MA 28: Bulk Materials: Soft and Hard Permanent Magnets

Time: Wednesday 9:30–10:45 Location: POT 6

MA 28.1 Wed 9:30 POT 6

Local stiffness tailoring of magneto-active composites produced by laser powder bed fusion — •Kilian Schäfer[1], Matthias Lutzi[1], Muhammad Bilal Khan[1], Sebastian Bruns[2], Claas Hartmann[3], and Oliver Gutfleisch[1] — [1]Functional Materials, Institute of Materials Science, TU Darmstadt, — [2]Physical Metallurgy, Institute of Materials Science, TU Darmstadt, — [3]Measurement and Sensor Technology Group, TU Darmstadt,

Magnetic actuation of mechanically soft actuators allows fast response, wireless operation and safe interaction with the human body. With additive manufacturing, the production of magneto-active composites in complex and bioinspired shapes is possible. To mimic the properties of biological systems, the fabrication of composites with locally different mechanical properties is needed. Here, we present a method to locally tailor the stiffness of a magneto-active compound, consisting of hard magnetic Nd2Fe14B particles in a thermoplastic polyurethane (TPU) matrix with laser powder bed fusion. By utilizing different laser parameters at different locations during the process, the mechanical properties of the composite are modified locally. The range in which the mechanical properties can be tailored is investigated with compression and tensile tests of the composite produced with different laser parameters. The stiffness can be increased tenfold when the laser power is increased from low to high values. The stiffness gradient within one sample is verified by line scans of Vickers indentations with a nanoindentation system. Then the actuation performance is evaluated for samples with and without stiffness gradients.

MA 28.2 Wed 9:45 POT 6

Magnetic properties of rare-earth-lean $ThMn_{12}$-type (Nd,X)Fe_{11}Ti (X: Y and Ce) compounds: A DFT study — •Stephan Erdmann, Thorsten Klüner, and Halil Ibrahim Sözen — Institute of Chemistry, Carl-von-Ossietzky University of Oldenburg, D-26129 Oldenburg, Germany

Due to the resource criticality of rare-earths (RE), an alternative to the well-known $Nd_2Fe_{14}B$ magnets with a lower amount of critical elements is required. In this work, we performed density functional theory (DFT) calculations to investigate the influence of partial Nd substitution with more abundant elements (X: Y and Ce) in $ThMn_{12}$-type (Nd,X)Fe_{11}Ti compounds. In order to have a systematic understanding, the intrinsic magnetic properties such as saturation magnetization M_S, Curie temperature T_C and magnetocrystalline anisotropy energy, are screened starting from binaries RFe_{12} (R: Y, Ce and Nd). Ti is considered for the thermodynamic stabilization and different concentrations of Ti are taken into account for ternaries $RFe_{12-y}Ti_y$, and quaternaries (Nd,X)$Fe_{12-y}Ti_y$ ($0.5 \leq y \leq 1$). In addition, the effect of nitrogenation is examined for each considered compound. In case of (Nd,Y)Fe_{11}Ti, $|BH|_{max}$ is found to be 384 kJ/m^3 and T_C is calculated to be 595 K. Similarly, $|BH|_{max}$ and T_C are calculated to be 365 kJ/m^3 and 593 K for (Nd,Ce)Fe_{11}Ti magnet, respectively. Both 50 % Nd-lean magnets exhibit higher $|BH|_{max}$ compared to Sm_2Co_{17} and T_C than $Nd_2Fe_{14}B$. For both cases, our theoretical magnetic hardness factor κ is calculated to be 1.20, which qualifies them as good candidates for RE-lean permanent magnets.

