MA 8: Magnetic Shape Memory Alloys

Time: Monday 15:15–19:00 Location: H22

MA 8.1 Mon 15:15 H22

Lattice dynamics and static displacements in Fe-based magnetic shape memory alloys — •Markus E. Gruner and Peter Entel — Faculty of Physics and Center for Nanointegration, CeNIDE, University of Duisburg-Essen, 47048 Duisburg

Within the framework of density functional theory, we provide a comparison between stoichiometrically ordered Fe_3Pt and disordered Fe-Pd magnetic shape memory alloys. We compare the analytic modelling of disorder within the coherent potential approximation (CPA) referring to the ideal lattice positions with an explicit description by supercell calculations allowing for the relaxation of the atomic positions. The calculations demonstrate that static displacements provide an important contribution to the variation of the total energy along the Bain path and are thus essential for the correct prediction of the ground state lattice structure. Distinct static relaxations are also present in all $L1_2$ ordered Fe-rich alloys with Ni-group elements, which can be described by an orthorhombic distortion of the Fe-octahedra encaged by the Ni-group sublattice. These manifest in a complete softening in the phonon dispersion at the M-point which we relate to nesting features of the Fermi surface.

MA 8.2 Mon 15:30 H22

Anomalous phonon behaviour in Ni-based Heusler alloys — •Mario Siewert, Markus E. Gruner, Peter Entel, and Alfred Hucht — Faculty of Physics and CeNIDE, University of Duisburg-Essen, 47048 Duisburg, Germany

Ferromagnetic shape memory alloys (FSMAs) are of large scientific interest due to their applicability in actuators and sensors based on magnetic fields. The martensitic transformation in the Ni_2MnGa reference system to a modulated low symmetry phase that is responsible for the magnetic shape memory behaviour is preceeded by anomalous temperature dependent phonon softening along the [110] direction in the parent phase. The occurence of the soft mode has been linked to Fermi surface nesting in the past. In this work we report systematic studies of magnetic Ni-Mn-X (X=Al, Si, Zn, Ga, Ge, In, Sn, Sb) based Heusler alloys by means of density functional theory. Our calculations reveal that a phonon softening along the [110] direction up to imaginary frequencies can be found for all compounds in the cubic phase. Furthermore, an inversion of the optical modes can be observed. A systematic investigation of the reconstruction of the Fermi surface as a function of the valence electron number per atom (e/a) allows to predict materials with particular nesting behaviour.

MA 8.3 Mon 15:45 H22

Dynamical properties of Ni-Mn-Ga alloys — •Semih Ener[1], Jürgen Neuhaus[1,2], Klaudia Hradil[2,3], Richard Mole[2], Peter Link[2], and Winfried Petry[1,2] — [1]Technische Universität München, Physik Department E13, Garching, Germany — [2]Technische Universität München, Forschungsneutronenquelle Heniz Maier-Leibnitz (FRM II), Garching, Germany — [3]Georg-August-Universität Göttingen, Institut für Physikalische Chemie, Göttingen, Germany

In this work we investigate the vibrational properties of Ni-Mn-Ga alloys by using the Three Axis Spectrometers (TAS) PUMA (for thermal neutrons) and PANDA (for cold neutrons) which are located in FRM II, Garching. To approve the first principle calculations the whole dispersions of stoichiometric sample were measured in high temperature austenite and low temperature martensite phases. The temperature dependence of the vibrational properties in both stoichiometric and off-stoichiometric sample were investigated. In the austenite phase we observe a softening at TA2[q q 0] branch in both stoichiometric and off-stoichiometric samples. In stoichiometric sample the softening is more prominent than the off-stoichiometric one and the minimum of the softening is at 0.33 and 0.27 for stoichiometric and off-stoichiometric samples, respectively. The temperature dependence of vibrational properties of TA2[q q 0] branch in pre-martensitic phase were investigated in stoichiometric sample. The results showed that in the vibrational point of view the 5-layered martensite phase and the pre-martensite phase have the same behavior but it is not the case in low energy excitations.

