

## MA 41: Joint Session Magnetic Shape Memory Alloys I (jointly with DS, MM)

Time: Thursday 10:15–12:00

Location: H 0106

MA 41.1 Thu 10:15 H 0106

**Different types of twin boundaries in 14M modulated Ni-Mn-Ga** — ●CHRISTIAN BEHLER<sup>1,2</sup>, BERND RELLINGHAUS<sup>1</sup>, ANJA BACKEN<sup>1</sup>, SANDRA KAUFFMANN-WEISS<sup>1</sup>, LUDWIG SCHULTZ<sup>1,2</sup>, and SEBASTIAN FÄHLER<sup>1,2</sup> — <sup>1</sup>IFW Dresden, Institute for Metallic Materials, P.O. Box 270116, 01171 Dresden, Germany — <sup>2</sup>Dresden University of Technology, Institute for Solid State Physics, Department of Physics, 01062 Dresden, Germany

Recent studies [L. Straka et al. *Acta Mat.* 59 (2011) 7450-7463] have found that various types of twin boundaries, such as type I, type II and modulation twins, with different mobilities can exist in the magnetic shape memory alloy Ni-Mn-Ga. In a 1.5  $\mu\text{m}$  thin epitaxial Ni-Mn-Ga film we observe two types of twin boundaries. This film was investigated by means of scanning electron microscopy (SEM), transmission electron microscopy (TEM) imaging and selected area diffraction (SAED) to clarify the type of the observed boundaries. From the orientations of neighboring variants, determined by SAED, conclusions can be drawn about the type of the interfaces. These analyzed interfaces can be attributed to type I twin boundaries as well as modulation twins. The 14M modulation is generated by nanotwins, which were observed by High Resolution TEM. However, this modulation is not perfect due to the existence of stacking faults.

MA 41.2 Thu 10:30 H 0106

**A multi-phase field model to investigate the elastic and magnetic hysteresis behaviour of twinned Ni<sub>2</sub>MnGa** — ●MARCUS JAINTA<sup>1</sup>, CHRISTIAN MENNERICH<sup>1</sup>, FRANK WENDLER<sup>1</sup>, and BRITTA NESTLER<sup>1,2</sup> — <sup>1</sup>IMP, Karlsruhe University of Applied Sciences — <sup>2</sup>IAM-ZBS, Karlsruhe Institute of Technology

In the last years, magnetic shape memory alloys became an important matter for material scientists. Due to their fast response time, their large recoverable strain and the good cost efficiency, this material class is well suited to be used as components of actuators or dampers. The microstructure evolution of magnetic shape memory alloys depends on the formation of magnetic domains and on the elastic strains induced by external magnetic fields and mechanical loads. To represent this behaviour, we applied a multi-phase field model of Allen-Cahn type based on a Helmholtz free energy density formulation. It is coupled with a model for linear elasticity and with an implementation of the Landau-Lifshitz-Gilbert equation. The order parameters are related to the different eigenstrains of the twin variants and to the spontaneous magnetization. In this contribution, we describe the model and compare simulation results of our combined micromagnetic phase-field solver with numerical results from the literature. We present simulation results of twinned structures in martensitic Ni<sub>2</sub>MnGa performing elastic and magnetic hysteresis behaviours under external forces. We also show the applicability of the model to polycrystalline systems.

MA 41.3 Thu 10:45 H 0106

**Modulated martensite and its twin boundaries in Ni-Mn-Ga films** — ●ANJA BACKEN<sup>1,2</sup>, SANDRA KAUFFMANN-WEISS<sup>1,2</sup>, ANETT DIESTEL<sup>1,2</sup>, LUDWIG SCHULTZ<sup>1,2</sup>, and SEBASTIAN FÄHLER<sup>1</sup> — <sup>1</sup>IFW Dresden, Institute for Metallic Materials, P.O. Box 270116, 01171 Dresden, Germany — <sup>2</sup>Dresden University of Technology, Institute of Materials Science, 01062 Dresden, Germany

The magnetic shape memory alloy Ni-Mn-Ga has gained much attention due to the high achievable strains of up to 10 % when applying an external magnetic field. The reorientation of martensitic variants is achieved by movement of twin boundaries. An external magnetic field can only overcome a twinning stress of 2 MPa or less, which brings the modulated martensite in the center of research interest. The 14-layer modulated martensite exhibits different generations of twin boundaries. The first generation are nano twin boundaries between non-modulated variants which are formed in order to decrease elastic energy at the austenite-martensite interface. The second generation connects variants of the 14M structure. This second generation is highly mobile and can be moved by an external magnetic field. We analyzed two types of microstructures which represent two cases of the 2nd generation of twinning. Although they appear to be completely different, X-ray diffraction and pole figure measurements reveal that both microstructures are composed of 14M twins. Magnetization measurements show, that only one type of twin boundaries can be moved

by a magnetic field which is important for future application in microsystems. This work is funded by DFG via SPP 1239.

