MA 13: Magnetic Heuslers and Semiconductors

Time: Monday 15:00–17:15 Location: POT/0361

MA 13.1 Mon 15:00 POT/0361

Investigation on the interplay of antisite disorder and magnetic ordering in $Co_2FeAl_{1-x}Si_x$ Heusler system — •Ahmad Omar[1], Matthias Frontzek[2], Robin Kramer[1], Bernd Büchner[1], and Sabine Wurmehl[1] — [1]Leibniz Institute for Solid State and Materials Research Dresden, Germany — [2]PSI Villigen, Switzerland

Quaternary Co-based Heusler compounds such as $Co_2FeAl_{1-x}Si_x$ system are predicted to demonstrate half-metallic ferromagnetism for the $L2_1$ ordered structure. However, the observed physical properties, are often in contrast to theory due to antisite disorder commonly present in practical samples. The $L2_1$-B_2 order-disorder transition is further convoluted with the ferromagnetic transition and is not well understood. Therefore, it is pertinent to understand the ordering phenomenon and develop routes to improve the order for practical realization of the desired properties. Herein, we present a systematic study of the impact of synthesis route and annealing parameters on the obtained order fraction in the samples, through detailed structural and magnetic characterization. In-situ neutron diffraction is performed during annealing to directly investigate the order-disorder transition. The interplay of disorder and the magnetic ordering is further studied through magnetic field annealing experiments. We aim to elucidate the structure-property relationships in the quaternary $Co_2FeAl_{1-x}Si_x$ system, developing methodology for tuning of the disorder through synthesis or post-processing routes, thus enabling a practical realization of half metallic ferromagnetism in the Heusler system.

MA 13.2 Mon 15:15 POT/0361

Impact of disorder on magnetic and vibrational properties of Ni-Mn-Sn Heusler alloys — •Olga Miroshkina[1], Benedikt Eggert[1], Benedikt Beckmann[2], Franziska Scheibel[2], Katharina Ollefs[1], Oliver Gutfleisch[2], Heiko Wende[1], and Markus E. Gruner[1] — [1]University of Duisburg-Essen, Duisburg, Germany — [2]Technical University of Darmstadt, Darmstadt, Germany

Ni-Mn-Sn Heusler alloys are attractive candidates for multi-stimuli caloric cooling. They undergo a magneto-structural phase transition at temperature that can be tuned via chemical disorder. In this work, we investigate the austenitic and martensitic phases near the composition $Ni_{50}Mn_{35}Sn_{15}$ by means of density functional theory complemented by magnetometry and nuclear resonant inelastic x-ray scattering (NRIXS). Bain-path calculations reveal strong competition between ferro-(FM) and ferrimagnetic (FiM) states in austenite and a clear FiM configuration in the $L1_0$ martensite. The FiM contribution in the cubic phase is confirmed by comparing the calculated Sn vibrational DOS with that extracted from NRIXS. In martensite, frustrated exchange introduced by Mn excess can prevail in the tetragonal FiM $L1_0$ phases and make nano-twinns competitive. We find that twins constructed according to the continuum theory of martensite are energetically even more favorable than $L1_0$. A striking outcome is that all Mn/Sn-disordered configurations are energetically more favorable than the ordered ones, with the FiM 4O and 10M phases remaining the most competitive structures. Financial support within the DFG Projects MI 3273/1 and CRC/TRR 270 is gratefully acknowledged.

MA 13.3 Mon 15:30 POT/0361

Finite Size-Effects in Martensite Microstructure of Magnetic Shape Memory Films — Satyakam Kar[1,2], Aman Singh[1], Kornelius Nielsch[1], Heiko Reith[1], and •Sebastian Fähler[3] — [1]Leibniz IFW Dresden, 01069 Dresden, Germany — [2]TU Dresden, Institute of Materials Science, 01062 Dresden, Germany — [3]Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden, Germany

Magnetic shape memory alloys, owing to their multifunctional properties, are a promising material system for integration into microsystems. Their multifunctionality arises from the coexistence of ferroelasticity and ferromagnetism. While size-effects in ferromagnetic microstructure are well understood, corresponding experiments on the influence of finite size on the ferroelastic martensite microstructure are sparse. In this study, we use epitaxially grown Ni-Mn-Ga-based films as a model system to investigate the influence of a finite size in the martensite microstructure under constrained and freestanding conditions. Our results show that the microfabricated patterns, in both conditions, retain the characteristics of their continuous film microstructures. Film thickness has a strong influence, as this is the smallest extension investigated in our study. We analyze similarities and differences between ferromagnetic and ferroelastic microstructure, as understanding finite size effects is decisive for using these multifunctional materials in microsystems with reduced size.

