MA 37: Magnetic Heuslers

Time: Thursday 9:30–11:00 Location: HSZ 403

MA 37.1 Thu 9:30 HSZ 403

Enhanced magnetism of antiphase boundaries in Fe_2CoAl compound — Martin Friák[1], Josef Gracias[2], Jana Pavlů[2], and •Mojmír Šob[2,1] — [1]Inst. Phys. Mat., Czech Acad. Sci., Brno, Czech Rep. — [2]Dept. Chem., Fac. Sci., Masaryk Univ., Brno, Czech Rep.

We performed a quantum mechanical examination of thermodynamic, structural, elastic, and magnetic properties of single-phase ferromagnetic Fe_2CoAl with a chemically disordered B2-type lattice with and without antiphase boundaries (APBs) with (001) crystallographic orientation. Fe_2CoAl was modeled using two different 54-atom supercells with atoms on the two B2 sublattices distributed according to the special quasi-random structure (SQS) concept. Both computational models used exhibited very similar formation energies (−0.243 and −0.244 eV/atom), B2-structure lattice parameters (2.849 and 2.850 Å), magnetic moments (1.266 and 1.274 μ_B/atom), practically identical single-crystal elastic constants (C_{11} = 245 GPa, C_{12} = 141 GPa, and C_{44} = 132 GPa) and auxetic properties (the lowest Poisson ratio close to -0.1). In contrast to these similarities, the averaged APB interface energies were observed to be 199 and 310 mJ/m^2 for the two models. The studied APBs increased the total magnetic moment by 6 and 8 % due to a volumetric increase as well as local changes in the coordination of Fe atoms (their magnetic moments are reduced for increasing number of Al neighbors but increased by the presence of Co). The APBs also enhanced the auxetic properties.

MA 37.2 Thu 9:45 HSZ 403

VTaNbAl: A new class of spin gapless semiconductor with topological non-trivial features — •Deepika Rani[1], P. C. Sreeparvathy[2], K. Gopi Suresh[2], Ratnamala Chatterjee[1], and Aftab Alam[2] — [1]Department of Physics, Indian Institute of Technology Delhi, Hauz Khas, New Delhi 110016, India — [2]Department of Physics, Indian Institute of Technology Bombay, Mumbai 400076, Maharashtra, India

We report the theoretical prediction of a new class of spin gapless semiconductor (SGS) hosting topological non-trivial features along with a fully compensated ferrimagnetic state in VTaNbAl, a quaternary Heusler alloy. Unlike conventional SGS, this new class of compound acquires a unique band structure with opposite spin characters in the valance and conduction band edges making them potential candidates for spin valves and large anomalous Nernst effect. Interestingly, despite of a compensated ferrimagnetic (CF) behavior, VTaNbAl shows a reasonably large anomalous Hall effect possibly arising from the intrinsic non-vanishing Berry curvature. The CF state breaks the time-reversal symmetry and hence opens the possibility of Weyl nodes. We found four pairs of Weyl nodes located near the Fermi level leading to the non-zero Berry curvature, and hence a large anomalous Hall conductivity (~ 100 S/cm). Our experimental synthesis confirms NbVTaAl to crystallize in a cubic Heusler structure with an A2-type disorder. Magnetization measurement shows a very small saturation moment, which agrees fairly well with our theoretical findings of fully compensated ferrimagnetism in the alloy.

MA 37.3 Thu 10:00 HSZ 403

Long range ordering in NiCoMnAl magnetic shape memory thin films with martensitic intercalations — •Inga Ennen, Dario Stierl, Laila Bondzio, and Andreas Hütten — Thin Films and Physics of Nanostructures, Physics Department, Bielefeld University, 33615 Bielefeld, Germany

Magnetic shape memory Heusler alloys, like NiMnX (X=Al,Ga,Sn,In), are considered as promising materials for magnetocaloric cooling applications due to their magnetoelastic coupling near room temperature. In order to reduce the thermal hysteresis in NiCoMnAl thin films, the usage of alternating active transforming austenitic and martensitic intercalation layers are beneficial. Therefore, the stoichiometry of these two layers is chosen in such a way that their thermal hysteresis does not overlap. If the austenite active layers have a similar thickness compared to the martensite intercalations a 3D check board pattern becomes visible in HRTEM cross section images. The contrast is due to alternating martensite/austenite domains.

In this contribution we aim for an improved understanding of the 3D check board pattern formation. Therefore, the number of the alternating layers as well as the ratio between the thicknesses of the two different layers have been varied. The phase transition has been characterized by temperature dependent XRD and TEM analysis. Furthermore, freestanding Heusler films have been prepared and analyzed in comparison to the substrate-bounded systems.

