MA 17: Magnetic Shape Memory Alloys

Time: Wednesday 15:15–19:15 Location: H10

MA 17.1 Wed 15:15 H10

First-principles study of the magnetoelastic behavior of magnetic shape memory alloys — •Peter Entel, Markus Gruner, Alfred Hucht, and Georg Rollmann — Physics Department, University of Duisburg-Essen, 47048 Duisburg

We investigate the magnetoelastic properties of magnetic shape memory alloys (MSMA) by large-scale *ab initio* calculations, which have been performed on massively parallel platforms like the Blue Gene/L at NIC (FZ Jülich). In particular, we focus on the change of elastic properties with composition and, in addition, under the action of uniaxial strain or external magnetic fields close to the magnetic, structural or combined magnetostructural phase transitons in the systems Ni-Mn-Z (Z = Ga, In, Sn). We highlight the atomistic details and origin of the austenitic to martensitic transformation in the MSMA, the latter of which is connected to the anomalous forces acting on the Ni atoms in Ni-Mn-Z. Note that the X atoms in X_2(Y = Mn)Z are usually responsible for the formation of the cubic $L2_1$ Heusler structure and its stability. However, in case of X = Ni, the high-temperature cubic structure is *band-Jahn-Teller instable* with respect to tetragonal distortions leading to a modulation of valence electron charges and a more favorable crystal field environment for the Ni atoms. We show how the interplay of Fermi surface nesting (and its change when the structure undegoes a tetragonal distortion) and the impact of anomalous force constants allows to understand most of the physical properties of the MSMA.

MA 17.2 Wed 15:30 H10

Ab initio determination of symmetry reduced structures by a soft-phonon analysis in Ni_2MnGa — •Tilmann Hickel, Blazej Grabowski, Matthé Uijttewaal, and Jörg Neugebauer — Max-Planck-Institut für Eisenforschung GmbH, Postfach 140444, 40074 Düsseldorf, Germany

The ferromagnetic shape memory compound Ni_2MnGa undergoes a martensitic phase transition from a high to a low symmetry structure at 200 K. In the low symmetry phase several shuffling structures have been observed experimentally, but their appearance and importance for the shape memory effect are not yet completely understood. In order to identify the stable structures and the phase transition paths, we have calculated free energy surfaces as function of key reaction coordinates (lattice constants, c/a-ratio) in DFT. Due to the large phase space of possible atomic positions and their small formation energies of only a few meV per unit cell, the determination of the shuffling structures is a major challenge in these studies. To overcome this issue, we have developed a scheme which is based on the computation of the phonon spectra using the quasiharmonic approximation. Starting with the symmetric structure, the TA_2 phonon dispersion shows a softening along the [110] direction. From the eigenvectors of the unstable phonon modes and by setting up the corresponding modulated harmonics in supercell calculations, we were able to systematically and efficiently identify stable shuffling structures. Using these structures, the effect of symmetry breaking on magnetic properties has been computed and the results have been compared with recent experiments.

MA 17.3 Wed 15:45 H10

Lattice dynamics in austenitic and martensitic phase of Ni_2MnGa from inelastic neutron scattering — •Tarik Mehaddene[1], Jürgen Neuhaus[2], Winfried Petry[2,1], Klaudia Hradil[3,2], and Peter Link[2] — [1]Physik-Department E13, Technische Universität München, 85748 Garching — [2]Forschungsneutronenquelle Heinz Maier-Leibnitz (FRM II), 85748 Garching — [3]Institut für Physikalische Chemie, Universität Göttingen, 37077 Göttingen

We report on the investigation of the normal modes of vibration in the martensitic and austenitic phase of Ni_2MnGa by inelastic neutron scattering. Phonon dispersions of both acoustic and optical phonons in a $Ni_{49}Mn_{31}Ga_{20}$ single crystal have been measured on the three-axis spectrometer PUMA (Forschungsneutronenquelle Heinz Maier-Leibnitz, Garching). The sample undergoes a martensitic transformation at M_s=350 K and orders ferromagnetically below T_c=385 K. We focus on the optical phonons and their temperature dependence, which, to our knowldge, has not been reported yet despite of the intensive previous works on Ni_2MnGa. Acoustic phonons of an orthorhombic 7-layered martensitic variant of the same sample have been measured on both thermal (PUMA) and cold (PANDA) three-axis spectrometers. The measurements revealed low-lying $TA_2[\xi\xi0]$ phonon frequencies with a Brillouin zone boundary frequency of 2.5 THz.

