MA 32: Bulk Materials: Soft and Hard Permanent Magnets

Time: Thursday 15:00–17:00 Location: H43

MA 32.1 Thu 15:00 H43

High-Entropy/Compositionally-Complex B2 Heusler alloy — •Asli Cakir[1,2], Mehmet Acet[2], and Michael Farle[2] — [1]Department of Metallurgical and Materials Engineering, Mugla University, 48000, Mugla,Turkey — [2]Fakultät für Physik, Universität Duisburg-Essen, Forsthausweg 2, 47057 Duisburg, Germany

High entropy alloys (HEAs) emerge as a new alloy concept contrary to conventional alloy design that includes one or two main elements with additional amounts of property-tuning elements. It has been established that the general physical properties of 3d-metallic HEAs can be understood within the known valence-electron-concentration scheme. Using this scheme alloys with particular physical properties can be designed. Here, we present a compositionally-complex alloy consisting of a HEA-component, MnFeCoNiCu, with 25 at% added Al. The resulting material is identical to a stoichiometric B2-Heusler alloy (HEA)50(HEA)25Al25. We have performed X-ray diffraction, energy-dispersive x-ray spectroscopy studies, and magnetization measurements. The alloy exhibits the ordered B2 structure with saturation-magnetization of 1.3 Bohr magneton and Curie temperature of 550 K.

MA 32.2 Thu 15:15 H43

Magnetic-field-, temperature- and time-dependence of structural and magnetic properties of shell-ferromagnets — •Nicolas Josten[1], Steffen Franzka[2], Mehmet Acet[1], Franziska Scheibel[3], Asli Çakir[4], Franziska Staab[5], and Michael Farle[1] — [1]Faculty of Physics and Center for Nanointegration (CENIDE), University Duisburg Essen, Duisburg, 47057, Germany — [2]Interdisciplinary Center for Analytics on the Nanoscale (ICAN), Carl-Benz-Straße 199, 47057 Duisburg, Germany — [3]Functional Materials, Institute of Materials Science, Technical University of Darmstadt, Alarich-Weiss-Str. 16, 64287 Darmstadt, Germany — [4]Department of Metallurgical and Materials Engineering, Mugla University, 48000 Mugla, Turkey — [5]Physical Metallurgy, Institute of Materials Science, Technical University of Darmstadt, Alarich-Weiss-Str. 2, 64287 Darmstadt, Germany

The strong pinning of magnetic moments in off-stoichometric $Ni_{50}Mn_{45}X_{05}$ (X= Al, Ga, In, Sn, Sb) Heusler alloys after magnetic annealing at 650K is known as the shell-ferromagnetic effect. This pinning leads to coercive fields larger than 6 Tesla and is interesting for the development of novel ultrahard permanent magnets. We report on the optimization of the strength of this effect by varying the annealing field, time, and temperature. The origin of the effect is discussed based on these results combined with magnetic force microscopy images.

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MA 32.3 Thu 15:30 H43

Effects of disorder on the magnetic properties of $L1_0$-FeNi — Ankit Izardar and •Claude Ederer — ETH Zürich, Switzerland

$L1_0$-ordered FeNi is a promising candidate for cheap mid-range permanent magnets. However, since the synthesis of fully ordered samples is very challenging, it is important to understand how deviations from perfect chemical order affect the magnetic properties of FeNi, in particular the magneto-crystalline anisotropy and Curie temperature. We use DFT in combination with a sampling over different supercell configuration to address effects of chemical disorder in FeNi. Our results show that a decrease in chemical order of up to 25 % does not cause a significant reduction of the magneto-crystalline anisotropy, and that the anisotropy can even be increased for Fe-rich compositions. We also show that the dominant magnetic coupling is strongly dependent on the specific chemical environment and vary drastically in the partially disordered system. We discuss these results in relation to alternative approaches to disorder, such as, e.g., the coherent potential approximation.

MA 32.4 Thu 15:45 H43

Influence of filler morphology, arrangement and filling fraction on the magnetic properties of polymer-bonded magnets produced by laser powder bed fusion — •Kilian Schäfer[1], Tobias Braun[1], Stefan Riegg[1], Jens Musekamp[2], and Oliver Gutfleisch[1] — [1]1Functional Materials, Institute of Materials Science, , Technical University Darmstadt, Darmstadt — [2]2Institute for Materials Technology (MPA-IfW), Technical University Darmstadt, Grafenstraße 2, D-64283 Darmstadt

Bonded permanent magnets are key components in many energy conversion, sensor and actuator devices. These applications need high magnetic performance, customizability, and freedom of shape. With additive manufacturing processes, for example laser powder bed fusion (LPBF), it is possible to produce bonded magnets with tailored stray field distribution.