MA 8.4 Mon 16:00 H22

Ab initio characterization of new ferromagnetic Fe-Ni-Co-Zn-Ga shape memory alloys — •Antje Dannenberg[1], Markus Ernst Gruner[1], Manfred Wuttig[2], and Peter Entel[1] — [1]Faculty of Physics, University of Duisburg-Essen, 47048 Duisburg, Germany — [2]Department of Materials Science and Engineering, University of Maryland, College Park, MD 20742, USA

Ferromagnetic shape memory alloys (FSMA) have received increasing interest, due to their potential use as smart materials for actuator and sensor applications, but for a technological breakthrough the operation temperatures are still too low.

In this report, we present a systematic investigation of the structural, electronic and magnetic properties of various systems based on Fe-Co-Ni-Ga-Zn. The results of our ab initio and Monte Carlo calculations predict high Curie temperatures for the Fe-based systems and show competing ordering between the conventional X_2YZ Heusler and the inverse (XY)XZ Heusler structure. The new Zn-based alloys may be promising new FSMA as they combine high T_C and the required structural properties but at the expense of structural stability.

MA 8.5 Mon 16:15 H22

A phase-field model for twin boundary motion in martensitic microstructures — •Christian Mennerich, Marcus Jainta, Frank Wendler, and Britta Nestler — Karlsruhe University of Applied Sciences, Karlsruhe, Germany

Magnetic shape memory (MSM) alloys are of great interest, e.g. for building actuators providing large deformations and rapid responses. Fundamental for the magnetic shape memory effect is the microstructure evolution in the twinned martensitic state of MSM materials under applied external magnetic fields. An existing phase-field model, basing on a free energy functional of the Ginzburg-Landau type, is extended by micromagnetic and elastic energy contributions, with the aim to model and predict the magnetically induced twin boundary evolution in martensitic microstructures. Assuming an isothermal setting below the Curie temperature and the martensitic start temperature, this model is appropriate to describe the diffusionless phase transition responsible for twin boundary motions. We give the derivation of the model extensions, resulting in a system of coupled partial differential equations, and solution strategies for a scheme using finite differences. With this model, the time-spatial evolution of the volume fractions of martensitic variants, of the displacement field for elasticity and of the micromagnetic domain wall structure can be described. Finally, we present simulation results demonstrating magnetically induced twin boundary motions.

MA 8.6 Mon 16:30 H22

Magnetization processes during field and stress induced twin boundary motion in NiMnGa — •Andreas Neudert, Yiu-Wai Lai, Rudolf Schäfer, and Jeffrey McCord — IFW Dresden, Helmholtzstr. 20, 01069 Dresden

We have studied the twin boundary motion in bulk single crystals of the ferromagnetic shape memory alloy NiMnGa using polarized light microscopy. Magnetic domains were imaged by using magnetic indicator films that are placed on top of the sample. Those indicator films consist of a soft-magnetic garnet film that senses the out of plane stray field of the sample. Twin boundaries can be moved by either applying a magnetic field or a mechanical stress to the sample, but there are qualitative differences between the two mechanisms. After moving a twin boundary by applying an external magnetic field, the domain state consists of wide antiparallel domains with 180° domain walls. Moving the twin boundary by applying external stress results in a different domain state. Here the magnetization rotates as the twin boundary passes through and a patchy domain structure is created. After demagnetizing the sample in a decaying ac magnetic field the domain state consists of mainly 180° domain walls again. This suggests that the magnetization after stress-induced reversal is not in a global energy minimum and rather trapped in local minima. The involved energies and effective fields for the two mechanisms will be discussed in the presentation.

