MA 26: Magnetic Shape Memory Alloys II

Time: Wednesday 14:45–16:30 Location: HSZ 103

MA 26.1 Wed 14:45 HSZ 103

First principles determination of phase transitions in magnetic shape memory alloys — •Tilmann Hickel, Matthe A Uijttewaal, and Jörg Neugebauer — Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Str.1, 40237 Düsseldorf, Germany

Magnetic shape memory alloys have recently attracted a lot of excitement, since they allow shape changes of more then 10% with a frequency in the kHz regime. The fundamental origin of this property is related to a martensitic phase transition. The material system Ni_2MnGa is the most promising candidate for applications, but its operation temperatures and ductility still need to be improved. Hence, an extension of the currently limited knowledge on the phase diagram is decisive. In order to identify the stable structures and their transitions we performed ab initio calculations of free energies for the austenite, the (modulated) pre-martensite and the unmodulated martensite. Quasiharmonic phonons and fixed-spin magnons are considered, employing density functional theory. Using this approach we were able to successfully describe the phase transition in detail, to reveal the involved delicate interplay of vibrational and magnetic excitations and to accurately determine the transition temperature. The methods are used to interpret the experimental findings and to make predictions for modified material compositions.

MA 26.2 Wed 15:00 HSZ 103

Binding energies of tetragonally distorted magnetic Heusler alloys — •Mario Siewert, Markus Ernst Gruner, and Peter Entel — Fachbereich Physik, Universität Duisburg-Essen

Binding surfaces of the magnetic Heusler Alloys Ni_2MnX (X=Al, Ga, In, Zn, Ge, Si, Sn, Sb, As) and Cu_2MnY (Y=As, Ga, Ge, Sb) have been calculated by using density functional theory. The binding surfaces tend to show a global minimum of the total energy at c/a-ratios larger than 1.0 with increasing valence electron density e/a. The c/a-ratios refer to a tetragonal distortion that can be linked to the low-temperature martensitic state. In some systems with large values of e/a the minimization of the energy is linked to a decrease of the volume which can be as large as 3.9%.

Fixed-spin moment calculations (FSM) reveal that the energy barrier between two minimums can be lowered or shifted in some systems by applying a magnetic field.

MA 26.3 Wed 15:15 HSZ 103

A general phase-field model for polycrystals with elastic and micromagnetic contributions — •Christian Mennerich, Andreas Melcher, and Britta Nestler — Institute of Computational Engineering, Karlsruhe University of Apllied Sciences, Germany

A phase-field model coupled with elastic and micromagnetic contributions is introduced to describe the time spatial evolution of a polycrystal under the influence of strains and in the presence of a magnetic field. We introduce the model in terms of a general Ginzburg-Landau free energy functional and derive a coupled system of partial differential equations for the vector valued phase-field variables, for the displacement-field and for the spontaneous magnetisation. Applications of the model to cubic and tetragonal crystal symmetries of the polycrystal are discussed. Finally we give a short insight into the numerical implementation.

MA 26.4 Wed 15:30 HSZ 103

Modelling the phase diagram of Ni-Mn-X (X = In, Sn, Sb) alloys:*A q-state Potts model monte Carlo study — •P. Entel[1], V. D. Buchelnikov[2], S. V. Taakaev[2], V. V. Sokolovskiy[2], A. Hucht[1], M. Ogura[3], H. Akai[3], M. E. Gruner[1], and S. K. Nayak[1] — [1]Physics Department, University of Duisburg-Essen, 47048 Duisburg, Germany — [2]Department of Condensed Matter Physics, Chelyabinsk State University, 454021 Chelyabinsk, Russia — [3]Department of Physics, Osaka University, Osaka 560-0043, Japan

On the basis of Monte Carlo simulations using Heisenberg and Potts model Hamiltonians, we investigate the complex temperature dependence of the phase diagram of Ni-Mn-X (X = In, Sn, Sb) Heusler alloys. For Mn excess concentration, we find Mn atoms on the X sites, whose magnetic moments interact antiferromagnetically with the Mn spin moments on the Mn sublattice. Using ab initio data for the magnetic exchange interactions, it is shown that this antiferromagnetic exchange is responsible for metamagnetic behavior and a series of magnetic phase transitions, which compete or act in favor of the martensitic transformation being present in the Heusler alloys. This scenario is finally responsible for the occurrence of magneto-structural phase transitions in this class of ferromagnetic Heusler alloys.

