MM 36: Phase Transitions II

Time: Thursday 11:45–13:00 Location: H 0107

MM 36.1 Thu 11:45 H 0107

First Principles Investigation of Twin Boundary Motion in Magnetic Shape Memory Heusler Alloys — •Markus Ernst Gruner and Peter Entel — Fachbereich Physik, Universität Duisburg-Essen, 47048 Duisburg, Germany

In the martensitic phase of the magnetic shape memory (MSM) Heusler alloy Ni_2MnGa, strains of up to 10 % can be induced by external magnetic fields, making the material a technologically relevant candidate for magneto-mechanical actuators. The MSM effect in near stoichiometric Ni_2MnGa is connected with a modulated pseudotetragonal martensitic phase with $c/a < 1$. It is attributed to a high mobility of the twin-boundaries in connection with a large magneto-crystalline anisotropy allowing the reorientation of martensitic twins with the help of a magnetic field thereby changing the shape of the crystal. So far, the origin of the high mobility of twin-boundaries in this phase is unresolved and empirical potentials permitting the simulation on the relevant length and time scales do not exist. We therefore attempt to close this gap by large scale ab initio calculations in the framework of density functional theory allowing the investigation of simplified models of martensitic twin boundaries for the different martensitic structures of Ni_2MnGa with the help of contemporary supercomputers. First results indicate that for the low-temperature, non-modulated martensitic $L1_0$ structure with $c/a > 1$, the energy needed for shifting a twin boundary is too large to be overcome by magneto-crystalline anisotropy.

[1] M. E. Gruner, P. Entel, I. Opahle, M. Richter, J. Mater. Sci. (accepted for publication)

MM 36.2 Thu 12:00 H 0107

Strain measurements in ferromagnetic martensitic Heuslers and magnetization easy axis — •Seda Aksoy, Mehmet Acet, and Eberhard F. Wassermann — Experimentalphysik, Universität Duisburg-Essen, Duisburg, Germany

The temperature-dependence of strain under constant magnetic-fields is studied in Ni-Mn-X (X: Ga, In, Sn, Sb) and Ni-Mn-In-X (X: Ga, Sn, Sb) polycrystalline ferromagnetic Heusler alloys which undergo a martensitic transformation close to room-temperature. The applied magnetic-field influences the nucleation of martensite so that decreasing the temperature under a magnetic field leads to large length changes between the austenite and martensite states. The length-change within the martensitic state varies with the magnitude of the cooling-field. This is related to the variant-orientation during martensite nucleation. These strain-data provide information on the easy axis of magnetization.

MM 36.3 Thu 12:15 H 0107

Phase transformations of Ni_2MnGa shape memory alloy from first principles. — •Matthe' Uijttewaal, Tilmann Hickel, and Joerg Neugebauer — MPI für Eisenforschung, Düsseldorf, Germany

Ni_2MnGa is a typical example of a Heusler alloy that undergoes a martensitic transformation. The high-temperature austenite has a cubic $L2_1$ structure, whereas below 200 K the structure is orthorhombically distorted. The transformation is completely reversible despite lattice deformations of up to 10% and large strains connected to this change. Ni_2MnGa is attractive for application in actuators and sensors because magnetism can control its phases. Central to the shape memory properties is a soft phonon mode in the austenite, leading to modulated (pre-) martensitic phases. Despite ample research, the physics of this soft mode is not well understood. We, therefore, systematically studied the soft mode in the various phases (austenite, pre-martensite and modulated martensites) and their transitions using ab initio DFT (GGA, PAW). First, phonon spectra were computed in the quasiharmonic approximation. The eigenvectors of the unstable phonon modes were used next to set up the corresponding modulated harmonics in supercell calculations and to identify the stable shuffling structures. Based on the derived double-well potentials we successfully explained the mechanism of the transitions and determined the corresponding temperatures. We conclude that for the pre-martensitic transition the dynamics of the phonons are important. The resulting temperature dependence of the phonon frequencies compares favorably to available neutron scattering experiments for this material.

MM 36.4 Thu 12:30 H 0107

Beyond the standard analysis of magnetic shape memory alloys-Comparison of Ni-Fe-Ga and Ni-Mn-Ga single crystals — •Oleg Heczko[1], Alexander Vasiliev[2], Yuriy Chumlyakov[3], and Sebastian Fähler[1] — [1]IFW Dresden, Institute for Metallic Materials, P. O. Box 27 01 16, 01171 Dresden, Germany — [2]Moscow State University, Moscow, 119991, Russia — [3]Tomsk State University, Tomsk, 634050, Russia

Some ferromagnetic Heusler alloys exhibiting martensitic transformations are known to change their shape by an external magnetic field (MSM effect). Here we analysed in depth and compared the magnetic properties of Ni54Fe19Ga27 and Ni50Mn29Ga21 single crystals; at low temperature using Bloch spin wave theory, at high temperature in the vicinity of the ferromagnetic transition using the equation of state and Arrot analysis. Temperature dependence of reciprocal paramagnetic susceptibility indicates a ferrimagnetic ordering in Ni-Fe-Ga compound. Magnetic anisotropy is determined from the magnetization curves measured in different temperatures. The transformation to martensitic phase is accompanied by the increase of the spontaneous magnetization and large increase of magnetocrystalline anisotropy in both compounds. The consequences of observed differences of magnetic properties for existence of the MSM effect are discussed.

MM 36.5 Thu 12:45 H 0107

The study on the structure, magnetism and shape memory effect of the ferromagnetic shape memory alloy CoNiGa. — •Xuefang Dai and Claudia Felser — Institute of Inorganic and Analytical Chemistry, Johannes Gutenberg - University, 55099 Mainz

The structure, magnetic properties and shape memory effect of CoNiGa alloys were investigated in the bulk, as-spun and single crystal samples. It was found by experiments that the ternary CoNiGa alloys have good shape memory effect, and the shape memory strain can be easily controlled by temperature, magnetic field and stress. For optimizing the mechanical properties, the iron was doped in the CoNiGa alloys. Excellent superelasticity was obtained in the quaternary CoNiFeGa single crystal samples. The superelastic strain of 6.7% can be induced by compressed stress and 11% can be obtained in tension test. In addition, the perfect superelasticities also showed up in bending and torsion tests. Special CoNiFeGa crystals with regular defects have also been grown in a deep super-cooling condition. These defects result in a large energy barrier which leads to a very sharp martensitic transformation within a temperature window of only 2 K. On the other hand, we also prepared Si-doped CoNiGa alloys, which exhibit larger magnetic-field-induced strain than the ternary CoNiGa alloys. This improvement in magnetic-field-induced strain can be attributed to the increase of the magnetic anisotropy induced by the Si-dopant.

Xuefang Dai acknowledges the support by the Institute of Physics, Chinese Academy of Sciences, Beijing 100080.