MA 17.4 Wed 16:00 H10

Investigation of structure and microstructure transformations of Ni-Mn-Ga single crystal exhibiting magnetic shape memory effect by neutron diffraction — •Heczko Oleg[1,3] and Prokes Karel[2] — [1]IFW Dresden,Helmholtzstrasse 20, 01069 Dresden, Germany — [2]Berlin Neutron Scattering Center, Hahn-Meitner-Institut Berlin, Glienicker Straße 100, D-14109 Berlin (Wannsee), Germany — [3]Laboratory of Materials Science, Helsinki University of Technology, Vuorimiehentie 2A, P.O. Box 6200, FI-02015 TKK, Espoo, Finland

Neutron diffraction of single crystal of alloy $Ni_{49.7}Mn_{29.3}Ga_{21}$ exhibiting 6% MSM effect was carried out in HMI, Berlin. The single crystal was mounted into cryostat with one of 100 directions along the magnetic field and perpendicular to diffraction plane. The set of nuclear Bragg reflections was recorded by 2D position sensitive detector after zero-field cooling and cooling in 5T magnetic field at different temperatures above and below martensitic transformation temperatures. The martensitic variants distribution and quality and inhomogeneity of the single crystal were studied using ω scan. Using measurement in reciprocal space we recorded a set of reflections that appear due to structural modulation (5M) of the martensite, however, the set seems to be incomplete with missing or very weak reflections of second order compared with X-ray diffraction. No sharp magnetic reflection of suggested antiferromagnetic ordering of excess Mn was observed.

MA 17.5 Wed 16:15 H10

Characterization of Ni2MnGa Single Crystal for Sensor Applications — •Christoph Bechtold[1], Andreas Gerber[1], and Eckhard Quandt[1,2] — [1]Stiftung caesar, AG Smart Materials, Ludwig-Erhard-Allee 2, 53175 Bonn — [2]CAU Kiel, Technische Fakultät, Inst. f. Materialwissenschaft, Anorg. Funktionsmaterialien, Kaiserstr. 2, 24143 Kiel

In the past 10 years MSM materials received attention as actuator materials on account of their large magnetically induced strains. Sensor applications were almost not pursued. However, those are very attractive and are the focus of this work. The corresponding sensor approaches are the use of MSM/polymer composites as mechanical sensors or as magnetic field sensors by employing piezoelectric polymers.

In this presentation the properties of Ni2MnGa single crystals were characterized with respect to features important for these sensor applications. Especially strain versus pre-stress and change of permeability as a function of strain were measured and will be discussed in view of the envisaged applications.

MA 17.6 Wed 16:30 H10

Structural and mechanical properties of NiMnGa shape memory ferromagnets — •Uwe Gaitzsch[1], Stefan Roth[1], Andrea Böhm[2], Bernd Rellinghaus[1], and Ludwig Schultz[1] — [1]IFW Dresden, P.O. Box 270116, D-01171 Dresden, Germany — [2]Fraunhofer IWU, Nöthnitzer Str. 44, D-01187 Dresden, Germany

Magnetic shape memory alloys are of significant research interest owing to their capability to deform quasi-plastically by some percent via twin boundary motion under the influence of a magnetic field. These materials are supposed to react faster than conventional shape memory materials because neither heating nor cooling are involved. We present the structural and mechanical properties of polycrystalline, textured $Ni_{50}Mn_{30}Ga_{20}$ and $Ni_{50}Mn_{29}Ga_{21}$. Upon cooling, these alloys undergo austenite-martensite transitions at 100^oC and 55^oC, respectively. The evolving martensitic structure is either orthorhombic or tetragonal and depends on the thermomechanical history of the samples and their composition. Since only two of the three possible martensitic structures are capable of providing the mandatory highly moblile twin boundaries, it is essential to understand and control the phase formation process by appropriate thermal and mechanical treatment. Once the sample is given a suitable structure, samples for magnetomechanical testing are hot mold cast for directional solidification and investigated in magnetic fields of up to 0.8 T in compression tests.

