Magnetic Multiscale Modelling Suite

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1. Introduction

Magnets are crucial for many of today's technologies, from the motors that power electric vehicles to computers, smartphones and the generators in wind turbines which help to reduce global warming. The EU demand for rare earth metals, used in wind turbines and electric vehicles is expected to increase six to seven-fold by 2050 [1]. The EU relies almost exclusively on imports for rare earth elements used in high-performance magnets. Substitution of critical raw materials and recycling are facilitated by computational materials design. The project entitled MAgnetic Multiscale MOdelling Suite (MaMMoS) is funded under the umbrella of the call Adaptive multi-scale modelling and characterisation suites from lab to production (HORIZON-CL4-2023-DIGITAL-EMERGING-01-12) and aims at the development of an open-source software platform for magnetic materials modelling.

2. Multiscale simulations and artificial intelligence

The macroscopic properties of magnets arise from the interaction of phenomena at different length and time scales. This often limits the application of numerical methods for magnetic materials development. The goal of MaMMoS is the design and optimisation of magnetic materials and devices based on multiscale modelling, characterisation, and numerical optimisation. To achieve interoperability between software and analysis tools, we will establish a domain ontology for magnetic materials. We aim to create standards for linking simulation software for magnetic materials from first principles simulations and micromagnetics to device level simulators (see Figure 1). MaMMoS will use artificial intelligence (AI) to fuse modelling and characterization data. AI methods will identify and correct systematic errors in the simulation data, enabling more accurate predictions. Moreover, AI models can fill gaps where measurements are not available. AI models can also serve as a surrogate in multi-objective optimisation. Optimisation will guide further experiments or simulations, reducing the development time. In MaMMoS, we will apply this approach to speed up the development of permanent magnets with reduced critical elements for electric machines and to

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optimise the layout of magnetic field sensors for high linearity range. The MaMMoS software will be validated against benchmarks defined according to the industrial requirements for electric machine and sensor design. The multiscale magnetic materials modelling suite will be made open source to enable easy access to high-end simulation tools. Interoperability will facilitate data sharing and reuse among researchers and industries. Interpretable machine learning will reveal insights into the physics and chemistry of magnetic materials and guide the discovery of new materials.

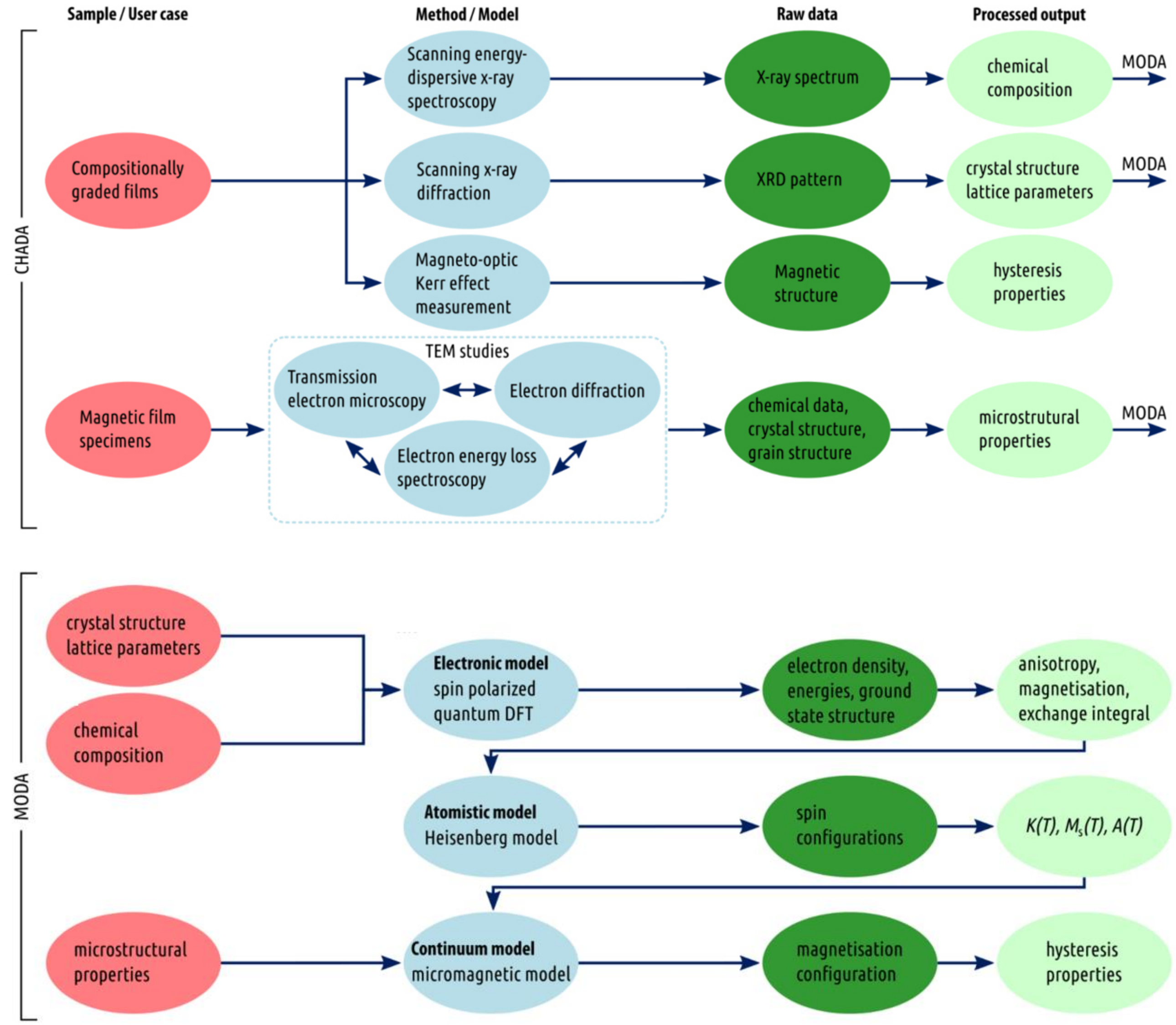

Figure 1: Linking of experimental data (CHADA) and modelling data (MODA) for the evaluation of the temperature dependent intrinsic magnetic properties and the hysteresis properties of magnetic materials.

3. Acknowledgement

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Digital Executive Agency (HADEA). Neither the European Union nor the granting authority can be held responsible for them.

4. References

[1] European critical raw materials act, Fact sheet, March 2023.