SYGM 1: Green Magnets for Efficient Energy Conversion

Ever increasing demands for efficient, low cost energy conversion require the development of new materials, which can be used in e-mobility, power generation, robotics and refrigeration. The class of magnetic materials covers all of these technologies; in fact hard and soft magnets as well as caloric materials are often overlooked key enablers of a net-zero CO2 emission scenario. In e-mobility, every battery needs a magnet, i.e. either the mass of the battery is reduced or the range is extended when highly efficient hard and soft magnets are employed in motor and generator. The complexity of magnetostructural phase transitions offers ample opportunities to design (magneto-) caloric and elastic properties for efficient, climate friendly future cooling technologies, smart actuators and soft magnetic robotics. Organizers: Oliver Gutfleisch (TU Darmstadt) and Michael Farle (U. Duisburg-Essen)

Time: Monday 15:00–17:45 Location: HSZ 01

Invited Talk SYGM 1.1 *(1)* Mon 15:00 HSZ 01
Data mining protocols for functional magnetic materials — •olle Eriksson — Uppsala University, Uppsala, Sweden

Theory of functional magnetic materials for use in permanent magnet applications or for magneto caloric cooling is described in this presentation. Using a high-throughput approach of calculations based on density functional theory together with a data-mining algorithm, several new rare-earth-free permanent magnets are reported. An interesting set of elements is found for materials containing 3d and p-elements, in particular Fe2C, Mn2MoB4, and Mn2WB4. For these systems doping protocols were also investigated and, in particular, (Fe0.75X0.25)2C (X = Mn, Cr, V, and Ti), Mn2XB4 (X = Mo and W) along with Mn2(X0.5Y0.5)B4 (X,Y = Mo, W, Ta, Cr) are suggested here as promising permanent magnets. Screening algorithms for magneto caloric materials are also discussed, and promising compounds will be presented.

Invited Talk SYGM 1.2 *(2)* Mon 15:30 HSZ 01
High performance permanent magnets; elements criticality, new demands, and extrinsic magnetic properties — •Hossein Sepehri-Amin, Xin Tang, Tadakatsu Ohkubo, and Kazuhiro Hono — National Institute for Materials Science, Tsukuba, Japan

Permanent magnets are widely used in the green energy conversions and they play an important role toward realization of carbon neutrality. In order to maintain sustainable production of permanent magnets in a long term, efforts are required to eliminate the permanent magnets* reliance on critical elements such as Dy and to diverge rare-earth usage while maintaining sufficiently large coercivity and energy product in the magnets. we will first present our research efforts on development of high coercivity Dy-free Nd-Fe-B magnets for applications in traction motor of hybrid/electric vehicles and generator of wind turbines. We will demonstrate how grain boundary/interface engineering in the hot-deformed Nd-Fe-B magnets has led to a large coercivity of 2.5 T, remanent magnetization of 1.32 T and excellent thermal stability of coercivity. In the second part of the talk, the potential of Fe-rich SmFe12-based magnets and the current challenges to realize these materials as new permanent magnets will be discussed. we will show our recent success in realizing a sufficiently large coercivity of 1.0 T in rare-earth lean SmFe12-based anisotropic sintered magnets assisted by machine learning. Based on detailed microstructure characterizations, modeled thin films, and micromagnetic simulations, we will discuss the optimum microstructure which can lead to a larger coercivity and remanent magnetization in the SmFe12-based magnets.

Invited Talk SYGM 1.3 *(3)* Mon 16:00 HSZ 01
Magnetic shape memory Heuslers: microstructure-related effects on the martensitic transformation — •Franca Albertini — Institute of Materials for Electronics and Magnetism (IMEM) - CNR, Parma, Italy

The vast family of magnetic shape memory Heuslers provides an extended playground of physical properties. The interplay between a martensitic transformation and magnetically ordered states gives rise to a series of functional properties that can be exploited in different technological sectors, among which solid state refrigeration, thermomagnetic generation, and robotics. Their excellent responsiveness to external fields, i.e. magnetic field, pressure and stress and their combined application, makes them promising for multifunctional exploitation. On the other hand, the hysteretic character of the martensitic transformation limits the performances of these materials in cyclic operations. In my talk I report some recent results on micro and nanoscale materials obtained by different fabrication methods, i.e. epitaxial thin films, micro/nanostructures obtained by lithographic techniques, and mechanically-milled particles. Thin films and micro/nanostructures are of particular interest not only for the realisation of miniaturised devices, but also for providing insights into the magneto-structural coupling at the different length scales. The talk will focus on microstructure tuning and microstructure-related effects on the martensitic transformation, in view of the fully exploitation of this class of materials in caloric and smart applications.

15 min. break

Invited Talk SYGM 1.4 *(4)* Mon 16:45 HSZ 01
Thin film combinatorial studies of hard magnetic materials — •Nora Dempsey — Univ. Grenoble Alpes, CNRS, Grenoble INP, Institut NEEL, 38000 Grenoble, France

Combinatorial thin film studies are used for the screening and optimization of a range of functional materials. The basic idea is to produce compositionally graded films, to allow high throughput characterisation of materials properties as a function of composition, as well as other processing parameters such as deposition temperature and post-deposition annealing conditions. This approach holds much potential for the development of green magnets for efficient energy conversion. In particular, it can be used to study the effect of element substitution in Rare Earth - Transition Metal hard magnetic phases, so as to reduce dependence on critical rare earth elements.

In this talk I will present both recent [1] and on-going studies of compositionally graded hard magnetic materials produced by sputtering asymmetric targets or co-sputtering of multiple targets followed by annealing under different conditions. I will discuss the influence of composition and processing parameters on structural and magnetic properties, as probed using high throughput scanning mode characterisation tools (EDX, XRD and MOKE). I will finish up by presenting future prospects for such studies, in particular when combined with ab-initio calculations on the one hand and machine learning on the other.

[1] Y. Hong et al., J. Mater. Res. Technol. 18 (2022) 1245

Invited Talk SYGM 1.5 *(5)* Mon 17:15 HSZ 01
Magnetocaloric materials for energy-efficient thermal control systems — •Victorino Franco, Aun N. Khan, Jorge Revuelta-Losada, Álvaro Díaz-García, Luis M. Moreno-Ramírez, and Jia Yan Law — University of Seville, Spain

Energy efficient and environmentally friendly thermal management have a direct impact on the sustainability of our way of life, with magnetocaloric refrigeration being promising for achieving a greener cooling technology [1]. However, appliances are not yet on the consumer market due to relevant limitations of the active materials. In addition to applications point of view, the effect can be used to perform studies of phase transitions. Focusing on rare earth free materials, two new types of have a promising future: high entropy alloys and materials for additive manufacturing. We will present a novel fabrication procedure for obtaining homogeneous composite filaments for additive manufacturing and we will demonstrate that the magnetocaloric response of the fillers is not affected by the manufacturing procedure [2]. We will also highlight magnetocaloric high-entropy alloys, for which new compositions have allowed to close the gap between traditional HEA and high-performing magnetocaloric materials [3,4].

[1] V. Franco et al., Progress in Materials Science 93 (2018) 112; [2] Á. Díaz-García et al., Composites Communications 35 (2022) 101352;

[3] J.Y. Law et al., APL Materials 9, (2021) 080702; [4] J.Y. Law et al., Journal of Materials Research (2022). https://doi.org/10.1557/s43578-022-00712-0