MA 17.7 Wed 16:45 H10

Untersuchungen zur Ermüdung von Ni_2MnGa unter zyklischer Belastung — •Katrien Huysmans, Matz Haaks, Torsten Staab und Karl Maier — Helmholtz Institut für Strahlen- und Kernphysik, Universität Bonn, Nußallee 14-16, D-53115 Bonn

Die magnetische Formgedächtnislegierung Ni_2MnGa ist ein neuartiger Werkstoff, dem z.B. in der Automobilindustrie und Medizintechnik hohes Potential zugesprochen wird. Eine bisherige Studie zeigt, dass bei bis zu 10^6 Magnetisierungszyklen ohne Last keine Materialermüdung nachweisbar ist. Im Rahmen einer Diplomarbeit wurde das Verhalten des einkristallinen Materials unter Last untersucht. Dabei zeigte sich lastabhängig bereits nach geringer Zyklenzahl eine signifikante Verschlechterung der Aktuatoreigenschaften. Untersuchungen mit Positronen (PAS) an technischen Legierungen (Fe, Al, Ti,...) zeigten eine deutliche Abhängigkeit der Zerstrahlungsparameter vom Ermüdungszustand. Bei der untersuchten MSMA-Probe wurden während der Ermüdung ortsaufgelöste Untersuchungen mit der Bonner Positronenmikrosonde (BPM) durchgeführt. Zur Aufklärung der bei der Ermüdung enstehenden Fehlstellentypen werden sowohl Untersuchungen mit Positronen (Lebensdauer, Hochimpulsanalyse) als auch Elektronenstrukturrechnungen durchgeführt.

MA 17.8 Wed 17:00 H10

Directional solidification of $Ni_{48}Mn_{30}Ga_{22}$ magnetic shape memory alloys — •Martin Pötschke, Uwe Gaitzsch, Stefan Roth, Bernd Rellinghaus, and Ludwig Schultz — IFW Dresden, P.O. Box 270116, D-01171 Dresden, Germany

NiMnGa ferromagnetic shape memory (FSM) alloys have gained large research interest because of their possible application as actuator materials. The FSM effect is caused by the movement of twin boundaries by virtue of an external magnetic field. So far, this effect has only been observed in single crystals. The preparation of single crystals, however, is a long time and cost intensive process and both compositional changes along the crystal and segregation may occur. This is why for technical applications, there is a great interest in polycrystalline FSM materials. In order to extend the FSM effect to polycrystals, directional solidification was applied 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 from the top of the cylindrical samples to the bottom and thereby a directional solidification in the opposite direction. The martensite start temperatures were checked by DSC, and the preferred growth direction and resulting textures were determined by EBSD. Further annealing, which is necessary for chemical homogeneity, results in grain coarsening and stress relaxation and affects the texture. The results of the investigation of the texture development during annealing will be presented.

MA 17.9 Wed 17:15 H10

Stress-Induced Twin Boundary Motion in NiMnGa-Polymer-Composites — •Nils Scheerbaum[1], Dietrich Hinz[1], Jian Liu[1], Oliver Gutfleisch[1], Werner Skrotzki[2], and Ludwig Schultz[1] — [1]IFW Dresden, Institut für Metallische Werkstoffe, P.O. Box 270116, D-01171 Dresden, Germany — [2]Technische Universität Dresden, Institut für Strukturphysik, D-01062 Dresden, Germany

Composites were prepared by embedding magnetic shape memory (MSM) particles in a polyester matrix. Single-crystalline MSM particles were obtained by mortar grinding of melt-extracted and subsequently annealed Ni50.9Mn27.1Ga22.0 (at.%) fibres. The crystal structure of the martensite is tetragonal (5M) and of uniaxial magnetocrystalline anisotropy with c being the short and easy magnetisation axis. Previous magnetic characterisation of these composites showed indirect evidence for stress-induced twin boundary motion in the MSM particles, as the compressed composite becomes easier to magnetise in the direction of compression [1]. Therefore, the texture of the embedded Ni-Mn-Ga particles is investigated before and after compression by means of synchrotron radiation. In the initial state, the MSM particles have a random texture, i.e. there is no preferred orientation of the c-axis. After a 30% compression of the composite, the MSM particles have a [004]-fibre texture in direction of compression [2]. This confirms stress-induced twin boundary motion.

[1] N. Scheerbaum, D. Hinz, O. Gutfleisch, K.-H. Müller, L. Schultz, Acta Mater., accepted. [2] N. Scheerbaum, D. Hinz, O. Gutfleisch, W. Skrotzki, L. Schultz, J. Appl. Phys., accepted.

