Ontology for magnetic materials based on EMMO

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ABSTRACT

The EU-project MaMMoS focuses on developing a software suite for the multiscale simulation of magnetic materials, aiding the design and optimization of magnetic devices. A key component is the Magnetic Materials Ontology, created by domain experts. Built on the Elementary Multiperspective Material Ontology (EMMO), it supports SI units for all magnetic properties, ensuring data consistency. The ontology is publicly available on GitHub and Zenodo, with detailed documentation and examples. Adhering to FAIR principles, it enhances data reproducibility, collaboration, and integration of diverse datasets and tools.

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COOPERATION

Leibniz Institut für Festkörper und Werkstoffforschung, Uppsala Universitet, Centre National de la Recherche Scientifique CNRS, Max-Planck-Gesellschaft zur Förderung der Wissenschaften e.V., Siemens Aktien-gesellschaft, Robert Bosch GmbH

Introduction

The MaMMoS project [1] aims to develop a comprehensive software suite for the multiscale simulation of magnetic materials, facilitating the design and optimization of innovative magnetic devices. A key component of this suite is the Magnetic Materials Ontology, created by domain experts. This ontology provides a standardized, machine-readable framework for describing magnetic material properties and their interrelationships across various length scales.

Main Aspects

- Built upon the Elementary Multiperspective Material Ontology (EMMO) [2]
- Organizes information from intrinsic and microstructural properties, and hierarchical spatial structure
- Encompasses a wide range of variables and units used in magnetics
- Utilizes the EMMOntoPy Python library for implementation
- Supports the use of SI units for all magnetic properties
- Publicly available on GitHub and Zenodo [3, 4]
- Detailed documentation and example Jupyter notebooks provided
- Adheres to the FAIR principles

Summary

The MaMMoS project focuses on developing a software suite for the multiscale simulation of magnetic materials, aiding the design and optimization of magnetic devices. The Magnetic Materials Ontology, created by domain experts, provides a standardized framework for describing magnetic material properties across various length scales. Built on the EMMO, it supports SI units for all magnetic properties, ensuring data consistency. The ontology is publicly available with detailed documentation and examples, promoting open science and innovation while adhering to the FAIR principles.

