Domain ontology for sharing data related to sustainable metallurgical and manufacturing industry

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1. Introduction

An overview is given of the ongoing work of developing a new domain ontology for metallic microstructures based on the Elementary Multiperspective Material Ontology (EMMO) [1]. This ontology is developed in the context of European Materials Modelling Council (EMMC) [2] and the Norwegian *Centre for Sustainable and Competitive Metallurgical and Manufacturing Industry* (SFI PhysMet) [3], for which the overall objective is to enable and accelerate the transformation of the national metal industry towards more sustainable and cost-efficient production, future material products, solutions, and improved processing methods.

2. The microstructure domain ontology

Ontologies have been successfully used for more than two decades in biomedical sciences to categorise and structure scientific data, to facilitate the description of the human genome and for the rapid development of new vaccines. Until recently there have been very few successful attempts towards ontologies in the domain of material sciences. The main reason for this is the large complexity of materials science, which consists of many scientific communities and has a large variety of characterisation techniques and modelling tools producing and requiring very heterogeneous types of data. However, during the last years, especially in Europe, an increasing interest in utilising ontologies for materials sciences has been observed. These developments to a large extend are driven by the EMMO.

Figure 1 shows a few selected concepts from the microstructure ontology and how they connect to EMMO.

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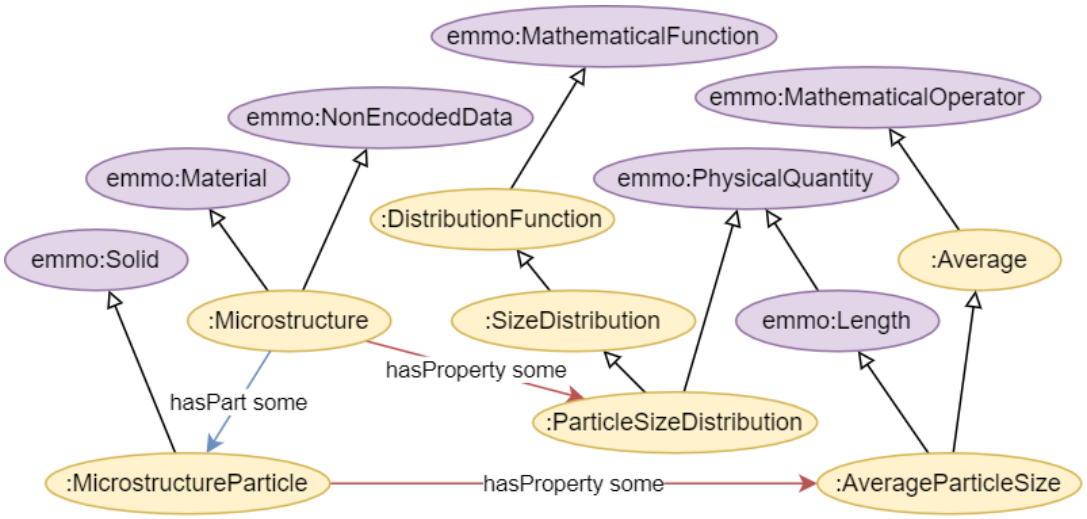

Figure 1. Some selected classes from the microstructure ontology (yellow) and how they connect to EMMO (purple). Three different types of relations/class restrictions are also shown; `rdfs:subClassOf` *(open arrows),* `emmo:hasPart` *(blue arrow) and* `emmo:hasProperty` *(red arrows).*

A microstructure is here described as an `emmo:Material` (real world object representing an amount of a physical substance), which is also an `emmo:NonEncodedData`. EMMO defines data in accordance with Floridi [4], as the variation of properties of a physical object that can be recognised and eventually interpreted, where non-encoded data is data that occurs naturally with no intentional encoding by an agent. A microstructure has (among others) a `MicrostructureParticle` part and a `ParticleSizeDistribution` property.

3. Enabling interoperability

Ontologies provide a common language and enables semantic interoperability, i.e. the ability to connect different models and data sources that have been developed independent of each other into complex workflows. The key is to create simplistic data models describing the underlying datasets and map them to ontological concepts. A simple example of this is shown in Figure 2, which also makes use of the Function Ontology (FNO) [5] to ontologically describe how the `mean_size` property of a data model for a simulation automatically can be instantiated from an experimental dataset of the precipitate size distribution in an aluminium alloy.

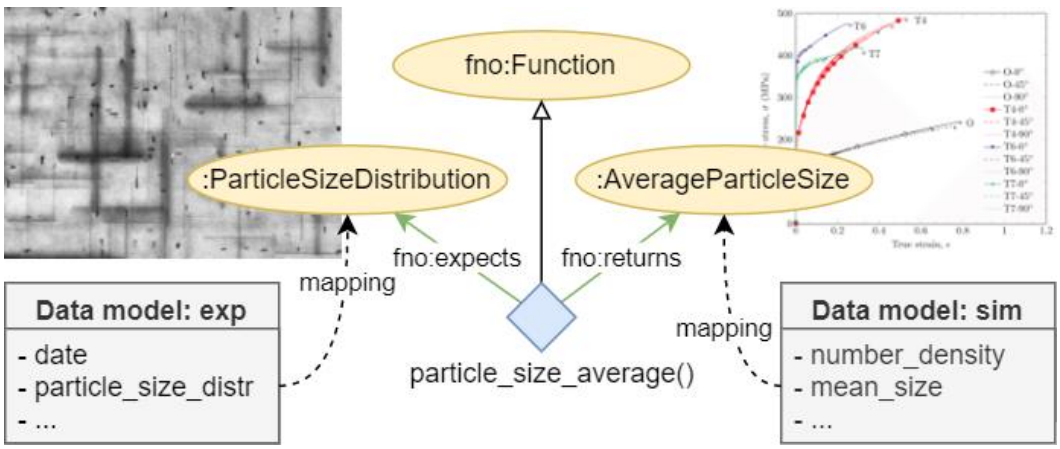

Figure 2. Example of two data models with properties mapped to ontological concepts. FNO is used to ontologically describe how an average particle size can be calculated from a particle size distribution.

4. Conclusions

The microstructure domain ontology provides a straightforward way to semantically document of physical metallurgical data and enable exchange of digital data between characterisation and modelling, across scales and processes and between physical metallurgy and other domains. An example is given on how this ontology can be used in practice to enable semantic interoperability.

5. References

[1] Elementary Multiperspective Material Ontology: https://github.com/emmo-repo/EMMO

[2] European Material Modelling Council: https://emmc.eu/

[3] Centre for Sustainable and Competive Metallurgical and Manufacturing Industry: https://www.ntnu.edu/physmet

[4] Luciano Floridi, "Information - A very Short Introduction", Oxford University Press., (2010) ISBN 978-0199551378.

[5] The Function Ontology (FNO): https://fno.io/