MA 26.5 Wed 15:45 HSZ 103

Reversibility of magnetostructural transition in Ni-Mn-In-Co magnetic shape memory alloys — •Jian Liu, Julia Lyubina, Nils Scheerbaum, and Oliver Gutfleisch — IFW Dresden, Institute for Metallic Materials, P.O. Box 270116, D-01171 Dresden, Germany

For Ni-Mn-based Heusler alloys showing a magnetic-field induced martensitic transition, the reversibility of the magnetostructural transition is of crucial importance for magnetic-shape-memory actuator materials. It is desirable that the austenite induced by the magnetic field is able to transform back to the initial martensite when the magnetic field is removed. A complete recovery of the initial martensite state may bring about magneto-elasticity (two-way shape memory effect), while the irreversible magnetostructural transition would result in magneto-plasticity (one-way shape memory effect). Here, by analyzing isothermal magnetization curves under magnetic field cycling, the reversibility of the magnetostructural transition was investigated in Ni45Mn37In13Co5 in form of bulk sample and melt-spun ribbons. Hysteresis in the thermally and magnetically induced martensitic transformation plays an important role in the reversibility of the magnetostructural transition. In ribbons with a large hysteresis of 18 K, a residual field-induced austenite is present after removing the magnetic field, while, in the bulk sample, the magnetostructural transition is reversible at moderate temperatures due to a relatively smaller hysteresis of 8 K. Additionally, the magnetocaloric effect strongly depends on the sample history due to the occurrence of the irreversible magnetostructural transition, especially for the ribbons.

MA 26.6 Wed 16:00 HSZ 103

Orientation characterisation of NiMnGa MSM — •Claudia Hürrich, Martin Pötschke, Stefan Roth, Bernd Rellinghaus, and Ludwig Schultz — IFW Dresden, PF 27 01 16, 01171 Dresden

Magnetic shape memory alloys (MSMA) have gained a large research interest due to their capability of showing magnetic field-induced strain (MFIS). In contrast to conventional shape memory alloys, plastic deformation in the martensitic phase, which is due to twin boundary motion, may be caused not only by mechanical stress but also by an external magnetic field. $Ni_{50}Mn_{29}Ga_{21}$ shows magnetic field induced strain (MFIS) in single crystals. Polycrystalline $Ni_{50}Mn_{29}Ga_{21}$ was prepared by directional solidification and was cut erosively from a cast ingots into cubes with a 5 mm edge length. These samples have a martensite - austenite transformation at approximately 60°C. The change in surface topography during this transformation is followed by an optical microscope. The configuration of the twin boundaries was analysed before and after compressing the samples.

Financial support by the DFG within SPP 1239 is gratefully acknowledged.

MA 26.7 Wed 16:15 HSZ 103

Influence of alloying Ni-Mn-Ga with cobalt on structural, mechanical, and magnetic properties — •Katharina Rolfs[1,2], Markus Chmielus[1,3], Peter Müllner[3], Robert C. Wimpory[1], Winfried Petry[2], and Rainer Schneider[1] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie, Glienicker Str.100, D-14109 Berlin, Germany — [2]Technische Universität München, Lichtenbergstr. 1, D-85747 Garching, Germany — [3]Department of Materials Science and Engineering, Boise State University, 1910 University Dr., Boise, Idaho 83725, USA

Magnetic Shape-Memory Alloys (MSMAs) can potentially substitute giant magnetostrictive materials as well as piezoelectrical ceramics in actuating devices due to their large magnetically induced strain. By alloying the most commonly studied MSMA Ni-Mn-Ga with 5 at-% Co, the martensite- and Curie-temperature was increased to values above 160°C. Two structures have been observed in Ni-Co-Mn-Ga single crystalline samples. Besides the non-modulated tetragonal structure, one of the common structures of Ni-Mn-Ga, a non-modulated orthorhombic structure, has been observed, which shows a cyclic permutation of

all three crystallographic axes by applying a mechanical stress. The stress-strain analysis and the crystallographic characterization will be discussed here in detail. The giant magnetocaloric effect at the first order phase transition in Ni-Mn-Ga is well known. This effect is strongly influenced by alloying Ni-Mn-Ga with Co. Depending on the Mn-Ga-ratio the entropy change at the phase transition is still huge, however with an opposite sign. The results will be discussed here as well.