The role of AI and ML in the development of a multiscale modeling suite for sustainable magnetic materials

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Soft and hard magnets are essential components of several devices of utmost importance in various high-tech manufacturing industries. As an example, they play a central role in the functioning of electric motors, which are a pivotal element in the ongoing transition from fossil fuels to renewable energy encouraged by the EU. Magnetic materials are also employed in the manufacturing of magnetic sensor devices, which are widely used in many consumer and industrial applications. The current manufacturing process of high-performing magnets heavily relies on the use of rare-earth elements, whose mining and processing produce a remarkable amount of polluting waste. Moreover, EU countries are currently importing 98% of their rare-earth elements requirements, thus facing a serious risk of supply shortage and price volatility [1]. To reduce the environmental footprint of rare-earth supply and to mitigate the consequences of their supply shortage, private and governmental entities in the EU have been fostering the search for alternatives to rare-earth elements in the development of novel magnetic materials. In this talk, we are going to introduce the MaMMoS (MAgnetic Multiscale MOdeling Suite) project [2], one of the most recently funded by the EU to accelerate the sustainable manufacturing of high-performing permanent magnets. Established by a consortium comprising both private companies (Robert Bosch GmbH, SIEMENS AG) and academic institutions (Danube University Krems, Max Planck Society, University of Uppsala, Leibnitz Institute for State and Materials Research, Centre National de la Recherche Scientifique), MaMMoS aims at developing an integrated toolchain for the characterization and modeling of magnetic materials from the nanoscale to the magnetic device scale, focusing primarily on improved critical-rare-earth-reduced and rare-earth-free hard magnetic materials in the systems Nd-Ce-Fe-B, Mn-Al and Fe-N (cf. Fig. 1). AI and ML will play a central role in the development of the proposed toolchain, especially for the integration of experimental and simulation data. In particular ML models will be employed to correct the systematic error of *ab-initio* simulations [3], to complement simulation data in domains not covered by the simulations, and to make predictions of materials properties. Specific feature engineering and dimensionality reduction techniques are currently being applied to the training data, with the purpose of encoding magnetic material properties into a low-dimensional vector space. We will then train ML models of increasing complexity to unveil the hidden patterns in our datasets. The feature encoding map, the best-fit model parameters, the model outcomes, and their limitations will be interpreted and validated iteratively by domain scientists, also exploiting existing optimization toolkits like Dakota [4]. The final models and all generated data will be publicly shared open-source, in accordance with the FAIR principles. In conclusion, the MaMMoS project is expected to have a remarkable impact on the materials science community. The final modelling and characterization suite, powered by AI, will be unique in its nature, as has been designed to simulate the behavior and properties of magnetic materials at different length scales, from the atomic to the macroscopic. It can help researchers and engineers design and optimize advanced magnetic materials with new functionality for various critical applications, such as electric motors and magnetic sensors. By using and improving methods of AI, it can also accelerate the material discovery and innovation process by learning from data and building new predictive models.

References

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Figures

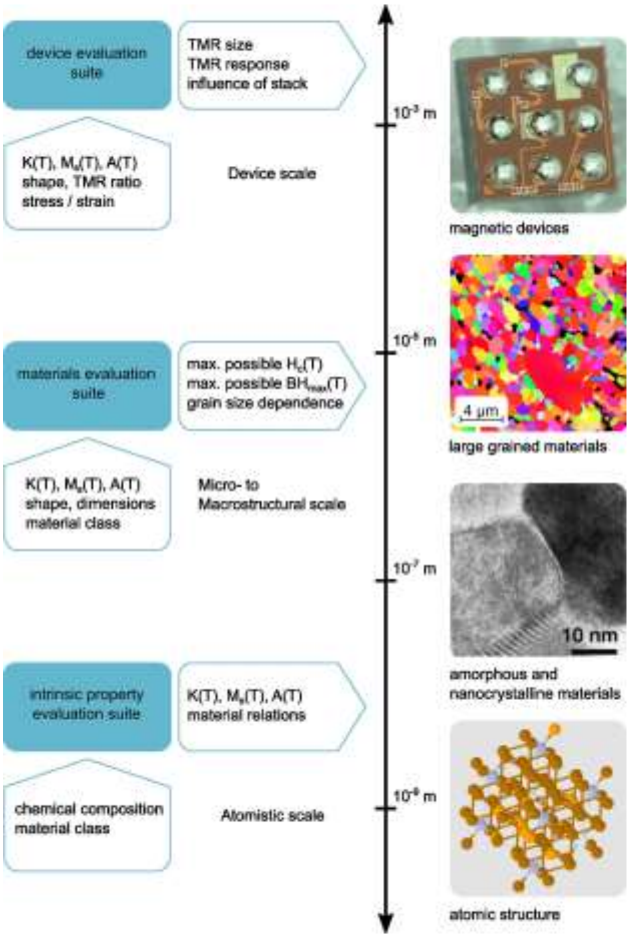

Figure 1. Bridging the length scales for magnetic materials modeling. MaMMoS will provide a modeling and simulation suite for intrinsic property evaluation, materials evaluation, and device evaluation. The temperature-dependent intrinsic magnetic properties are the anisotropy K(T), the spontaneous magnetization M_s(T), and the exchange constant A(T). They arise from the crystal structure of the material. Together with the specific internal structure of the magnet, they influence the hysteresis properties, such as the coercive field H_c(T) and the energy density product BH_{max}(T). The former is the strength of the magnet against demagnetization, the latter is a measure for the strength of the magnetic field produced by a permanent magnet. Tunnel magnetoresistive (TMR) magnetic field sensors measure the electric resistance through a stack of magnetic layers.