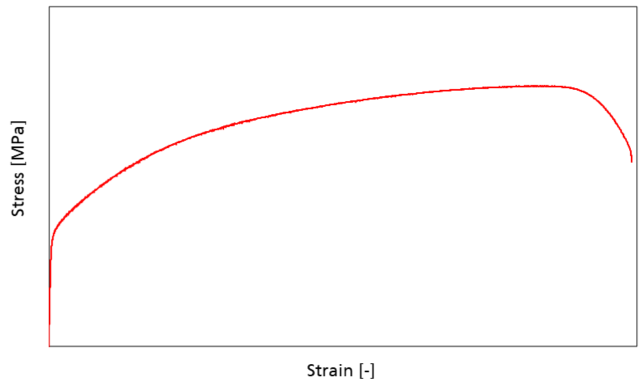


Fig. 2. Example of a stress-strain curve.

  - *quenching*, fast cooldown to room temperature, generally by water.
  - *aging*, storage at room temperature or at moderate higher temperature to enable segregation processes.
- *Specimen extraction* from the ready-to-use *component* and its processing to a standardised *geometry* of a tensile test *specimen*, including the subprocesses:
  - *extraction* of a block of material from the component at a desired position
  - *turning* process according to the geometric requirements of a standard specimen
  - *grinding* process (optionally) to reach the required surface quality (roughness).
- *Tensile test*

At each of these steps, the material experiences a set of factual process parameters, which variously affect its properties. The extent of these effects depends on the parameters' particular values as well as on the material state and properties of the material's previous stage. The result of the entire process chain can be accessed by the tensile test at the end of the workflow. This disregards other characterization methods that could be applied to derive the material's properties, e.g. hardness testing or microscopy.

4 Materials Science Perspectives for Ontology Design

As for any digital representation of physical phenomena, one has to define the model's system boundaries. The project aims to define an ontology that represents the workflow described above including the consideration of MSE knowledge. Generally, we consider our workflow to be an alternating chain of objects and processes of which the latter lead to changes in the status of the object (material properties and structure) according to the individual process parameters (Figure 3).

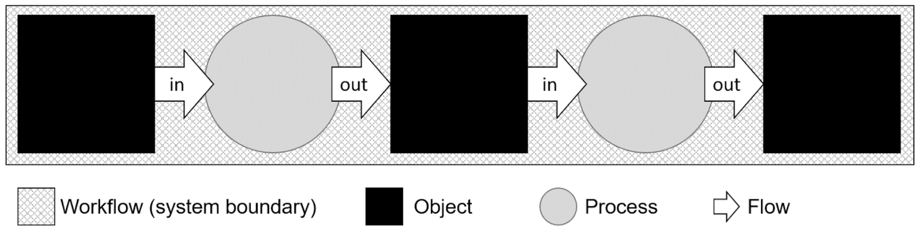


Fig. 3. Alternating chain of manipulated objects and processes within the system boundary.

Every process comes with its own parameters that represent all the regarded variables, under which a specific process can be distinguished. The decision, which parameters to regard, is up to the ontologist and should theoretically incorporate all relevant factors as known by domain experts. Furthermore, parameters must be well distinguished between the nominal ("desired" by engineering design), the environmental and the factual ("experienced") parameters. The factual parameters are the result of the composition of the nominal, technological and the environmental parameters. For example a heat treatment might be supposed to be conducted under a certain nominal temperature. However, due to the oven's poor calibration and additional environmental effects the locally experienced temperature history generally diverges from the control input.

We proceed by disregarding time as its own continuous dimension and replace it with the workflow, which is the chain of processes happening at discrete time points[10]. Generally, an object leaving one process is therefore assumed to be identical to the one entering the next process. This leads to further assumptions since everything not explicitly represented in the workflow chain is disregarded. However, for example storage times under specific weather conditions, rough transport conditions or further thinkable scenarios that the practical world encounters do have an influence on a material. Theoretically, one would thus have to incorporate these scenarios as additional processes along the workflow or add them to one of the others. The workflow-representing part of our ontology starts after the completion of the casting process with a wrought material component at room temperature. An expansion of this framework to include the casting process or the chemical composition of the material and its variation by sourcing parameters is possible.

We consider process parameters to have various effects on the material, which can be described on the different granularity levels. While basically all effects can be comprehended on a material's atomistic level, this representation does not lend itself to the description of macroscopic behaviour. In fact, all the structural granularity levels cover different features related to a material's properties. This relation between the structure of a material, which is affected by its experienced

[10] However, regarding time is possible via its consideration as an individual process parameter, like e.g. the process duration.

history (processing) and its interlinked properties and performance is the key in incorporating domain knowledge of MSE. This interaction is illustrated in Figure 4. A weak back coupling from the materials properties to the process is possible. For example during cutting, the materials surface hardness can undergo changes through plastic deformation increasing the required process energy to cut the sample.

