MM 41: Topical Session Diffussionless Transformations II

Time: Thursday 16:15–17:45 Location: IFW D

MM 41.1 Thu 16:15 IFW D

Martensitic transformations in thin epitaxial films of the NiTi shape memory alloy — •Joerg Buschbeck, Jason Kawasaki, Alexander Khozanov, and Chris Palmstrom — ECE Department, University of California, Santa Barbara, US

Phase formation and martensitic transformations are studied on molecular beam epitaxy (MBE) grown Ni-Ti films over a wide range of Ti contents from 43 to 56 at.%. Ordering of the B2 phase is investigated as function of growth temperature. Lattice mismatch stabilizes the NiTi B2 phase in a tetragonally distorted structure. Despite the epitaxial interface constraining the only 35 nm thick films, we observe reversible martensitic transformations in temperature dependent X-ray diffraction and resistivity. Ti-content and epitaxial interface control the transformation temperatures. In similarity to the B2-R-B19' sequence in bulk, a two-stage martensitic transformation is observed. This transformation occurs without tilt of the normal lattice vector, as temperature dependent reciprocal space mappings show.

MM 41.2 Thu 16:30 IFW D

Smart Heusler materials from first-principles calculations — •Peter Entel, Antje Dannenberg, Mario Siewert, and Markus E. Gruner — Faculty of Physics, University of Duisburg-Essen, 47048 Duisburg, Germany

The interplay of structural and magnetic phase transitions vastly determines the properties of ternary intermetallics such as X_2YZ Heusler alloys. Here, X and Y are ransition metal elements and Z is an element from the III-V group. In order to give a precise prescription of the possibilities to optimize the magnetic shape memory and magnetocaloric effects of these alloys, we use density functional theory calculations. From these calculations we can infer the martensitic driving forces and reveal the dominant role of the *d*-electrons in the formation of both, the different martensitic structures as well as the different magnetic spin orderings as a function of the atomic composition. In particular, we outline how one may find new intermetallics which show higher Curie and martensitic transformation temperatures when compared with the prototypical magnetic-shape memory compound Ni_2MnGa. Higher operation temperatures are needed for technological applications. On the other hand, the optimization of the magnetocaloric effect is strongly related to find alloys for which the magnetic and structural phase transitions merge in a narrow temperature interval. This allows for larger adiabatic temperature changes across the transitions in an external magnetic field.

MM 41.3 Thu 16:45 IFW D

Ab initio derivation of chemical trends in the phase temperatures of Ni_2MnGa-based shape memory alloys — •Ali Al-Zubi, Tilmann Hickel, and Jörg Neugebauer — Max Planck Institut für Eisenforschung, 40237 Düsseldorf

Since martensitic phase transitions are essential for the shape memory effect, their dependence on the chemical composition is of utmost importance for the application of these alloys. In this study we systematically investigated chemical modifications of the magnetic Heusler alloy Ni_2MnGa, with a particular focus on an excess Ni content. We combine density functional theory with thermodynamic concepts in order to derive accurate temperature dependencies of the free energies for the austenitic, pre-martensitic and martensitic phase. Vibrational excitations are treated in the quasiharmonic approximation and magnetic excitations are considered in a fixed-spin moment approach, yielding a delicate interplay of these two degrees of freedom. Particular care has been taken to determine the shuffling structures related to soft phonons. Using this approach we were able to successfully describe the phase transitions for different chemical compositions. In very good agreement with experiment, we find an increase of the martensitic phase transition temperature with x in $Ni_{2+x}Mn_{1-x}Ga$ and revealed a sensitive dependence of this behaviour on the Curie temperature of the system. Further, a strong dependence of the pre-martensitic phase stability on the Ni content was resolved. The information have been combined in temperature-dependent phase diagrams.

MM 41.4 Thu 17:00 IFW D

First-principles investigation of the magnetic shape memory system Co-Ni-Ga — •Mario Siewert, Markus E. Gruner, Antje Dannenberg, and Peter Entel — Faculty of Physics and CeNIDE, University of Duisburg-Essen, 47048 Duisburg, Germany

The magnetic shape memory (MSM) system Ni-Mn-Ga still has limited applications because the operating temperatures are not suitable for many practical devices. Hence, the search for new ferromagnetic shape memory compounds is not only of scientific but also of industrial importance. One approach to find new MSM alloys are Heusler compounds based on Co. Here, we present first-principles results for the Co-Ni-Ga system. In particular, the structural, electronic and dynamic properties of stoichiometric Co_2NiGa and off-stoichiometric compositions have been investigated using density functional theory. Our results reveal that there is a competition between tetragonal distorted and bcc-like structures. In addition, a competition between different structural orderings, namely the regular Heusler structure and the so called inverse Heusler structure, occurs. In advance, no phonon softening along the [110] direction is found for Co-Ni-Ga in agreement with neutron scattering measurements. This is supported by the electronic structure which reveals no sign of Fermi surface nesting.

MM 41.5 Thu 17:15 IFW D

Competing structural ordering tendencies in new high-TC ferromagnetic Fe-Co-based Heusler alloys from ab initio investigations — •Antje Dannenberg[1], Markus 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

Fe-Co-based Heuslers are candidates for new ferromagnetic shape memory alloys (FSMA) as they promise higher operation temperatures compared with prototype Ni2MnGa. Of interest are also the corresponding binary systems FeZn and Fe3Ga which show a huge magnetostriction. We present results of ab initio and Monte Carlo calculations regarding structural, magnetic, and electronic properties of Fe2CoGa1-xZnx alloys in conventional X2YZ and inverse (XY)XZ Heusler structures. All systems exhibit high Curie temperatures TC. The preference of the cubic inverse structures is believed to originate from the bcc-like environment of two inequivalent Fe atoms and their strong hybridization with the Co- states. Weakening the Co-Fe hybridization by substitution of Ga by Zn reduces this preference and leads to higher TC but simultaneously reduces the miscibility. Despite the strong spin-dependent Fe-Co hybridization we find a localized character of the spin moments. Extraordinary Z-elements like Cu, Ag, and Au or further enhancement of the Zn content induces a martensitic instability also in the inverse structures. Thus, we conclude that it is possible to find new FSMA with rather high Curie temperatures.

MM 41.6 Thu 17:30 IFW D

Twin boundary rearrangement in magnetic shape memory alloys studied with a phase-field model — •Frank Wendler, Christian Mennerich, Marcus Jainta, and Britta Nestler — IMP, Karlsruhe University of Applied Sciences

The observed large magnetic field induced strain (MFIS) in magnetic shape memory alloys is characterized by a structural rearrangement of martensite variant fractions. The complicated interdependency of microstructure - stress - magnetic field in the alloy Ni2MnGa motivates this numerical study. The displacive phase transition in the free boundary problem is treated by a phase-field model, based on the formulation of chemical, micromagnetic and magneto-elastic free energy densities. For the isothermal situation of martensite nucleation in the parent phase and twin boundary motion in the martensitic state, order parameters for variants and parent phase are introduced and related to their eigenstrain. The parameters are evolved according to Allen-Cahn dynamics, whereas a time dependant wave equation is solved for the field of elastic displacements. The magnetization field is updated by solving the Landau-Lifshitz-Gilbert equation with a geometric integration scheme. First, a verification of the variational approach is given for the subproblems of either magnetic or elastic fields interacting with the variant structure. Then, we focus on the reversible transformation process in single crystals, where the coupled evolution of magnetic domains and twin variants is studied and examples for resulting magnetization and strain reaction are given. An extension of the approach to treat polycrystalline materials is discussed.