Up to now, most studies use spherical powders as magnetic fillers due to their good flowability. Here, the behavior of large SmFeN platelets with a high aspect ratio as filler material and its influence on the arrangement and the resulting magnetic properties were examined. To study the distribution and orientation of the magnetic filler in 3D, computed tomography measurements were conducted and analyzed with the open-source software ImageJ. It is shown that the plateletshaped particles align themselves perpendicular towards the buildup direction during the process. In addition, the effect of filling fraction on the magnetic properties of the composites is investigated.

MA 32.5 Thu 16:00 H43

magnetocrystalline anisotropy in easy-plane kagomé ferromagnet Fe_3Sn — •Lilian Prodan[1], Vladimir Tsurkan[1,2], and István Kézsmárki[1] — [1]Experimental Physics V, Institute of Physics, University of Augsburg, D-86159 Augsburg, Germany — [2]Institute of Applied Physics, MD 2028, Chisinau, Republic of Moldova

Kagomé magnets are expected to host exotic magnetic and electronic properties due to possible interplay of spin-orbit coupling (SOC) and specific topology of the energy band structures [1,2,3]. Here, we present the field-dependent and angular-dependent magnetization studies of the kagomé -lattice easy-plane ferromagnet Fe_3Sn. The SOC is probed by the measurements of the magnetocrystalline anisotropy in high-quality bulk single crystals. Measurements in high fields reveal the difference in the saturation magnetization along the a and the c axes, which does not vanish up to the highest applied field of 14 T. The anisotropy evidenced in the saturation moment indicates a possible contribution of the orbital moment. The temperature dependence of the magnetocrystalline anisotropy constants K_1 and K_2 was determined. [1] L. Ye et al., Nature 555, 638 (2018), M. Altthaler et al., Phys. Rev. Research 3, 043191 (2021), J. Watanabe, et al., arXiv:2202.06665 (2022).

MA 32.6 Thu 16:15 H43

First principles study of the complex magnetism in Ce_2Fe_{17} — Alena Vishina[1], Olle Eriksson[1,2], Anders Bergman[1], and •Heike C. Herper[1] — [1]Department of Physics and Astronomy, Uppsala University, Uppsala, Sweden — [2]School of Science and Technology, Örebro University, Örebro, Sweden

With its comparably low cost and high magnetization the intermetallic Ce_2Fe_{17} has potential to become a candidate for permanent magnets. Problems arising from the in-plane magnetocrystalline anisotropy and the low T_C could be overcome by doping with light elements. Despite that, there is an ongoing debate regarding the magnetic phases in Ce_2Fe_{17}. While a large number of partially seemingly contradicting experimental findings have been reported, only few theoretical studies exist and they do not capture the experimental findings. Performing a comprehensive study of the magnetic properties of Ce_2Fe_{17} we applied various approaches for the exchange-correlation functional to identify the best theoretical treatment of the system. To account for the mixed valent nature of Ce_2Fe_{17} we tested several approximations including an analysis of the hybridization function. We used a combination of ab initio methods (VASP, FP-LMTO RSPt) to obtain geometrical and magnetic data including magnetic exchange parameters.

Our results [1] clearly show that the ground state is non-collinear with a strong FM component which explains the low magnetic moment reported in experiment. At 93 K the FM component vanishes and we observe correctly the transition to the helical state.

[1] A. Vishina et al., JALCOM **888**, 161521 (2021)

MA 32.7 Thu 16:30 H43

High-throughput and data-mining search for novel rare-earth-free permanent magnets — •Alena Vishina[1], Heike

Herper[1], and Olle Eriksson[1,2] — [1]Department of Physics and Astronomy, Uppsala University, Se-75120 Uppsala, Sweden — [2]School of Science and Technology, Örebro University, SE-701 82 Örebro, Sweden

Rare-earth (RE) magnetic materials dominate the market when high-performance permanent magnets are needed (e.g. the area of 'green' energy technology, such as electric vehicles and windmills). At the same time, there is a growing interest in RE-free alternatives, since the heavier RE elements are quite expensive and are often mined with methods that leave an environmental footprint. We propose to use the data-mining approach to search for high-performance RE-free/lean magnetic materials. Filtering through a large number of known structures from ICSD database, we are looking for materials with high magnetization M > 1 T, uniaxial MAE > 1 MJ/m3, and Tc >300 K. Sometimes, additional elements alterations are attempted to make the material more cost-effective. Two searches have already been performed. New magnetic material has been found and consequently synthesized by experimental collaborators - Co3Mn2Ge. From the ab-initio calculations, the defect-free material was predicted to have the saturation magnetization of 1.71 T, the uniaxial magnetocrystalline anisotropy of 1.44 MJ/m3, and the Curie temperature of 700 K. Its magnetism depends critically on the amount of disorder of the Co and Ge atoms, a further improvement of the magnetism is possible.

MA 32.8 Thu 16:45 H43

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 the program MAELAS[1,2] to calculate 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[3]. 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.

References:[1-3] www.md-esg.eu/software and references therein