MA 8.7 Mon 16:45 H22

Free-standing epitaxial Ni_2MnGa films — •Tobias Eichhorn, Peter Klaer, Hans-Joachim Elmers, and Gerhard Jakob — Institut für Physik, Universität Mainz, Deutschland

Among the compounds crystallizing in the Heusler structure many systems are of interest due to their predicted high spin polarization making them potential materials for spintronic devices. On the contrary Ni_2MnGa is attracting high scientific interest by presenting a ferromagnetic shape memory effect in the low temperature phase (martensite). Moderate magnetic fields can induce large reversible length changes up to 10 % in martensitic single crystals. Thereby actuators and sensors with a compact design can be realised using single crystalline thin films of the material. The investigated films are prepared on heated Al_2O_3(11-20) and MgO(100) substrates by dc-magnetron sputtering from alloy targets of different stoichiometry. Samples deposited from a Mn-rich target are martensitic at room temperature and show a modulated orthorhombic structure (7M). The complex crystal structure is studied by x-ray diffraction in 4-circle geometry. Magnetic properties are investigated by magnetometry, x-ray absorption spectroscopy and magnetic circular dichroism measurements. Since rigid substrates block magnetically induced strains free-standing films will be needed. One route is to deposit on NaCl(100) substrates that can be easily dissolved in water. The released films are strongly textured, but not single crystalline as desired. Improved crystal quality can be reached by another approach, i.e. introducing a buffer layer on MgO(100) that can be etched selectively. This work is part of SPP 1239.

MA 8.8 Mon 17:00 H22

Microstructure of adaptive martensite in Ni-Mn-Ga — •Sebastian Fähler[1,2], Stefan Kaufmann[1,2], Robert Niemann[1,2], Tom Thersleff[1], Oleg Heczko[3,1], Bernhard Holzapfel[1,2], and Ludwig Schultz[1,2] — [1]IFW Dresden, PO Box 270116, 01171 Dresden — [2]Institute for Solid State Physics, Department of Physics, Dresden University of Technology, 01062 Dresden — [3]Institute of Physics, Czech Academy of Science, Na Slovance 2, CZ-182 21 Praha 8

Recently we showed that modulated phases in the Ni-Mn-Ga magnetic shape memory alloy can be interpreted within Khachaturyan's concept of adaptive martensite and described as a nanotwinned microstructure of a basic tetragonal martensite [S. Kaufmann et al. arXiv:0906.5365v1]. The observed coexistence of austenite, 14M and NM martensite in thin films indicated that the transition between 14M and NM proceeds through coarsening of twin boundaries. Here we present a detailed study of the microstructure of an epitaxial film using FIB, AFM and SEM. At the first glance, the microstructure images appear more like modern art than physics. However, it can be shown that this microstructure arises from simple geometrical concepts. A quantitative analysis demonstrates that branching of twin boundaries occurs down to atomic scale and it controls twin width and periodicity over lengthscales more than 3 orders of magnitude.

MA 8.9 Mon 17:15 H22

A comparison of substrate-constraint and freestanding thin Ni-Mn-Ga films — •Anja Backen[1,2], Srinivasa Yeduru Reddy[3], Manfred Kohl[3], Anett Diestel[1,2], Ludwig Schultz[1,2], and Sebastian Faehler[1] — [1]IFW Dresden, Institute for Metallic Materials, P.O. Box 270116, 01171 Dresden, Germany — [2]Dresden University of Technology, Department of Mechanical Engineering, Institute of Materials Science, 01062 Dresden, Germany — [3]Karlsruhe Institute of Technology, Institute of Microstructure Technology, Herrmann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen, Germany

The magnetic shape memory alloy Ni-Mn-Ga belongs to a class of active materials where an external magnetic field can cause a maximum strain of 10 % in bulk single crystals. In order to use this effect for microsystems, scaling down from bulk dimensions is a key issue and thus epitaxial thin films are of particular interest. Recently we have reported on epitaxial growth of Ni-Mn-Ga on single crystalline MgO (100) substrates, however, the substrate constraints hinder elongation by magnetically induced reorientation. Hence, it is crucial to release films from the substrates. We report on successfully releasing thin Ni-Mn-Ga films grown on MgO (100) by using Chromium as sacrificial layer. We observe epitaxial growth of both Cr on MgO (100) and Ni-Mn-Ga on Cr without interdiffusion. After deposition, Cr can be etched selectively without affecting the Ni-Mn-Ga film properties. In order to understand the influence of substrate constraint on the film properties, structure, microstructure and magnetic properties are analyzed and compared for films before and after their release.

