MM 15: Phase transitions I

Time: Tuesday 10:15–11:15 Location: H4

MM 15.1 Tue 10:15 H4

Combinatorial study of the phase transformation characteristics of Ti-Ni-X (X = Cu, Pd) shape memory thin film composition spreads — •Robert Zarnetta[1,2], Sigurd Thienhaus[1,2], Alan Savan[1], and Alfred Ludwig[1,2] — [1]Combinatorial Material Science group, caesar, Ludwig-Erhard-Allee 2, 53175 Bonn, Germany — [2]Ruhr-University Bochum, Institute of Materials, 44780 Bochum, Germany

The phase transformation properties of Ti-Ni-X (X=Cu,Pd) shape memory thin films prepared in the form of continuous composition spreads were investigated. The thin film materials libraries were fabricated from elemental targets using an ultra-high vacuum combinatorial magnetron sputter-deposition system. Alternating wedge-type layers of Ti, Ni, and Cu (Pd) were deposited on a thermally oxidized Si wafer and subsequently annealed at 500°C for 1h in situ. Automated temperature-dependent resistance measurements (R(T)), energy dispersive X-ray analysis (EDX) and X-ray diffraction measurements (XRD) revealed the compositional region in the ternary phase diagram where thermoelastic transformations occur. The transformation temperatures and the thermal hysteresis were determined from R(T) measurements.

MM 15.2 Tue 10:30 H4

Phonons in High-Pressure structures of Boron — •Jens Kortus[1] and Lilia Boeri[2] — [1]TU Bergakademie Freiberg, Institut for Theoretical Physics, Leipziger Str. 23, 09599 Freiberg, Germany — [2]Max-Planck Institut for Solid State Research, Heisenbergstr. 1, D-70569 Stuttgart, Germany

Boron has recently received a lot of interest in the search of new electron-phonon superconductors. Elemental boron has been shown to undergo a superconducting transition at high pressures. However, no experimental data about the actual crystal structure of the superconducting phase are available. In this work we examine the relative stability of different possible high-pressure phases of boron and calculate the phonon dispersions at the experimental pressures at which superconductivity is observed. The total-energy calculations show that the $\alpha - Ga$ phase of boron, which gives a metal with a low DOS, remains the most energetically favoured one up to very high pressures. Our linear-response results indicate further, that several of the in the literature proposed structures are actually unstable at high pressure.

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MM 15.3 Tue 10:45 H4

Diffuse x-ray scattering from the refractory alloy systems Mo-Ta and Nb-Ta — •Harald Reichert, John Okasinski, Markus Mezger, and Helmut Dosch — Max-Planck-Institut für Metallforschung, Heisenbergstrasse 3, 70569 Stuttgart, Germany

We have performed diffuse x-ray scattering experiments on the bcc refractory alloy systems Mo-Ta and Nb-Ta. Using high energy x-rays in transmission geometry we were able to map the diffuse scattering of single crystalline samples as a function of concentration and temperature. In addition to thermal diffuse scattering we found diffuse scattering from short-range order. Our results will be compared with recently published first-principles calculations [1].

[1] V. Blum, A Zunger, Phys. Rev. B 70, 155108 (2004).

MM 15.4 Tue 11:00 H4

Laser-induced phase transition in As under pressure — •Nils Huntemann, Eeuwe Sieds Zijlstra, and Martin Garcia — Theoretische Physik, Fachbereich Naturwissenschaften, Universität Kassel, Heinrich-Plett-Str. 40, 34132 Kassel, Germany

It has been experimentally shown [U. Häussermann et al., J. Am. Chem. Soc. **124**, 15359 (2002)] that As undergoes a structural transition from the A7 to the simple cubic (SC) structure for increasing pressure. This phase transition occurs in thermodynamical equilibrium. In the last years different nonthermal, ultrafast structural changes have been induced in solids by means of femtosecond laser pulses [A. Cavalleri et al., Phys. Rev. Lett. **87**, 237401 (2001)]. Based on first-principles electronic structure calculations we explored the possibility of inducing nonthermal structural changes in As by ultrashort laser pulses. For this purpose, we determined the potential energy surface (electronic free energy) as a function of the lattice parameters and atomic coordinates for different electronic temperatures, which simulates the ultrafast laser heating of the electrons. Our results indicated that a laser-induced phase transition may occur in As under a pressure of ~ 20 GPa.