MA 37.4 Thu 10:15 HSZ 403

Anomalous Hall effect in epitaxial thin films of the hexagonal Heusler MnPtGa noncollinear hard magnet — •Edouard Lesne[1], Rebeca Ibarra[1,2], Bushra Sabir[3], Bachir Ouladdiaf[4], Ketty Beauvois[4], Alexandr Sukhanov[2], Rafal Wawrzynczak[1], Walter Schnelle[1], Anton Devishvili[4], Dmytro Inosov[2], Jacob Gayles[3], Claudia Felser[1], and Anastasios Markou[1] — [1]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [2]Technische Universität Dresden, Dresden, Germany — [3]University of South Florida, Tampa, United States of America — [4]Institut Laue-Langevin, Grenoble, France

Centrosymmetric MnPtGa Heusler films grown by magnetron sputtering on (0001)−Al_2O_3 crystallize with an out-of-plane c-axis crystal orientation, along which they exhibit perpendicular magnetic anisotropy below their Curie temperature (T_C = 263 K). Further, below a thermally induced spin reorientation transition at 160 K, the magnetic groundtstate, determined by single-crystal neutron diffraction, is found to be a noncollinear spin-canted state where the Mn moments tilt 20° away from the c-axis [*Appl. Phys. Lett.* 120, 172403 (2022)].

Furthermore, the anomalous Hall conductivity (AHC) of 20−60 nm thick MnPtGa epitaxial films is found to exhibit a strongly nonmonotonic behaviour as a function of longitudinal conductivity and temperature, whereby the AHC changes sign at T^* = 110 K. Our findings, supported by first-principle calculations, hint at an anomalous Hall effect of intrinsic origin driven by a momentum-space Berry curvature mechanism [*Adv. Mater. Interfaces* 9, 2201562 (2022)].

MA 37.5 Thu 10:30 HSZ 403

Effect of increasing Mn content on twin mobility in Mn-excess Ni-Mn-Ga alloys — •Martin Heczko[1], Petr Šesták[2], and Martin Zelený[1] — [1]Institute of Materials Science and Engineering, Faculty of Mechanical Engineering, Brno University of Technology, Brno, Czech Republic — [2]Institute of Physical Engineering, Faculty of Mechanical Engineering, Brno University of Technology, Brno, Czech Republic

Martensitic phases of Ni-Mn-Ga ferromagnetic shape memory alloy are considered to be useful in various advanced engineering applications due to reported giant magnetic field induced strain (MFIS). The MFIS originates in the high mobility of twin boundaries combined with large magneto-crystalline anisotropy. We calculated the generalized planar fault energy (GPFE) curves using the spin-polarized DFT method implemented in the Vienna Ab Initio Simulation Package (VASP) to reveal the effect of increasing concentration of excess Mn and its magnetic ordering on formation and propagation of twin boundaries. Effects of local arrangement of excess Mn atoms in Ga sublattice has been considered as well.

Our results show that the barriers for nucleation and grow of a twin rise with increasing content of Mn. It results in more difficult twin formation and propagation in compositions far from stoichiometry. This effect is even more enhanced if excess Mn atom in Ga sublattice is located exactly in the planar fault, and when they are ordered antiferromagnetically.

MA 37.6 Thu 10:45 HSZ 403

The impact of disorder on the 4O-martensite of Ni-Mn-Sn Heusler alloy — •Martin Friák[1], Martin Zelený[2,3], Jiří Kaštil[4], Jiří Kamarád[4], Martin Míšek[4], Zdeněk Arnold[4], Ilja Turek[1], Oldřich Schneeweiss[1], and Mojmír Šob[5,1] — [1]Institute of Physics of Materials, Czech Academy of Science, Brno, CZ — [2]Institute of Materials Science and Engineering, Faculty of Mechanical Engineering, Brno University of Technology, Brno, CZ — [3]Faculty of Mathematics and Physics, Charles University, Prague, CZ — [4]Institute of Physics, Czech Academy of Sciences, Prague, CZ — [5]Department of Chemistry, Faculty of Science, Masaryk University, Brno, CZ

We have performed a quantum-mechanical study of thermodynamic, elastic, magnetic and structural properties of four different ferrimag-

netic states in $Ni_{1.9375}Mn_{1.5625}Sn_{0.5}$ martensite. They are modeled by the four-layer modulated 4O structures with Mn-excess atoms randomly distributed in Ni and Sn sublattices. The Mn atoms at the Ni sublattice turn out to play a key role in the system. A reversal of the orientation of their local magnetic moments has a huge impact on the properties of the whole system. The lowest-energy configuration exhibits anti-parallel local magnetic moments of these Mn atoms with respect to the orientation of the total magnetic moment. By testing both elasticity and phonons we conclude that the lowest-energy state is mechanically stable. Vibrational properties of individual atoms are found to be very sensitive to the chemical disorder. For details see Intermetallics 151 (2022) 107708, DOI:10.1016/j.intermet.2022.107708.