MM 49: Microstructure and Phase Transformations - shape memory alloys

Time: Wednesday 15:45–16:45 Location: IFW B

MM 49.1 Wed 15:45 IFW B

Role of nano-precipitates in thermoelastic martensitic transformation in Fe-Mn-Al-Ni shape memory alloys — •Toshihiro Omori[1], Makoto Nagasako[2], and Ryosuke Kainuma[1] — [1]Department of Materials Science, Tohoku University, Sendai 980-8579, Japan — [2]Institute for Materials Research, Tohoku University, Sendai 980-8577, Japan

Fe-Mn-Al-Ni alloy shows superelasticity associated with the α(bcc)/γ(fcc) martensitic transformation. Although Fe-Mn-Al ternary alloys show non-thermoelastic martensitic transformation, the addition of Ni results in the precipitation of fine β-NiAl (B2) particles and changes the transformation manner to thermoelastic. Therefore, it is considered that Ni plays a key role in the thermoelastic transformation. In this study, the effect of Ni on the martensitic transformation was investigated. The microstructures of Fe-36Mn-15Al-Ni (at%) alloys with different Ni contents were observed using TEM and HAADF-STEM. It was found that the β particle with about 10 nm is coherent with the martensite phase in 7.5Ni alloy, and the B2 lattice was distorted. In the martensite phase, the nano-twins were frequently introduced and the shear angle became smaller. These facts suggest that there is interaction between the β precipitate and martensite matrix due to the coherency, and it is deduced that the compatibility between the parent and martensite phases becomes high. The thermoelasticity comes from this microstructural feature.

MM 49.2 Wed 16:00 IFW B

Ordering Nanotwins in Modulated Martensite — Markus E. Gruner[1,2], Robert Niemann[2], Peter Entel[1], Rossitza Pentcheva[1], Ulrich K. Rössler[2], Kornelius Nielsch[2], and •Sebastian Fähler[2] — [1]Theoretical Physics and Center for Nanointegration, CENIDE, University of Duisburg-Essen, D-47048 Duisburg, Germany — [2]IFW Dresden, P.O. Box 270116, D-01171 Dresden, Germany

Modulated ferromagnetic martensites exhibit outstanding magnetocaloric and magnetic shape memory properties. Focusing on the Ni2MnGa prototype system, we use large scale density functional theory calculations to demonstrate that the formation of modulated martensite and key functional properties are governed by ordering nanotwins. Ordering is driven by the interaction between twin boundaries, which oscillates with the distance between twin boundaries. Minimizing the interaction energy results in the experimentally observed ordered modulations at the atomic scale, it explains a particular type of stacking fault at the mesoscale, known as a/b twin boundaries, and contributes substantially to the macroscopic hysteresis losses. Furthermore, an analysis of the relaxation process reveals that phonon softening paves the way for the transition towards the nanotwinned martensite, which unifies both competing concepts to explain modulated martensite.

MM 49.3 Wed 16:15 IFW B

Impact of doping on the magnetic and structural transformations in magnetocaloric materials — •Biswanath Dutta, Vijaya Begum, Tilmann Hickel, and Jörg Neugebauer — Max-Planck-Institut für Eisenforschung GmbH, D-40237 Düsseldorf, Germany

Understanding the magnetic and the martensitic transformations together with their coupling in magnetocaloric materials (MCMs) is crucial to tailor and optimize them for magnetic refrigeration. Specifically, any application of the MCMs requires a detailed knowledge of their underlying phase transformations. Within this study, we employ density functional theory along with Monte Carlo (MC) simulations to understand the impact of substitutional elements on the phase stability and the transformation behavior in Ni-Mn-based Heusler alloys. Our calculations reveal a reduction in the martensitic transformation temperature accompanied by a metamagnetic transition leading to a large entropy change due to Co substitution. We discuss the results in terms of calculated free energies, magnetic exchange interactions and the magnetic moments. The coupling of the magnetic and the structural degrees of freedom and its influence on the transformation behavior is addressed using MC simulations with the DFT input. Based on the achieved results, we provide new insights into the effect of doping on the martensitic and the magnetic transformations in Heusler alloys.

MM 49.4 Wed 16:30 IFW B

Vacancy annihilation and ordering kinetics in Ni_2MnAl studied by PALS — •Georg Zagler[1], Pascal Neibecker[1,2], Michael Leitner[1,2], Josef Schmidbauer[1,2], and Christoph Hugenschmidt[1,2] — [1]Physik Department, Technische Universität München, 85747 Garching, Germany — [2]Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universität München, Lichtenbergstr. 1, 85748 Garching, Germany

Heusler alloys are ternary intermetallic compounds with sum formula X_2YZ. These systems are of special interest due to them displaying the ferromagnetic shape memory effect (FSME) with strains larger than those of conventional actuators. While the protoypical ferromagnetic shape memory alloy Ni_2MnGa exhibits a martensitic transition and hence a pronounced FSME, the closely related Ni_2MnAl-System does not show this effect. Presumably this is due to a lack of atomic $L2_1$ order in the Ni_2MnAl system. Responsible for the reduced degree of order are the slow ordering kinetics in the temperature region of interest. Indirect measurements show that the achievable state of order in this system can however be influenced by quenched-in vacancies. A direct method to study vacancy concentrations in solids is positron annihilation lifetime spectroscopy (PALS). In the outlined work, we investigate the effect of quenched-in vacancies on the ordering kinetics of an off-stoichiometric Ni_2MnAl-alloy by means of PALS. We show a clear reduction of the average positron lifetime with the annealing time in isothermal annealing studies and correlate vacancy concentrations to ordering kinetics as determined by calorimetric measurements.