MA 17.10 Wed 17:30 H10

EPITAXIAL FILMS OF THE MAGNETIC SHAPE MEMORY MATERIAL Ni_2MnGa — •Tobias Eichhorn, Gerhard Jakob, Michael Kallmayer, and Hans Joachim Elmers — Institute of Physics, Johannes Gutenberg University, 55099 Mainz

By dc-sputtering from a stoichiometric target onto sapphire and MgO substrates we prepared epitaxial films of Ni_2MnGa. Using temperature dependend X-ray diffraction, resistivity and magnetization measurements we find the austenite to martensite transition in these films. The characteristic temperatures are shifted with respect to the bulk values. The presence of two different phases at high and low temperature also shows up in a different behavior of the magnetic hysteresis curves measured in the austenitic state and the martensitic state of the sample, respectively.

The element specific magnetic moments for thin film samples have been determined by magnetic circular x-ray dichroism (XMCD) measurements. From these measurements we determine orbital and spin momentum in austenite and martensite phase.

Changing target and film stoichiometry the martensitic transition temperature can be tuned to be above room temperature.

MA 17.11 Wed 17:45 H10

Epitaxial growth of martensitic Ni-Mn-Ga films prepared by sputter deposition — •Michael Thomas, Jörg Buschbeck, Oleg Heczko, Ludwig Schultz, and Sebastian Fähler — IFW Dresden, Helmholtzstraße 20, 01069 Dresden

Bulk Ni-Mn-Ga material exhibits a large magnetic-field-induced strain up to 6% in the 5M phase and 10% in the 7M phase. While the phenomenology and requirements in bulk single crystals are understood quite well, only little work has been done on thin films until now. Ni-Mn-Ga films were deposited on MgO, Al_2O_3, $SrTiO_3$, $NaCl$ and Si single crystals with different orientations under variation of the deposition temperature by DC sputtering. The estimated film thickness was about 650 nm. The samples were analyzed with XRD using 2θ and pole figure measurements. At certain deposition conditions an epitaxial growth occured. A martensitic phase was observed on MgO, $SrTiO_3$ and $NaCl$ substrates at room temperature. The influence of substrate symmetry and misfit between the substrate and the Ni-Mn-Ga films on the existence of martensitic phase and martensitic variant orientation is discussed. This work is supported by the SPP 1239, project C3 (http://www.magneticshape.de).

MA 17.12 Wed 18:00 H10

In-situ magnetic domain observation during twin boundary movement in bulk Ni-Mn-Ga — •Ryan Yiu Wai Lai, Jeffrey McCord, Nils Scheerbaum, Oliver Gutfleisch, Rudolf Schäfer, and Ludwig Schultz — Leibniz Institute for Solid State and Materials Research IFW Dresden, Helmholtzstrasse 20, 01069 Dresden, Germany

A study of twin boundary movement in a Ni-Mn-Ga single crystal in connection with in-situ magnetic domain observation is presented. Polarization microscopy in connection with a magneto-optical indicator film (MOIF) technique was used to record the magnetic domain pattern's reorganization during the process. A magnetic field up to 330 mT in amplitude was applied to a single variant sample with the structural c-axis being also the magnetically easy axis, aligned perpendicular to the field direction. Structural reorientation by twin boundary movement was induced by the magnetic field. Images at different field strength display no domain wall movement, even during twin boundary movement. This result is different from the previously proposed model, which assumes domain wall movement under an external field [1]. Funding through the DFG priority program SPP1239 is gratefully acknowledged. [1] H.E. Karaca et al. Acta Materialia 54 (2006) 233-245

MA 17.13 Wed 18:15 H10

Controlling the martensitic transformation temperature at constant valence electron concentration in Heusler based Ni-Mn-In alloys — •Seda Aksoy[1], Mehmet Acet[1], Thorsten Krenke[1], Eberhard Wassermann[1], Xavier Moya[2], Lluis Manosa[2], and Antoni Planes[2] — [1]Experimentalphysik (AG-Farle), Universitaet Duisburg-Essen, 47048 Duisburg — [2]Departament d'Estructura i Constituents de la Materia, Facultat de Fisica, Universitat de Barcelona, Diagonal 647, E-08028 Barcelona

Although the martensitic transformation temperature Ms increases linearly with increasing valence electron concentration e/a in Ni-Mn-X Heusler alloys (X: group III or IV element), the slope varies depending on the X-species, i.e., Ms vs. e/a is not universal. This aspect can be favorably exploited to control Ms by holding e/a constant and replacing X by an isoelectronic X*, where X and X* are elements within the same group. Using this property we have substituted In in Ni50Mn34In16 (Ms˜200 K) with Ga to bring Ms close to room temperature. Here, we show how magnetic field induced phase transition properties and associated magnetocaloric effects in Ni50Mn34In16 are modified in Ni50Mn34(In,Ga)16.