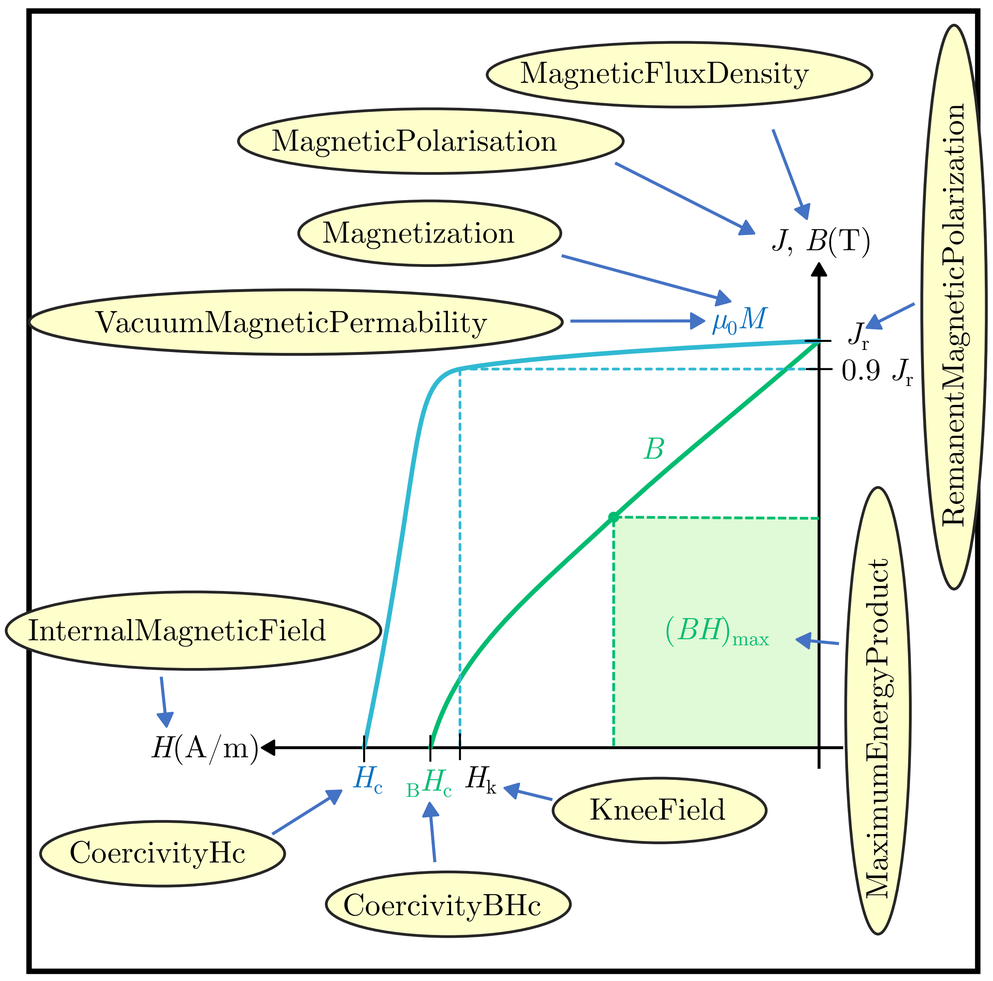

Figure 1: Parameters necessary for the description of a hysteresis loop and how they arenamed in the ontology.

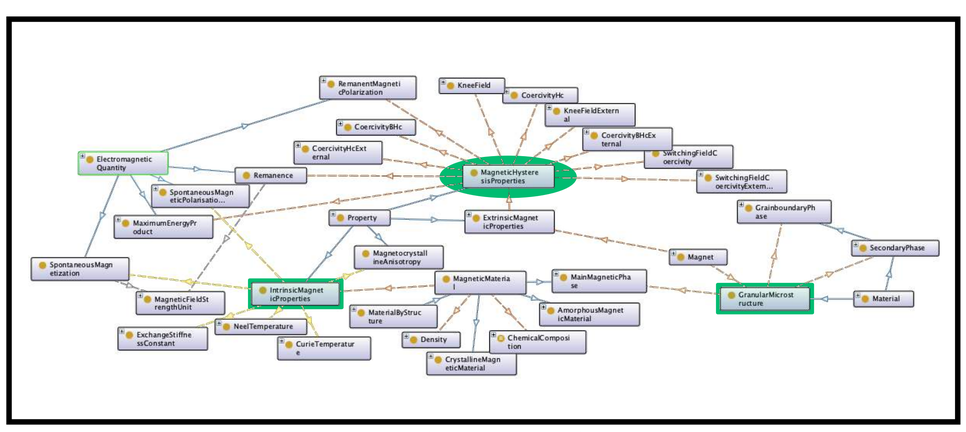

Figure 2: Three main categories of properties for magnetic materials together with therelated elements in the ontology.

References

[1] MaMMoS project on cordis https://doi.org/10.3030/101135546
[2] GitHub repository of EMMO, https://github.com/emmo-repo/EMMO
[3] The ontology is publicly available on GitHub (https://github.com/MaMMoS-project/MagneticMaterialsOntology/)
[4] Schrefl, Hortschitz, Holt, Pile, & Fangohr (2024). MagneticMaterialsOntology (0.0.3). https://doi.org/10.5281/zenodo.14547623