15 min. break

MA 8.10 Mon 17:45 H22

High resolution imaging of epitaxial Ni-Mn-Ga films with STM — •Philipp Leicht[1], Aleksej Laptev[1], Mikhail Fonin[1], Yuansu Luo[2], and Konrad Samwer[2] — [1]Fachbereich Physik, Universität Konstanz — [2]I. Physikalisches Institut, Universität Göttingen

Magnetic shape memory (MSM) alloys are of great interest due to their possible application as actuators or sensors. Upon cooling from the high temperature austenite phase a structural phase transformation to a distorted martensite phase occurs. MSM films deposited on substrates accommodate the strain associated with the martensite transition by formation of twin boundaries [1]. Here epitaxial off-stoichiometric Ni-Mn-Ga films were grown on MgO substrates by dc-magnetron sputtering. The surface of the films was investigated in ultra high vacuum conditions by means of scanning tunneling microscopy (STM) at room temperature. Austenitic areas reveal atomically flat terraces separated by steps with an average height corresponding to the distance between equivalent atomic planes of the bulk $L2_1$ structure. STM images on martensitic areas reveal a wavy-like structure due to the formation of twin boundaries. An additional superstructure on every second variant in form of narrow stripes running perpendicular to the twin boundaries was observed. The latter structure is explained on the basis of a structural model taking into account the twinning and the shuffling of atomic planes in layered martensites (5M, 7M) [2]. This work is supported by BMBF-projects MSM-Sens 13N10061 and 13N10062.

[1] J. Buschbeck et al., Acta Materialia **57**, 2516-2526 (2009)
[2] V. V. Martynov et al., J. Phys. III France **2**, 739-749 (1992)

MA 8.11 Mon 18:00 H22

Preparation and characterization of textured Ni-Mn-Ga to show MFIS — •Martin Pötschke, Claudia Hürrich, Stefan Roth, Bernd Rellinghaus, and Ludwig Schultz — IFW Dresden

Ni-Mn-Ga alloys are interesting because of their possible application as magnetic shape memory materials. This effect is caused by the motion of twin boundaries in a magnetic field. Up to now most of the research was concentrated on single crystals. However, the preparation of single crystals is a time consuming and cost intensive process and compositional changes along the growth axis as well as segregations may occur. This is why for technical applications there is a great interest in polycrystals, which are easier to produce. To achieve magnetic field induced twin boundary motion in polycrystals, directional solidification was applied to a 5M Ni-Mn-Ga alloy in order to prepare coarse grained, textured samples. Stationary casting in a pre-heated ceramic mold mounted on a copper plate was employed to generate a heat flow towards the bottom of the sample and thereby a directional solidification in the opposite direction. The preferred solidification-induced growth direction was determined by EBSD. Annealing is necessary for homogenization and stress relaxation. The martensitic transformation temperature which strongly depends on the composition was monitored by DSC, and it is shown that the chemical homogeneity along the sample axis is improved in likewise treated samples. After a mechanical training process MFIS was observed.