MA 13.4 Mon 15:45 POT/0361

Microstructure Design via Additive Manufacturing of Heusler Alloys for Multicaloric Applications — •Nene Narh Teinor[1,2], Adrian Guder[3], Johannes Puy[1], Christian Lauhoff[3], Thomas Niendorf[3], Oliver Gutfleisch[1], and Franziska Scheibel[1,2] — [1]Institute of Materials Science, Technical University of Darmstadt, Germany — [2]Additive Manufacturing Center, Technical University of Darmstadt, Darmstadt, Germany — [3]Institute of Materials Engineering, University of Kassel, Germany

Heusler alloys like NiMnSn and NiCoMnTi show strong potential for solid-state cooling due to their first-order magnetostructural transitions (FOMST). However, their functional performance is highly sensitive to processing conditions. In this work, bulk samples are produced via Laser Powder Bed Fusion (PBF-LB/M) using gas-atomized powders to explore the influence of additive manufacturing parameters on microstructure and caloric properties. By varying laser power, scan speed, and strategy, we achieve controlled tuning of martensitic, austenitic, and Curie temperatures, as well as reduced thermal hysteresis. Structural, compositional, and magnetic analyses reveal how rapid solidification enhances the sharpness and reversibility of FOMST. We demonstrate that additive manufacturing not only preserves the functional properties of these alloys but also enables active enhancement of their tunability of transition behavior compared to conventionally processed samples. We acknowledge Deutsche Forschungsgemeinschaft (DFG) support through the CRC/TRR 270 (Project ID 405553726)

MA 13.5 Mon 16:00 POT/0361

Modelling the martensitic transformation in Ni-Mn-based Heusler compounds with machine-learning force-fields — •Markus E. Gruner, Mike J. Bruckhoff, and Olga Miroshkina — Faculty of Physics and CENIDE, University of Duisburg-Essen, D-47048 Duisburg

Functional properties of Ni-Mn-based Heusler alloys, such as Ni_2MnGa, depend on the presence of hierarchically twinned, modulated structures in the martensite phase. These can be interpreted as an adaptive, self-organized arrangement of [101]-aligned nanotwins consisting of non-modulated tetragonal building blocks. Density functional theory (DFT) suggests that these martensites are connected to cubic austenite via a downhill transformation path. This is owed to a Fermi surface reconstruction, softening the corresponding acoustic phonons of austenite. Modeling free energy surfaces at finite temperatures or the dynamics of the martensitic transition as probed in recent ultrafast laser heating experiments [1] is too expensive for conventional DFT. Machine-learning force fields (ML-FF) trained on DFT data offer a possibility to account for electronic instabilities and allow to explore the impact of adaptive nanotwining on the martensitic transition using ML-FF in classical molecular dynamics simulations. Funding by the DFG via TRR270 (B06), SFB1242 (C02) and MI3273/1 is gratefully acknowledged.

[1] Y. Ge, F. Ganss, D. Schmidt, D. Hensel, M. J. Bruckhoff, S. Sadashivaiah, B. Neumann, M. Brede, M. E. Gruner, P. Gaal, K. Lünser, S. Fähler, arXiv:2509.06513.

MA 13.6 Mon 16:15 POT/0361

Enhanced anomalous Hall response via nodal line tuning in Co2VSn(1-x)Alx topological semimetal — •Sunil Wilfred DSouza[1], Shivani Rastogi[2], Gaurav Shukla[3], Nidhi Shukla[2], Jan Minár[1], and Sanjay Singh[2] — [1]New Technologies Research Centre, University of West Bohemia, 30100 Pilsen, Czech Republic — [2]School of Materials Science and Technology, Indian Institute of Technology (Banaras Hindu University), Varanasi 221005, India — [3]National Institute for Materials Science (NIMS), Tsukuba 305-0047, Japan

Topological semimetals (TSMs) with nodal-line states exhibit strong Berry-curvature driven transport. We Investigate Co2VSn(1-x)Alx (x = 0-0.75) to understand how hole doping tunes the nodal line relative

to the Fermi level. Al substitution shifts the nodal-line states upward, leading to a maximum intrinsic anomalous Hall conductivity (AHC) of 203 S/cm at x = 0.5, representing a significant enhancement over the undoped compound. First-principles calculations corroborate the nodal line in Co2VSn, its gapping under SOC, and its progressive alignment with the Fermi level upon Al doping. The correlation between nodal-line tuning and enhanced AHC highlights an effective strategy for controlling Berry-curvature driven transport in magnetic TSMs.

