MA 22: Caloric Effects in Ferromagnetic Materials

Time: Wednesday 9:30–11:30 Location: H19

MA 22.1 Wed 9:30 H19

Utilizing frustration in Gd- and Yb-based oxides for milli-Kelvin adiabatic demagnetization refrigeration — •Tim Treu[1], Prachi Telang[1], Marvin Klinger[1], Alexander Tsirlin[2], Anton Jesche[1], and Philipp Gegenwart[1] — [1]Experimental Physics VI, Center for Electronic Correlations and Magnetism, University of Augsburg — [2]Felix Bloch Institute for Solid-State Physics, University of Leipzig

Gadolinium- and Ytterbium-oxide based frustrated magnets have recently been characterised as excellent millikelvin adiabatic demagnetization refrigerants [1]. They offer several advantages over conventional paramagnetic hydrated salts, such as higher entropy density at similar minimum temperatures, chemical stability and UHV compatibility. We present a comprehensive study of the structural, magnetic and thermodynamic properties as well as the adiabatic demagnetisation refrigeration performance of several different Gd- and Yb-based oxides (including [1-2] and further unpublished results). For the temperature range between 0.03 and 2 K, a systematic comparison of the field-induced entropy density change and the refrigerant capacity is provided, demonstrating the advantages of frustrated magnets for low-temperature ADR.

Work supported by the German Research Foundation through the project 514162746 (GE 1640/11-1).

[1] T. Treu et al., J. Phys. Condens. Matter 37, 013001 (2025).
[2] P. Telang et al., arXiv:2411.04805

MA 22.2 Wed 9:45 H19

High-throughput design of all-d-metal Heusler alloys for transverse thermoelectric applications — •Fu Li, Hao Wang, Ruiwen Xie, and Hongbin Zhang — Technical University of Darmstadt, 64287 Darmstadt, Germany

Magnetic materials with prominent topological transport properties have been attracting significant attention due to the underlying intriguing physics and great potentials in various applications. Among these, Heusler alloys are particularly interesting because of their compositional flexibility which enables tunability of their physical properties via chemical doping. In this work, we perform high-throughput density functional theory calculations to evaluate the effects of chemical doping on the intrinsic anomalous Hall conductivity (AHC) and anomalous Nernst conductivity (ANC) in all-d-metal Heusler compounds, where chemical alloying with neighboring elements is considered using the virtual crystal approximation. The AHC and ANC are computed using the tight-binding Hamiltonian by automatically constructing the maximally localized Wannier functions. It is observed that rigid band model does not apply in all cases, because not only the Fermi energy has been shifted, but also the band structure has modified significantly. For (Pt0.7Ir0.3)2RhFe, detailed analysis reveals that the significant AHC and ANC are originated from the Weyl points close to the Fermi energy. These findings highlight the critical importance of chemical doping in the development of high-performance materials.

MA 22.3 Wed 10:00 H19

Electronic structure of all-*d*-metal Ni(-Co)-Mn-Ti vs. *p*-*d* Ni_2MnSn: DFT and XAS insights — •Olga Miroshkina[1], Johanna Lill[1], Benedikt Eggert[1], Benedikt Beckmann[2], David Koch[2], Franziska Scheibel[2], Katharina Ollefs[1], Wolfgang Donner[2], Oliver Gutfleisch[2], Heiko Wende[1], and Markus Gruner[1] — [1]University of Duisburg-Essen, Duisburg, Germany — [2]Technical University of Darmstadt, Darmstadt, Germany

All-*d*-metal Heusler alloys are a new class of promising caloric materials for energy efficient solid-state refrigeration [1]. We investigate the peculiar differences of the electronic structure between *d*-*d* Ni(-Co)-Mn-Ti and *p*-*d* Ni_2MnSn by combining density functional theory and x-ray absorption spectroscopy (XAS). To retrieve the distinctive characteristics of *d*-*d* orbital hybridization in K- and $L_{2,3}$-edges spectra, we correlate the features in the electronic densities of states (DOS) and XAS. The comparison of *d*-*d* Ni(-Co)-Mn-Ti with the conventional *p*-*d* Ni_2MnSn enables us to reveal the impact of the third *d*-element on magnetic and vibrational properties. The correlation of the calculated and measured XAS shows the presence of (partial) disorder not only in all-*d*-metal systems, but also in *p*-*d* Ni_2MnSn sample. This is consistent with our earlier findings of the traces of atomic disorder in the vibrational DOS [2]. Therefore, the interatomic hybridization in all-*d*-metal Heusler compounds can be utilized as an intrinsic control parameter for designing high-performance caloric materials.

