MM 72: Magnetic Shape Memory Alloys (joint with MA)

Time: Friday 9:30–10:30 Location: TC 010

MM 72.1 Fri 9:30 TC 010

Magnetic ground state and compositional stability of epitaxial strain induced martensites in Fe_xRh_{1-x} thin films — •Ralf Witte[1], Markus E. Gruner[2,3], Richard A. Brand[1,2], Di Wang[1,4], Heiko Wende[2], Robert Kruk[1], and Horst Hahn[1,5] — [1]Institute of Nanotechnology, Karlsruhe Institute of Technology — [2]Faculty of Physics and Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen — [3]Forschungs-Neutronenquelle Heinz Maier-Leibnitz (FRM II), Technische Universität München — [4]Karlsruhe Nano Micro Facility (KNMF), Karlsruhe Institute of Technology — [5]KIT-TUD-Joint Research Laboratory Nanomaterials, Technical University Darmstadt

Recently we reported on the formation of an adaptive martensite structure observed in chemically disordered, equiatomic FeRh thin films which were subject to large epitaxial strains [1]. A magnetically disordered ground state of the resulting structure was predicted from density functional theory (DFT) calculations. In this contribution we will show by means of low temperature conversion electron Mössbauer spectroscopy that the strain induced structural change leads to a magnetic spin glass state at low temperature in agreement with DFT calculations. Additionally, structural and magnetic characterization of thin films with different Fe_xRh_{1-x} composition will be presented. The observed magnetic and strain adaption behavior is discussed with respect to the equilibrium binary alloy phase diagram and the existing metastable phases. We acknowledge funding by the DFG via HA1344/28-1. [1] R. Witte *et al.*, PRB 93, 104416 (2016).

MM 72.2 Fri 9:45 TC 010

Ab initio design strategies for NiMn-based magnetocaloric materials: The effect of Co and Fe — •Biswanath Dutta, Fritz Körmann, Tilmann Hickel, and Jörg Neugebauer — Max-Planck-Institut für Eisenforschung GmbH, 40237 Düsseldorf, Germany

In the quest to improve magnetocaloric properties of NiMn-based Heusler alloys, doping with ferromagnetic elements is found to be a promising strategy. Recent experiments show a large magnetization drop also known as metamagnetic transition and a giant inverse magnetocaloric effect (MCE) upon martensitic transformation in Co and Fe substituted NiMn-based Heusler alloys. In spite of this huge potential, a complete understanding of the role of different substitutional elements in these materials is still missing. Using ab initio calculations, we study the impact of Co and Fe on the martensitic transformation and the magnetic properties in Mn-excess Ni-Mn-Al alloy (B. Dutta et al., Phys. Status Solidi B 1700455 (2017)). Our calculations reveal an antiferromagnetic to ferromagnetic transition above a critical amount of Co or Fe doping in the austenite phase. The martensite phase, however, remains antiferromagnetic, which explains the experimentally observed metamagnetic transition in these alloys. The obtained magnetic properties are explained on the basis of magnetic exchange interactions. We also find that both Co and Fe substitution reduces the martensitic transformation temperature with the effect being larger in the case of the Fe containing alloy. Based on the achieved results on saturation magnetization and transformation temperature, Co containing alloys are found to be more promising for future MCE applications.

MM 72.3 Fri 10:00 TC 010

Martensitic transformations in Ni_2MnGa alloy: a first-principles study — •Martin Zelený[1,2], Ladislav Straka[2,3], Alexei Sozinov[4], and Oleg Heczko[2,3] — [1]NETME Centre, Faculty of Mechanical Engineering, Brno University of Technology, Brno, Czech Republic — [2]Faculty of Mathematics and Physics, Charles University, Prague, Czech Republic — [3]Institute of Physics, Czech Academy of Sciences, Prague, Czech Republic — [4]Material Physics Laboratory, Lappeenranta University of Technology, Savonlinna, Finland

The martensitic transformation paths in Ni_2MnGa alloy from cubic austenite to several low-symmetry martensitic structures have been studied by first-principles calculations combined with the generalized solid state nudged elastic band method. We determined the minimum energy path and corresponding changes in crystal lattice leading to the four-, five-, and seven-layered modulated phases of martensite (4O, 10M, and 14M) described as the relaxed nanotwinned non-modulated (NM) phase. In the transformation to the 10M phase there is no energy barrier on the path and energy decreases with a large negative slope. Initially, these transformations are driven by a softening of the TA_2 [$\xi\xi$0] phonon branch corresponding to the shift of (110) planes. Transformation paths to other structures exhibit more or less significant barriers in the beginning of the path, hindering such a transformation from austenite. This finding corresponds to experiment and demonstrates that the kinetics of the transformation is decisive for the selection of the particular low-symmetry structure of martensite.

MM 72.4 Fri 10:15 TC 010

Timedependent effects in martensitic transformations of Ni-Mn-X Heussler alloys with X = Ga, In and Snd — •Peter Entel — University Duisburg-Essen, Lotharstrasse, 47048 Duisburg

Martensitic transformation of rapidly and less rapidly cooled Heusler alloys of type Ni-Mn-X with X = Ga, In, and Sn are investigated by ab initio calculations. For the rapidly cooled alloys, we obtain the magnetocaloric properties near the magnetocaloric transition. For the less rapidly cooled alloys hese magnetocaloric properties start to change considerably. This shows that none of the Heusler alloys is in thermal equilibrium. Instead each alloy tranforms during temper annealing into a dual-phase composite. The two phases are identified to be cubic Ni-Mn-X and tetragonal NiMn.