MA 17.14 Wed 18:30 H10

Martensitic transformation and magnetic properties of Ni-Fe-Ga-Co magnetic shape memory alloys — •Jian Liu, Nils Scheerbaum, Dietrich Hinz, and Oliver Gutfleisch — IFW Dresden, Institute for Metallic Materials, P.O. Box 270116, D-01171 Dresden, Germany

To overcome the disadvantage of brittleness in Ni-Mn-Ga alloys, Ni-Fe-Ga-Co alloys with a Ga content of 27 at.% were reported as a new magnetic shape memory (MSM) system due to its good ductility, high mobility of twin boundaries and high martensitic transformation temperature Tm as well as magnetic transition temperature Tc [1]. In this work, the effects of substitution of Co for Ni on the martensitic and magnetic properties in Ni-Ga-Fe alloys with a wider composition range were studied. The influence of composition on the crystal structure of martensite phase was also presented. A series of polycrystalline alloys, Ni54-xFe20Ga26Cox, Ni54-xFe19Ga27Cox and Ni54-xFe18Ga28Cox (x = 0, 2, 4, 6) was produced using arc-melting. As-cast samples were homogenized at 1453 K to obtain a single-phase structure followed by annealing at 673 K to achieve a high degree of atomic order. Tm was measured by differential scanning calorimetry (DSC). Tc and magnetisation were determined by vibrating sample magnetometer (VSM). The structure was investigated by X-ray diffraction (XRD) and scanning electron microscopy (SEM). The results show that Tm and Tc can be tailored by adjusting the composition of the Ni-Fe-Ga-Co alloys.

[1] Morito, K. Oikawa, A. Fujita, K. Fukamichi, R. Kainuma, K. Ishida, T. Takagi, J. Mag. Mag. Mater. 290-291 (2005) 850.

MA 17.15 Wed 18:45 H10

Structural, magnetic and phase transformation properties of Fe-Pd thin film composition spreads — Hayo Brunken[1,2], Sven Hamann[1,2], Sigurd Thienhaus[1,2], Alan Savan[1], Michael Ehmann[1], and •Alfred Ludwig[1,2] — [1]caesar, Ludwig-Erhard-Allee 2, 53175 Bonn — [2]Institut für Werkstoffe, Ruhr-Universität Bochum, 44780 Bochum

Fe-Pd thin film composition spreads have been fabricated by sequential and co-sputtering of elemental targets, both on oxidized Si wafers and on micro-hotplate arrays. The micro-hotplates - microstructured Si3N4 membranes with Pt heaters and measurement electrodes - are used as a materials processing and characterization platform: films can be heated and cooled very quickly with rates of several 1000 K/s which allows for a wide variation of process parameters for the achievement of necessary phases. During the heat treatment, the resistance of the thin film on the micro-hotplate can be monitored, and phase transformations thus can be identified in situ. The films have also been characterized by EDX, XRD, macroscopic resistance versus temperature measurements, and temperature dependent VSM measurements. First results show a phase transformation close to a composition of Fe70Pd30 in an temperature interval from 40°C to 70°C.

MA 17.16 Wed 19:00 H10

Epitaxial Growth, Structure and Magnetic Properties of Fe-Pd films — •Jörg Buschbeck, Inge Lindemann, Ludwig Schultz, and Sebastian Fähler — IFW Dresden, Institute for Metallic Materials, P.O. Box: 270116, 01171 Dresden, Germany

Magnetic shape memory materials like Ni-Mn-Ga and Fe-Pd reach high strains in moderate applied magnetic fields below 1 T due to a selective growth of martensite variants. The maximum strain of Fe70Pd30 is about 3%. Films of this material are interesting candidates for micro-actuators and sensors, because of the materials high ductility and the ability to compensate internal stresses during the straining process. Fe(70+x)Pd(30-x) films are deposited by Pulsed Laser Deposition in UHV of p=10ˆ(-9) mbar at room temperature. It is observed, that the films grow (100) epitaxially on MgO (100) substrates. XRD measurements indicate martensitic phase formation in the films. In the as-depositied state the metastable phases change from fct to bct and bcc when reducing the Pd content. Temperature dependent magnetic measurements indicate a transition occurring in the fct phase. It is suggested that in the films stress induced martensite formation occurs. Furthermore annealing experiments are carried out. After annealing, the films are relaxed and instead of the fct phase the fcc phase is observed in X-ray measurements on Pd-rich films (X<0).