[1] B. Beckmann *et al.*, *Acta Materialia* **246** 118695 (2023).
[2] O. Miroshkina *et al.*, *Phys. Rev. B* **106**, 214302 (2022).

MA 22.4 Wed 10:15 H19

Magnetocrystalline anisotropy of magnetocaloric Fe_2AlB_2 single crystals — •Nicolas Josten[1], Ralf Meckenstock[1], Anna Semisalova[1], Benedikt Beckmann[2], Konstantin Skokov[2], Oliver Gutfleisch[2], Hanna Pazniak[3], Thierry Ouisse[3], Michael Farle[1], and Ulf Wiedwald[1] — [1]Faculty of Physics and Center for Nanointegration (CENIDE), University Duisburg Essen, Germany — [2]Functional Materials, Institute of Materials Science, Technical University of Darmstadt, Germany — [3]LMGP, Grenoble INP, CNRS, Université Grenoble Alpes, France

Fe_2AlB_2 is a low-cost, low weight and easily synthesized material composed of abundant elements for magnetocaloric applications near room temperature [1]. It is a ferromagnetic MAB phase with an orthorhombic crystal structure and a Curie-temperature T_C = 274 K [2]. The low crystal symmetry of Fe_2AlB_2 leads to a significant magnetocrystalline anisotropy up to around 1 $MJ{\cdot}m^{-3}$ at 10 K. We determined the temperature-dependent magnetocrystalline anisotropy constants of a bulk Fe_2AlB_2 single crystal using the Sucksmith-Thomson method and broadband ferromagnetic resonance measured along principal crystallographic directions. Both methods show perfect quantitative agreement.

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[1] B. Beckmann et al. J. Appl. Phys. 133, 173903 (2023)
[2] T. N. Lamichhane et al. Phys. Rev. Mater. 2, 084408 (2018)

MA 22.5 Wed 10:30 H19

Effect of boron doping on the magnetocaloric properties in La(Fe, Si)$_{13}$ — •M. Strassheim[1,2], C. Salazar-Mejía[1], J. Wosnitza[1,2], and T. Gottschall[1] — [1]Hochfeld-Magnetlabor Dresden (HLD-EMFL), HZDR, Dresden, Germany — [2]TU Dresden, Dresden, Germany

Traditional refrigeration methods rely on gases and toxic refrigerants, contributing to environmental degradation and energy inefficiencies. In contrast, magnetocaloric materials offer a promising alternative, with the ability to produce large, reversible thermal changes when exposed to magnetic fields. Among these, La(Fe,Si)$_{13}$-based compounds stand out due to their excellent magnetocaloric effect at near-room temperatures, relatively high transition temperatures, and comparatively low cost of the base elements, making them ideal candidates for practical applications. The influence of elements such as hydrogen and carbon on interstitial sites of the La(Fe,Si)$_{13}$ lattice is already well understood, but boron doping is not. We present a study of the latter in regard of magnetization and transition temperature with a perspective of both room-temperature and cryogenic applications.