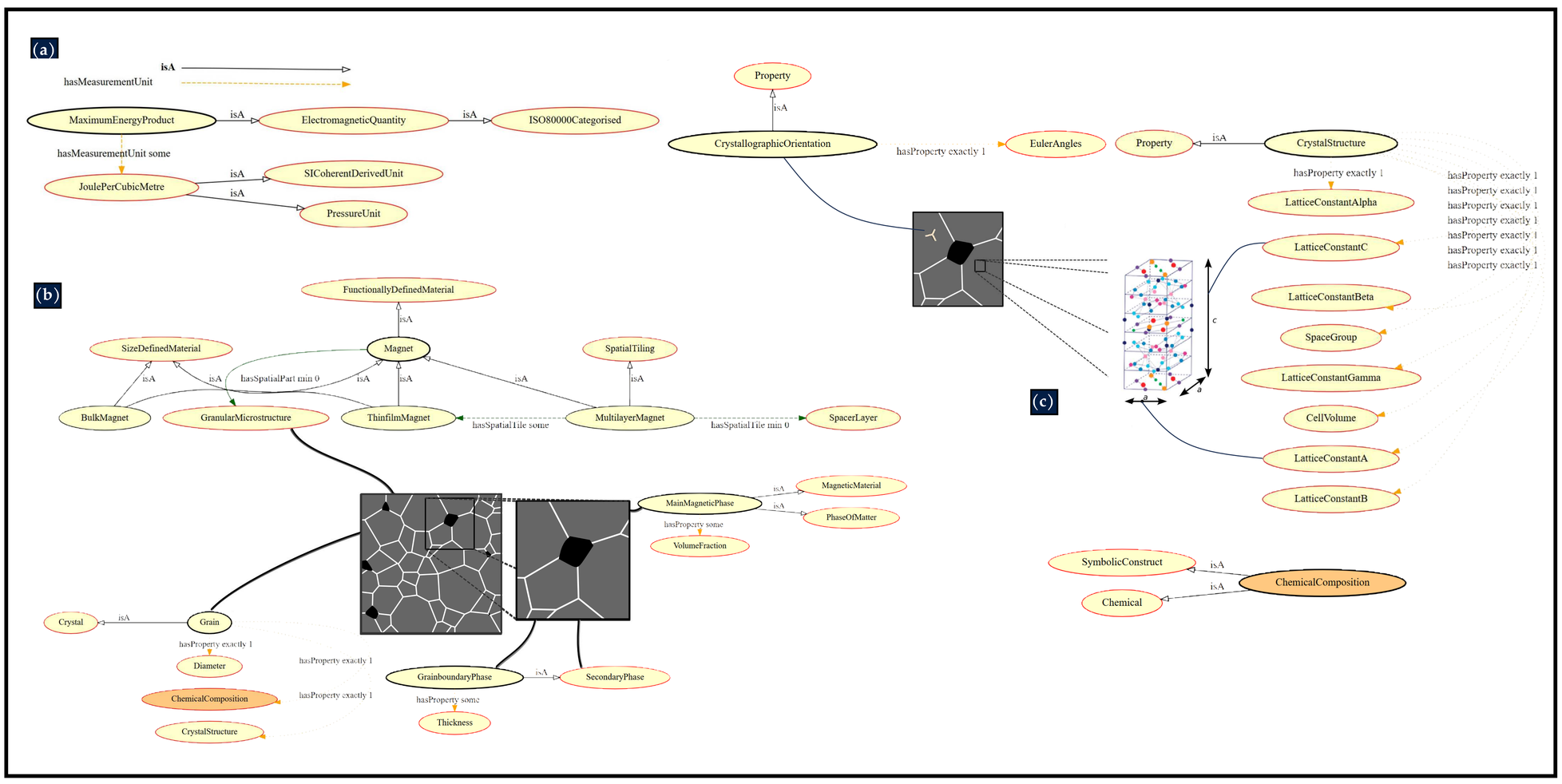

Figure 3: **a**) Quantities and their units are defined within the ontology. **b**) Magnet and its microstructure. The centre shows a sketch of the granular microstructure based on a scanning electron microscopy image of permanent magnet. **c**) A grain has a crystallographic orientation, a chemical composition, and a crystalstructure.

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