MA 13.7 Mon 16:30 POT/0361

Manipulating the first-order magnetostructural phase transition in Ni-Mn-Sn Heusler alloy through nano-functionalization — •Johannes Puy[1], Nadine Stratmann[2], Hamed Shokri[3], Bilal Gökce[3], Stephan Barcikowski[2], Oliver Gutfleisch[1], Anna Ziefuss[2], and Franziska Scheibel[1] — [1]TU Darmstadt, Darmstadt, Germany — [2]Universität Duisburg-Essen, Essen, Germany — [3]BU Wuppertal, Wuppertal, Germany

Ni-Mn-based Heusler alloys are considered as a promising candidate for magnetocaloric or multicaloric cooling applications, as they exhibit an inverse magnetocaloric and conventional elastocaloric effect, which arise from a first-order magnetostructural phase transition (FOMST). However, the practical use of these alloys is limited by the thermal hysteresis associated with the FOMST and their intrinsic brittleness. This work demonstrates a novel approach to tailor the FOMST characteritics and the mechanical stability of spark-plasma-sintered (SPS) Ni-Mn-Sn by nano-functionalization. Silver and zirconium diboride nanoparticles (NP) are synthesized by pulsed laser fragmentation of microparticles (MP-LFL) and subsequently used to functionalize Ni-Mn-Sn powder (150 - 75 μm) at varying mass loadings. This enables targeted modification of the sintered particle interfaces, which act as martensite nucleation sites, but also as origin of fracture under compressive stress. We systematically characterize the influence of NP-functionalization on the microstructure, the temperature-induced FOMST and the mechanical stability. This work was supported by the DFG within the CRC/TRR 270 (Project ID No. 405553726).

MA 13.8 Mon 16:45 POT/0361

Fe^{3+}-Centers as Structural Probes in Fe-Doped $Cs_2AgBiBr_6$ Semiconducting Perovskite — •Volodymyr Vasylkovskyi[1], Timur Biktagirov[2], Anastasiia Kultaeva[1], Carlos Canhassi[3], Mykola Slipchenko[4], Yakov Kopelevich[3], and Vladimir Dyakonov[1] — [1]Experimental Physics 6, University of Würzburg, 97074 Würzburg, Germany — [2]Physics Department, Paderborn University, D-33098 Paderborn, Germany — [3]Gleb Wataghin Institute of Physics, University of Campinas, 13083-859 Campinas, Brazil — [4]Institute for Scintillation Materials, Kharkiv, Ukraine

Fe-doping introduces new functionality into halide double perovskites alongside modifying optical properties. We report controlled growth of Fe-doped $Cs_2AgBiBr_6$ single crystals and correlate their structural, optical, and magnetic parameters. ICP analysis confirms Fe incorporation below 0.1% relative to Bi, which induce defect-related sub-gap absorption and photoluminescence shift. EPR measurements reveal an $S = 5/2$ Fe^{3+} spin center whose anisotropy follows the phase transition below 120 K. DFT calculations, guided by angular-dependent EPR, identify these centers as impurity-vacancy complexes, likely Fe_{Bi}-V_{Br}. SQUID magnetometry shows ferromagnetic-type hysteresis at room temperature, with rising spontaneous magnetization below 20-30 K and magnetization irreversibility under zero-field and field-cooling, confirming ferromagnetism from Fe-related defect complexes. Even small Fe amounts significantly alter optical and magnetic behavior of $Cs_2AgBiBr_6$, emphasizing the role of controlled doping and defect engineering in lead-free double perovskites.

MA 13.9 Mon 17:00 POT/0361

Pressure-dependence of the thermoelectric properties of $MnIn_2Te_4$ — •Shubham Rakesh Singh, Mohammed Ghadiyali, and Udo Schwingenschlögl — Physical Science and Engineering Division (PSE), King Abdullah University of Science and Technology (KAUST), Thuwal 23955-6900, Saudi Arabia

We investigate the thermoelectric properties of $MnIn_2Te_4$ in its two experimentally characterized phases. The tetragonal phase ($I\bar{4}2m$) undergoes a pressure-induced transition to an orthorhombic phase ($Pnma$) at 1.3 GPa. First-principles calculations reveal for both phases a small energy difference between antiferromagnetic and ferromagnetic states. The band gap is 1.04 (0.70) eV in the tetragonal phase and 1.25 (1.10) eV in the orthorhombic phase for the antiferromagnetic (ferromagnetic) state. A higher power factor is achieved by n-type than by p-type carriers. At 700 K, for example, the more densely packed orthorhombic phase exhibits a 56% reduction in the lattice thermal conductivity as compared with the tetragonal phase, yielding high thermoelectric figures of merit of 1.23 for n-type carriers and 0.96 for p-type carriers at optimal carrier concentration.