MA 22.6 Wed 10:45 H19

Direct measurements of the adiabatic temperature change of a dysprosium single crystal — •E. Bykov[1], T. Gottschall[1], J. Wosnitza[1,2], C. Salazar Mejia[1], M. D. Kuz'min[3], Y. Mudryk[4], and D. L. Schlagel[4] — [1]Hochfeld-Magnetlabor Dresden (HLD-EMFL), HZDR, Dresden, Germany — [2]Technische Universität Dresden, Dresden, Germany — [3]Aix-Marseille Université, IM2NP, Marseille, France — [4]Ames Laboratory, U.S. Department of Energy, Iowa State University, Ames, USA

Heavy rare-earth elements in the Gd-Tm series have unique magnetic properties due to their electronic structure. The exchange between 4*f* electrons occurs via RKKY interactions and, therefore, is extremely sensitive to the ionic radii of the elements, exhibits anisotropy, and shows pronounced magnetoelastic coupling. This leads to various magnetic phase diagrams with different helicoidal magnetic structures despite similar chemical and physical properties of the 4*f* elements. The high total angular momentum enables significant magnetocaloric effects, which is relevant for magnetic refrigeration applications. Gadolinium, for instance, exhibits a notable magnetocaloric effect at room temperature, serving as a comparative standard. Prior

research at the Dresden High Magnetic Field Laboratory demonstrated record magnetocaloric effects in terbium. Holmium's broad plateau in ΔT_{ad} at 5 T suggests potential in cryogenic applications, such as for hydrogen liquefaction. Continuing our study of the magnetocaloric effect of the $4f$ elements, we present our recent results for a dysprosium single crystal.

MA 22.7 Wed 11:00 H19

Estimation of the inverse giant barocaloric effect in Fe_2P — •Sven Wiesekopsieker[1,2], Tapas Samanta[1], Chris Taake[1], Judith Bünte[1], Andreas Hütten[1], and Luana Caron[1,2] — [1]Faculty of Physics, Bielefeld University, Bielefeld 33501, Germany — [2]Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin 12489, Germany

The Fe_2P system has so far been explored with respect to the magnetocaloric effect, linked to it's first-order magnetostructural transition between a ferromagnetic high volume phase at low T and a paramagnetic low volume phase at high T. Both phases show a hexagonal structure ($P\bar{6}2m$ space group) [1]. This transition also gives rise to the barocaloric effect (BCE), which we studied by means of an indirect method, consisting of magnetization measurements under pressure and ambient pressure differential scanning calorimetry [2]. Application of pressure shifts the transition by $-45.8(1.0)$ K/GPa. It is accompanied by a transition entropy change of $|\Delta S_{\mathrm{tr}}| = 1.06(0.16)$ J/(kg K), similar to that reported by Hudl et al. Under application of 0.74 GPa a moderate adiabatic temperature change of -0.65 K is observed.

[1] A. Koumina et al., Ann. Chim. Sci. Mat. 23, 177 (1998)
[2] X. J. He et al., J. Mater. Sci. 52, 2915 (2017)
[3] M. Hudl et al., Phys. Rev. B 90, 144432 (2014)

MA 22.8 Wed 11:15 H19

Towards the hydrogenation of DyCo2 for cryogenic magnetocaloric liquefaction applications — •Allan Döring, Imants Dirba, Fernando Maccari, Konstantin Skokov, and Oliver Gutfleisch — TU Darmstadt, Darmstadt, Germany

Hydrogen can play an important role in the carbon-neutral society. Liquid H2 stands out for its higher volume-to-energy ratio. However, the current liquefaction method sums up to 34% of the costs to liquefy H. The magnetocaloric cooling could be one alternative to improve the efficiency of this process. Hence, research for materials with intense magnetocaloric effect (MCE) between 20 K and 77 K is needed. Those materials exhibit the peak of the MCE at transition temperatures, such as the Curie temperature (TC). Further, the MCE is stronger in heavy rare-earth (Re) based compounds, such as ReCo2. However, some of the ReCo2 materials exhibit giant MCE in temperatures above 77 K, and one way to shift down TC of such compounds is by introducing H as interstitial atoms. The TC of DyCo2 was shifted down by 120 K through the hydrogenation processK. Further, partially hydrogenated samples showed two distinct TCs. By X-ray diffraction analysis a crystalline state was confirmed with distorted lattices. The magnetic entropy changes were measured in non-hydrogenates, partially and fully hydrogenated samples, revealing a peak of entropy change at 25 K after hydrogenation. The reversibility of hydrogenation and its microstructuctre was also investigated. We acknowledge the HyLICAL project through grant 101101461.