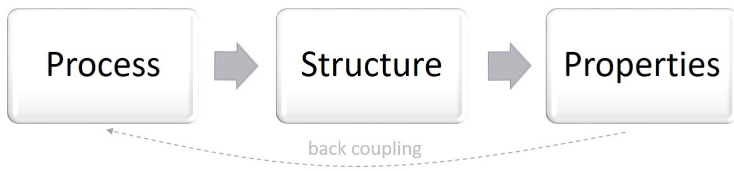


Fig. 4. Modelled interactions between processes, material structure and material properties according to materials science knowledge.

The solution to the problem of locally heterogeneous process parameters and thus material properties throughout the component can be derived by separating the component into a certain number of volumetric sub-areas, so called voxels. Therefore, the voxel becomes the object of the ontology and describes the conditions of the material with its individually experienced process parameters. If the description of a larger volumetric area of the component or even of its entire volume is desired, the ontology can be iterated over the relevant voxels regarding their respective local factual parameters. The size of the voxels and thus the resolution of the diverse description of the volumetric area has to be set according to the granularity level of the considered material properties. The technique to divide a component into several volumetric areas is well known e.g., from finite element (FE) modelling.

Additional to the implications of processes and their parameters on a voxel, traditional materials science theory, including physics and engineering, provides us with what we call intrinsic dependencies of different material properties. For example, the size and orientation of the grains in the microstructure affects the elastic behavior of the material. Many of these intrinsic dependencies are described in the literature qualitatively and in some cases even quantitatively by formulas. These dependencies allow to regard process effects on material properties indirectly via a well described process effect on a different structural granularity level. Therefore, materials science knowledge can help us to get more out of our mere measurements by consideration of the incorporated interdependencies. We aim to integrate equations in the sense that we introduce an ontological relationship called X "influences" Y, initially adding formulas exclusively according to their qualitative sense. Prospectively, numerical interdependencies shall be integrated in the knowledge graph in a processual manner.

5 Conclusions and Outlook

The setup to implement MSE into an ontology that represents a chain of technical processes has been discussed exemplarily. This was done according to the use case of a manufacturing workflow of a cylinder head component and a subsequent tensile test workflow of the component's material. The basic aim is the structured storage of all relevant knowledge including the dependency between material effects and process parameters as well as the consideration of the component's geometry. This aim led to the need for digitization of the relevant processes and of all available material effects on the different granularity levels. To define our system boundaries we distinguish between a workflow dimension and a material structure and properties dimension. The workflow dimension includes all relevant processes from an MSE point of view, ranging from the starting point of a wrought cylinder head material via the heat treatment to the tensile test workflow with the extraction and generation of a standardized tensile test specimen. The system boundaries in the material structure and properties dimension include the different granularity levels from the continuum to the atomistic level. In the ontology, we consider the workflow to be an alternating chain of objects that describe the material status on all granularity levels and processes, of which the latter lead to changes in the status of the material and thus of the information stored in the object. The component is separated into a certain number of volumetric sub-areas, so called voxels, since the factual process parameters naturally vary throughout the components volumetric area. Therefore, the object introduced above gives information only for the single voxel of material defined at a local position of the component. An iteration over several voxels enables a description of a larger volumetric area of the component. To provide a practical benefit, a capable MSE ontology needs to allow for comprehension of its various relevant dimensions. Therefore, this approach discusses the numerous necessary modelling considerations and enriches mere process and entity description with available domain knowledge. The benefit of a knowledge-describing ontology in MSE is to provide structured digitized information, which simplifies data access via expert queries. Such a query is defined as a request of data covering all available material properties related to process parameters by considering the entire workflow at any desired position of the component.

Perspectively, the structured data can be queried, for example within the Platform MaterialDigital (PMD), by an individual expert, as well as by a software agent, which might represent a digital twin of a component. The future work based on this paper would be the realization of the introduced approach for an ontology within the defined system boundaries. After the validation of the ontology by the application of real data, it may be transferable to other use cases. Combining observations with strongly supported scientific theory vastly increases the variety of options to predict a system's yet unobserved or entirely unobservable parameters, for example by relying on grey-box models [5]. In turn, this promises a strongly accelerated gain of new insights, while depending on much smaller amounts of data than what current AI requires.

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