MM 38: Topical Session Diffussionless Transformations I

Time: Thursday 14:00–16:00 Location: IFW D

Topical Talk MM 38.1 Thu 14:00 IFW D

Epitaxial films of the magnetic shape memory alloy Ni2MnGa — •Gerhard Jakob, Tobias Eichhorn, Richard Hausmanns, Peter Klaer, Michael Kallmayer, and Hans-Joachim Elmers — Institute of Physics, Johannes Gutenberg-University Mainz

While large magnetically induced strains up to 10% have been observed for bulk single crystals of Ni_2MnGa, these large effects have not been demonstrated for thin films of this compound yet. The preparation of free standing single crystalline films turns out to be a challenging task, but is a necessary precondition for applications on smallest scale.
We report on the preparation and investigation of thin epitaxial films of the NiMnGa-system via dc-magnetron sputtering from an alloy target to heated substrates as Al2O3(11-20), MgO(100) and NaCl(100). The complex crystal structure is studied by temperature dependent x-ray diffraction in 4-circle geometry, whereas magnetic properties are investigated by magnetometry. To avoid blocking effects of the substrate free standing films were prepared by introduction of a buffer layer on MgO(100) that can be etched away selectively.
Using X-ray absorption spectroscopy we determined the element specific magnetic moments and found a remarkable change of the Ni X-ray absorption spectra occurring at the temperature of the phase transition (Tm) which indicates specific changes of the electronic structure. The observed changes are in agreement with theoretical predictions.
This work is part of the DFG priority program SPP 1239.

MM 38.2 Thu 14:30 IFW D

Transition from modulated to non-modulated martensite in thin Ni-Mn-Ga films — •Anja Backen[1,2], Bernhard Holzapfel[1], Ludwig Schultz[1,2], and Sebastian Fähler[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

In Ni-Mn-Ga, an external magnetic field can induce strains of up to 10% by twin boundary motion. One condition for this MSM effect is a twinning stress of 2 MPa or less, which only the modulated martensite fulfills. The coexistence of 14-layer modulated (14M), non-modulated martensite (NM) and austenite in epitaxial films make them a model system to study the transition between the different martensitic phases. Kaufmann et al. [PRL 104 (2010) 145702] recently showed that 14M can be described as nanotwinned NM which forms at the austenite-martensite interface reducing elastic energy for the cost of twin boundary energy. With increasing distance to the interface, the elastic energy becomes less important and 14M transfers to NM by coarsening. To probe this, we examined Ni-Mn-Ga films of varying thickness deposited on MgO(100) substrates with a Cr buffer layer. Taking the integrated XRD-intensity ratio as a measure of phase fraction, we observe an increase of NM with increasing film thickness up to a maximum value of 63%. We conclude that for films on rigid substrates coarsening is inhibited by the elastic energy at the interface for one third of all possible 14M variants. This work is funded by DFG via SPP 1239.

MM 38.3 Thu 14:45 IFW D

Correlating twinning periodicity and film thickness of epitaxial Ni-Mn-Ga films — •Anett Diestel[1,2], Anja Backen[1,2], Ludwig Schultz[1,2], and Sebastian Fähler[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

In order to probe the theoretical geometrical theory by Kiselev et al. [1] about the periodicity of stripe domains in magnetic shape memory alloys, we have analysed the finely twinned microstructure of 14M martensite in epitaxial Ni-Mn-Ga films. Epitaxial Ni-Mn-Ga films with different thicknesses ranging from 30 nm to 2 μm have been deposited by sputter deposition on single crystalline MgO(100) substrates with a chromium buffer layer. The characteristic microstructure of 14M martensite was quantified by atomic force microscopy. The periodic height profiles of the mesoscopic twin boundary formation were analysed according to the geometrical model of a twinned surface by Buschbeck et al. [2]. We observed an increasing twin boundary periodicity with the square root of the film thickness. We did not observe the increase of variant size below a critical thickness predicted by Kiselev et al. We attribute this to the finite number of unit cells involved, an aspect not considered in continuum theory. This work was funded by DFG through SPP 1239. [1] N.S. Kiselev et al. Eur. Phys. J. Special Topics 158 (2008) 119 [2] J. Buschbeck et al. Acta Mater. 57 (2009) 2516

MM 38.4 Thu 15:00 IFW D

Modelling Bain path and adaptive martensite in Fe-based magnetic shape memory alloys — •Markus Ernst Gruner[1], Sandra Weiss[2], Sebastian Fähler[2], Ludwig Schultz[2], and Peter Entel[1] — [1]Faculty of Physics, University of Duisburg-Essen, 47048 Duisburg — [2]IFW Dresden, P.O. Box 270116, 01171 Dresden

