MM 43: Phase Transitions IV

Time: Thursday 16:00–17:15 Location: H 0107

MM 43.1 Thu 16:00 H 0107

Effect of composition and heat treatment on martensitic transformation and magnetic properties in Ni-Fe-Ga-Co magnetic shape memory alloys — •Jian Liu, Nils Scheerbaum, Dietrich Hinz, and Oliver Gutfleisch — IFW Dresden, Institute for Metallic Materials, P.O. Box 270116, D-01171 Dresden, Germany

Ni-Fe-Ga-Co is a promising alloy system for magnetic shape memory alloy applications, due to its good ductility, mobile twin boundaries and high transformation temperatures. Here, the martensitic transformation and magnetic properties in a large composition range with Ni54-xFe20Ga26Cox, Ni54-xFe19Ga27Cox, Ni56-xFe17Ga27Cox and Ni54-xFe18Ga28Cox (x = 0, 2, 4) are investigated. The martensitic transformation temperature Tm and the Curie temperature Tc can be tailored in a wide range by changing composition and heat treatment (ageing temperature, time and cooling rate), Tm ˜ -100 to 100 C and Tc ˜ 10 to 130 °C. A coupling of martensitic and magnetic transformations at a relatively high temperature (˜ 90 °C) is found for Ni52Fe17Ga27Co4. In this composition, increasing the degree of atomic order by long ageing and slow cooling decreases Tm but keeps Tc unchanged. Compared to ageing at 300 °C, after ageing at 400 °C there is no obvious change in Tm and Tc, but the transformation hysteresis is increased and the transformation interval is decreased significantly. However, the presence of γ precipitates induced by ageing at 500 °C suppresses the occurrence of the martensitic transformation itself.

MM 43.2 Thu 16:15 H 0107

First-principles study of hexagonal to cubic phase transformations in Laves phases $NbCr_2$ and $TaCr_2$ — •Olena Vedmedenko[1], Frohmut Rösch[1], and Christian Elsässer[2] — [1]Institut für Theoretische und Angewandte Physik, Universität Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart — [2]Fraunhofer-Institut für Werkstoffmechanik, Wöhlerstr. 11, 79108 Freiburg

The Laves phases $NbCr_2$ and $TaCr_2$ are two technically attractive intermetallic compounds with high melting temperature, high oxidation resistance, and low density. The thermodynamically most stable phases of both are hexagonal (C14) at high temperatures and cubic (C15) at low temperatures. However, the kinetics of the phase transformations leads to significantly different microstructures. To get a deeper scientific understanding of their evolution from the atomic scale, we have systematically studied the hexagonal to cubic phase transformations with respect to a synchroshear deformation mechanism. Total energies of structurally optimised atomistic supercell models have been calculated from first principles, by means of density functional theory with the local density approximation and a mixed-basis pseudopotential method. We obtain a quantitative description of activation energy profiles for deformation paths from hexagonal (high-temperature) to cubic or twinned cubic (low-temperature) phases. Based on these activation energy profiles we discuss differences in the transformation behaviour and interpret recently reported experimental observations of microstructural features for the two compounds.

MM 43.3 Thu 16:30 H 0107

Genuine Metal-Insulator Transition of V_2O_3 Revealed by Hard X-ray Photoemission — •Hidenori Fujiwara[1,2], Akira Sekiyama[1], Junnichi Yamaguchi[1], Gen Funabashi[1], Shin Imada[1], Sung-Kwan Mo[3,4], James W. Allen[3], Patricia Metcalf[5], Atsushi Higashiya[6], Makina Yabashi[7], Kenji Tamasaku[6], Tetsuya Ishikawa[6,7], and Shigemasa Suga[1] — [1]Graduate School of Engineering Science, Osaka University, Toyonaka, Japan — [2]II. Physikalisches Institut, Universität zu Köln, Köln, Germany — [3]Randall Laboratory of Physics, University of Michigan, Ann Arbor, USA — [4]Department of Physics, Stanford University, Stanford, USA — [5]Department of Physics, Purdue University, West Lafayette, USA — [6]SPring-8/RIKEN, Sayo, Japan — [7]SPring-8/JASRI, Sayo, Japan

V_2O_3 is a paradigmatic example of Mott-Hubbard (MH) metal-insulator transition (MIT) materials; it displays the 1st-order transition from the paramagnetic metal (PM) to the antiferromagnetic insulator (AFI) at 150 K. In order to reveal the mechanism of the Mott-Hubbard metal-insulator transition (MH-MIT) in V_2O_3, we have performed the hard X-ray photoemission (HAXPES) with $h\nu = 8170$ eV at BL19LXU in SPring-8. The energy resolution was set to 130 meV. The clean surface of the single crystalline sample was obtained by cleavage in situ in ultra-high vacuum. The significant spectral transfer of the V 3*d* states is observed through the MH-MIT. We reveal the simple Mott-Hubbard scenario does not describe the transition, and new reliable model is required to explain"the MH-MIT on V_2O_3.

MM 43.4 Thu 16:45 H 0107

Photoinduced ultrafast volume changes in intermediate valence solids — •momar diakhate and martin garcia — Institut für Physik, Universität Kassel, D-34132 Kassel, Germany

We present a theoretical model for the description of the ultrafast structural response of intermediate valence solids to femtosecond laser excitation. Based on the promotional Ramirez-Falicov model we consider the femtosecond laser heating of γ Cerium and the subsequent ultrafast lattice expansion dynamics.

In particular we determine the thermodynamic and electronic properties of cerium metal at very high electronic temperatures (simulating the laser excitation). The possibility for a non-equilibrium photoinduced inverse volume collapse transition is discussed. The p-v-T equation of state is obtained from the Helmoltz free energy in the usual way of thermodynamic derivatives by considering an adiabatic expansion of the crystal at high temperature.

We take into account both the laser excited and the unexcited parts of the system, in oder to account for inertial confinement. The thermodynamic properties were obtained as function of time and used to calculate the shock velocity variation and in the surrounding (unheated) part of the sample.

MM 43.5 Thu 17:00 H 0107

An *ab-initio* study of the phase transitions in the interstitial Fe-C solid solutions — •Alexander Udyansky, Martin Friák, and Jörg Neugebauer — Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Str. 1, 402 37, Düsseldorf, Germany

The Fe-C system constitutes the backbone of the steel industry that has long been altering our daily life. The Fe-C phase diagram is very rich in different phases exhibiting both low-carbon concentration, like ferrite or martensite, and high-carbon content, as e.g. austenite or cementite. An important prerequisite for the nucleation and formation of the latter is the existence of regions in the Fe matrix with diffusion-enhanced carbon concentration. In order to gain a detailed insight into properties of the high-C regions we have theoretically determined the formation energies, magnetic moments, and structural properties of selected interstitial Fe-C solid solutions employing density functional theory (DFT) in the generalized gradient approximation (GGA). The interstitial solid solutions have been modeled using the super-cell approach. Both magnetic and structural phase transformations induced by increasing carbon concentration are predicted and the very strong interplay between the C-content and both structural and magnetic degrees of freedom is found and analyzed.