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MA 8.12 Mon 18:15 H22

Training of polycrystalline NiMnGa alloys — •Robert Chulist[1], Martin Pötschke[2], Andrea Böhm[3], Carl - Georg Oertel[1], Werner Skrotzki[1], and Erik Rybacki[4] — [1]Institut für Strukturphysik, Technische Universität Dresden, D-01062 Dresden, Germany — [2]Institut für Metallische Werkstoffe, Leibniz-Institut für Festkörper- und Werkstoffforschung, D-01069 Dresden, Germany — [3]Fraunhofer-Institut für Werkzeugmaschinen und Umformtechnik, D-01187 Dresden, Germany — [4]Geoforschungszentrum Potsdam, D-14473 Potsdam, Germany

In order to achieve magnetic field induced strain in NiMnGa alloys a training process is applied. This process consists of successively compressing the sample along two or three axes. As a result the twinning stress is reduced and the strain is maximized. To study the effect of training, two samples with 5M modulated structure were used: bicrystal and polycrystal deformed by high pressure torsion. Within the individual parent austenitic grains the initial orientation is characterized by three different martensitic variants separated by twin boundaries. Compression of the samples results in the motion of the twin boundaries changing the volume fraction of particular variants. Local orientation measurements by electron backscatter diffraction directly confirm twin boundary motion. The training process finally leading to a single variant state will be discussed with respect to initial microstructure and number of martensitic variants.

MA 8.13 Mon 18:30 H22

Training effects of polycrystalline Ni50Mn29Ga21 magnetic shape memory alloy — •Claudia Hürrich, Martin Pötschke, Stefan Roth, Bernd Rellinghaus, and Ludwig Schultz — IFW Dresden, Institute for Metallic Materials, P. O. Box 270116, 01069 Dresden, Germany

The alloy Ni-Mn-Ga arose great interest for its application as a magnetic shape memory material. This effect is caused by reorientation of twin variants by an external magnetic field. So far most of the experiments were concentrated on single crystals. But, this effect can also be realised in polycrystals which can be prepared much more efficiently. Here, polycrystalline samples were prepared by directional solidification with a <100> fibre texture of the high temperature cubic phase parallel to the heat flow. Afterwards a heat treatment was applied for chemical homogenization and stress relaxation in the austenitic state. Then the samples were heated up to the austenitic state and cooled down under load. The microstructure was analysed by Electron Back Scatter Diffraction (EBSD) before and after that treatment. Mechanical training in three directions was tracked by recording stress-strain curves. With increasing the number of training cycles the strain also increases. This work is supported by DFG within SPP 1239.

MA 8.14 Mon 18:45 H22

Magnetic field induced strain in Ni_2MnGa-Polymer-Composites — •Sandra Weiss[1], Nils Scheerbaum[1], Jian Liu[1], Ludwig Schultz[1], Oliver Gutfleisch[1], Edith Mäder[2], and Gert Heinrich[2] — [1]IFW Dresden, Institute for Metallic Materials, P.O. Box 270116, D-01171 Dresden — [2]Leibniz-Institut für Polymerforschung e.V., Hohe Straße 6, 01069 Dresden

Ni-Mn-Ga single- and polycrystals show large magnetic field induced strain (MFIS) but are in general difficult and expensive in preparation and also very brittle. An alternative to single- and polycrystals are Ni-Mn-Ga/polymer-composites. Here, small single-crystalline $Ni_{50.9}Mn_{27.1}Ga_{22.0}$-particles, produced by gently crushing melt-extracted and subsequently annealed fibres, were embedded in a soft polymer matrix. The particles have a 5M martensitic structure. The Young's Modulus of the polymer-matrix is 2 MPa and 175 MPa, for polyurethane and epoxy respectively. In response to the applied magnetic field, the MSM particles are prone to relocation within the polyurethane due to its low Young's modulus, leading to a very little effect of magnetic field-induced twin boundary motion. By contrast, the Ni_2MnGa-epoxy-composite shows a pronounced MFIS up to 0.1 % because the stiffness of epoxy fits better the one for Ni-Mn-Ga. Furthermore, the interface stability between Ni-Mn-Ga and epoxy-matrix was investigated by quasistatic Pull-Out Tests. First tests with silan-coupling-agent treated fibres indicate significant improvements of interface.