Magnetic shape memory (MSM) exhibit macroscopic strains of several percent in realistic magnetic fields. Apart from the prototypical system Ni-Mn-Ga also Fe-based alloys as fct $Fe_{70}Pd_{30}$ are considered for technological applications. Within this contribution we investigate the ground state behavior and finite temperature magnetism of MSM Fe-Pd alloys by means of large scale density functional theory calculations with up to 500 atoms including atomic relaxations, which are essential for an accurate description of structural properties [1]. On the essentially flat binding surface the ground state is found to be bct, while for tetragonal distortions beyond fcc an adaptive structure consisting of bct building blocks effectively decreases the energy. Also, magnetic excitations are capable of substantially altering the binding surface. The results agree closely with experimental evidence obtained from strained Fe-Pd MSM alloys epitaxially grown on different substrates, which cover the Bain path [2] and beyond confirming that adaptive structures can be deliberately grown in Fe-based MSM films.

This work is supported by the DFG through SPP 1239 and the supercomputing resources of the NIC, FZ Jülich.
[1] M. E. Gruner, MRS Symp. Proc. **1200E**, 1200-G04-04 (2010)
[2] J. Buschbeck *et al.*, Phys. Rev. Lett. **103**, 216101 (2009)

MM 38.5 Thu 15:15 IFW D

Probing the electronic origin of a martensitic transformation in frozen intermediate stages. — •X. Kozina[1], S. Weiss[2], L. Schultz[2], S. Fähler[2], G. Stryganyuk[1], S. Ouardi[1], G. H. Fecher[1], C. Felser[1], S. Ueda[3], and K. Kobayashi[3] — [1]Institute of Inorganic and Analytical Chemistry, Johannes Gutenberg - University, Mainz, Germany — [2]IFW Dresden, Germany — [3]National Institute for Materials Science, SPring-8, Hyogo, Japan

An energetically unfavourable high density of states close to Fermi level had been suggested as driving force for martensitic transformation in metals. Here we present a direct experimental proof for the $Fe_{70}Pd_{30}$ magnetic shape memory alloy. By coherent epitaxial film growth we stabilize intermediate stages along the Bain transformation path, connecting *bcc* and *fcc* structure. This allows a detailed analysis at a constant temperature of 300 K, in vicinity of the martensitic transformation temperature. For probing the electronic structure of these 50 nm-thick films hard X-ray photoelectron spectroscopy (HAXPES) at BL15XU at SPring-8 was used. High probing depth of this method makes it a unique, non-destructive tool for studying electronic properties of thin films without taking into account the quality of the surface. Further, at high excitation energies one reaches nearly equal spectral weight for all states. Our measurements reveal that the density of states at 2 eV below the Fermi energy is reduced by 4,6% when the structure changes from the *fcc* austenite towards the *bcc* martensite. This confirms the proposed band Jahn Teller effect. *This work is supported by DFG through SPP 1239 and DfG-JST (FE633/6-1).*

Topical Talk MM 38.6 Thu 15:30 IFW D

Phase Transformations in Bi-based lead-free piezoceramics — •Jürgen Rödel and Wook Jo — Institute of Materials Science, Technische Universität Darmstadt,, Darmstadt, Germany

Piezoceramics in the application as an actuator experience electric fields between 0 and 3 kV/mm and temperatures between -30°C and 150°C with uniaxial stress up to 40 MPa. Lead-containing materials have relied on the concept of a morphotropic phase boundary (MPB), where similar free energy functions between rhombohedral and tetragonal afford easy polarization rotation and domain switching.

In this talk, the focus will be placed on the main lead-free piezoceramic material with MPB. Bismuth-Natrium-Niobate (BNT) - Bar-

ium titanate (BT)exhibits a pseudocubic structure at the MPB, which transforms irreversibly into a mixture of tetragonal and rhombohedral phases upon poling. this transformation, however, is reversible, if small amounts of Niobates are added. This leads to a very field-induced strain (poling strain+unipolar strain). the phase transition behavior will be presented utilizing in-situ (under electric field) investigations under synchrotron diffraction, neutron diffraction and in the TEM. Further, first diffuse scattering measurements on single crystals will be presented. Some of these measurements have been performed as function of temperature and are always discussed with respect to salient electrical performance.