MA 41.4 Thu 11:00 H 0106

**Freestanding single crystalline Fe-Pd ferromagnetic shape memory membranes: structural, morphological and magnetic characterization** — ●YANHONG MA<sup>1</sup>, A. SETZER<sup>3</sup>, J. W. GERLACH<sup>1</sup>, F. FROST<sup>1</sup>, P. ESQUINAZI<sup>3</sup>, and S. G. MAYR<sup>1,2</sup> — <sup>1</sup>Leibniz-Institut für Oberflächenmodifizierung e.V., 04318 Leipzig — <sup>2</sup>Translationszentrum für Regenerative Medizin und Fakultät für Physik und Geowissenschaften, Universität Leipzig — <sup>3</sup>Faculty of Physics and Earth Sciences, Institute for Experimental Physics II, Division of Superconductivity and Magnetism, Universität Leipzig

Miniaturized single crystalline Fe<sub>70</sub>Pd<sub>30</sub> ferromagnetic shape memory alloy membranes in the correct fct phase are synthesized by employing molecular beam epitaxy on MgO (001) substrates at deposition temperatures of 850°C and higher without post-annealing treatment. Atomic force microscopy images of these martensitic Fe-Pd thin films directly reflect formation of twin structure on the surface and reveal, how martensite variants grow. Martensitic phase transformation in the freestanding thin films is investigated with temperature dependent x-ray diffraction and magnetometry using a superconducting quantum interference device. The XRD patterns measured at various temperatures for freestanding martensitic Fe-Pd thin films show reversible (fcc-fcc) and irreversible (bcc/bct-fcc) structural transformations.

This project is funded by the Leipzig Graduate School of Natural Sciences "Building with Molecules and Nano Objects" through the German Science Foundation (DFG), as well as by the German Federal Ministry of Education and Research (BMBF, PTJ-BIO, 0313909).

MA 41.5 Thu 11:15 H 0106

**Adaptive nanostructures in Fe-Pd magnetic shape memory alloys** — ●MARKUS ERNST GRUNER<sup>1</sup>, SANDRA KAUFFMANN-WEISS<sup>2</sup>, SEBASTIAN FÄHLER<sup>2</sup>, LUDWIG SCHULTZ<sup>2</sup>, and PETER ENTEL<sup>1</sup> — <sup>1</sup>Faculty of Physics, University of Duisburg-Essen, 47048 Duisburg — <sup>2</sup>IFW Dresden, P.O. Box 270116, 01171 Dresden

Apart from the prototypical Ni-Mn-Ga Heusler alloy, also Fe-based alloys as Fe<sub>70</sub>Pd<sub>30</sub> exhibit significant magnetic field induced strains in moderate magnetic fields. This is bound to a slightly tetragonal fct structure (fct) which finds no correspondence on the low temperature binding surface which has been determined from density functional theory (DFT) calculations [PRB **83**, 214415 (2011)]. Instead, the energy decreases rather uniformly along the Bain path towards the absolute minimum close to bcc. Recent experiments reveal the possibility of growing Fe<sub>70</sub>Pd<sub>30</sub> films with  $c/a_{\text{fct}} = 1.09$  extending the Bain path beyond fcc [PRL **107**, 206105 (2011)]. XRD spectroscopy reveals that this is accompanied by a novel relaxation mechanism leading to a nanotwinned pattern consisting of fct building blocks. DFT modelling confirms this process showing a second minimum on the binding surface. This owes to the extremely low formation energy of fct twins causing the autonomous evolution of a twinned superstructure in the simulation cell along [110]. This corresponds to the experimentally observed soft transversal acoustic phonon in this direction, which is also a central feature of the Ni<sub>2</sub>MnGa magnetic shape memory alloy. We demonstrate further that magnetic excitations significantly alter the binding surface and thus potentially influence the transformation.

MA 41.6 Thu 11:30 H 0106

**Functional properties of magnetic Heusler alloys from an ab initio point of view** — ●PETER ENTEL, MARIO SIEWERT, MARKUS E. GRUNER, HEIKE C. HERPER, and SANJUBALA SAHOO — Faculty of Physics, University of Duisburg-Essen, 47048 Duisburg, Germany

Magnetic Heusler alloys exhibit complex magnetic phases and multiple intermediate martensitic structures. The strong interplay of magnetic and structural degrees of freedom is decisive for the functional properties associated with the magnetic shape-memory effect and the magneto-, elasto- and barocaloric effect. In this contribution we will discuss how the different functional properties arise from the complex spin interactions between the magnetic ions. We will show that this knowledge can be used to tune and optimize the various functional properties of the Heusler alloys as recently discussed for quaternary magnetic shape memory compounds [1].

[1] M. Siewert *et al.*, Appl. Phys. Lett. **99**, 191904 (2011).

MA 41.7 Thu 11:45 H 0106

**Failure of the Maxwell relation for the quantification of caloric effects in ferroic materials** — ROBERT NIEMANN<sup>1,2</sup>, OLEG HECZKO<sup>3</sup>, LUDWIG SCHULTZ<sup>1,2</sup>, and SEBASTIAN FÄHLER<sup>1,2</sup> — <sup>1</sup>IFW Dresden, P.O. Box 270116, 01171 Dresden, Germany — <sup>2</sup>Department of Physics, Institute for Solid State Physics, Dresden University of Technology, 01062 Dresden, Germany — <sup>3</sup>Institute of Physics, Academy of Science of the Czech Republic, Na Slovance 2, 182 02 Prague, Czech Republic

Giant caloric effects were reported in elasto-, electro- and magnetocaloric materials near phase transformations. Commonly, their entropy change is indirectly evaluated by a Maxwell relation. We report the fundamental failure of this approach. We analyze exemplarily the Ni-Mn-Ga magnetic shape memory alloy. An applied field results in magnetically induced reorientation of martensitic variants, which form during the phase transformation. This results in a spurious magnetocaloric effect, which only disappears when repeating the measurement a second time. This failure is universal as the vector character of the applied field is not considered in the common scalar evaluation of a Maxwell relation.