MA 28.3 Wed 10:00 POT 6

Ab initio thermodynamic modelling for Ce-based alternative hard magnetic materials — •Halil Ibrahim Sözen[1], Tilmann Hickel[2], and Thorsten Klüner[1] — [1]Institute of Chemistry, Carl-von-Ossietzky University of Oldenburg, D-26129 Oldenburg, Germany — [2]BAM Federal Institute for Materials Research and Testing, 12489 Berlin, Germany

The utilization of the RE-lean $ThMn_{12}$ materials system in combination with the abundant RE element Ce is a promising strategy for modern hard magnet applications. One of the main challenges for the Ce-based hard-magnetic materials is the formation of detrimental Laves phases next to the $ThMn_{12}$-type compound $CeFe_{11}$Ti. In this contribution, we present an ab initio-based approach to modify the stability of these phases in the Ce-Fe-Ti system by additions of 3d and 4d-elements. The results are used to provide two fundamental methodological insights. One of them is our recently developed modeling concept of partial decomposition, which considers the enrichment of the added solutes in phases that would at the considered temperature not be stable in a conventionally used full decomposition model. The second conclusion is the dominant impact of 0 K formation enthalpies on the solute-enhances phase stability compared to finite temperature entropy terms. Based on this, a screening approach is developed, considering the substitution of all 3d and 4d-elements. We show that substituted elements with more than a half-filled 3d-shell or with less than a half-filled 4d-shell mainly reduce the formation temperature of the 1:12 phase.

MA 28.4 Wed 10:15 POT 6

Rare earth lean permanent magnets from computational design and the challenge of the 4f electrons — •H. C. Herper[1], K. P. Skokov[2], S. Ener[2], P. Thunström[1], L. V. B. Diop[3], O. Gutfleisch[2], and O. Eriksson[1,4] — [1]Department of Physics and Astronomy, Uppsala University, Sweden — [2]Functional Materials, Department of Material Science, TU Darmstadt, Germany — [3]Université de Lorraine, CNRS, IJL, Nancy, France — [4]School of Science and Technology, Örebro University, Örebro, Sweden

Computational design has been proven to be a powerful tool to tailor properties of functional materials but it becomes challenging in presence of 4f electrons. Here, $NdFe_{11}$Ti and YFe_{11}Ti serve as prototypes for rare-earth (RE) lean or RE-free magnets with the $ThMn_{12}$ structure. Though, for Sm (Ce) counterparts a core (valence) treatment was sufficient to describe the magnetic properties, the complex low temperature magnetism of $NdFe_{11}$Ti could only be reproduced with an intermediate sized LDA+U or a DMFT approach (full potential LMTO). We compare our calculations to experimental values obtained from single crystals. The investigations clearly demonstrate the crucial dependence of the calculated magnetic properties of $NdFe_{11}$Ti on the treatment of the 4f electrons.[1]

Using $Nd_{1-x}Y_xFe_{12-y}Ti1+y$ as a test case we investigated how far the strong dependence of the magnetic properties on the description of the Nd 4f states influences the prediction of new phases.

[1] H.C. Herper et al., Acta Materialia 242, 118473 (2023)

MA 28.5 Wed 10:30 POT 6

MAELAS: MAgneto-ELAStic properties calculation via computational high-throughput approach — Pablo Nieves[1], Sergiu Arapan[1], Shihao Zhang[2], Andrzej Kadzielawa[1], Ruifeng Zhang[2], and •Dominik Legut[1] — [1]IT4Innovations, VSB-TU Ostrava, Ostrava, Czech Republic — [2]School of Mat. Sci. and Eng., Beihang University, Beijing, China

Magnetostriction is a physical phenomenon in which the process of magnetization induces a change in the shape or dimension of a magnetic material. Nowadays, materials with large magnetostriction are used in many electromagnetic microdevices as actuators and sensors. By contrast, magnetic materials with extremely low magnetostriction are required in applications such as electric transformers. In this work, we present results based on the in-house developed code MAELAS to determine anisotropic magnetostriction coefficients and magnetoelastic constants in an automated way by quantum-mechanical calculations. The behavior of the magnetocrystalline anisotropy energy and magnetostrictive coefficients under a general external magnetic field could be visualized as a relative length change using our MAELASviewer tool. To verify accuracy and our approach in general we present a number of examples of each crystal symmetry class with calculated magnetostriction and magnetoelastic constants and compare them with recorded data. One of our highlights with this novel approach is an ability to separate exchange-striction (ω_s) from the magnetic part and to avoid the calculation of the paramagnetic state that is still a challenge.