MM 33: Phase Transitions I

Time: Wednesday 14:45–16:30 Location: IFW B

MM 33.1 Wed 14:45 IFW B

Stoichiometrical trends in differential scanning calorimetry measurements on phase-change materials — •Michael Klein, Malte Linn, and Matthias Wuttig — I. Physikalisches Institut (IA), RWTH Aachen University, Aachen, Germany

Phase-change materials are alloys which can be rapidly switched between two metastable states, the amorphous and the crystalline phase. At the same time they show pronounced contrast in their electrical and optical properties. They are widely used as the functional layer in rewritable optical discs. Prototypes of electrical devices employing phase change materials as non-volatile memory are already entering the market.

Here we present calorimetric measurements, mainly on ternary Ge-Sb-Te alloys. Scratched-off thin film samples were heated in a differential scanning calorimeter to measure the transition from as-deposited amorphous to metastable crystalline phase and finally to the stable crystalline phase. The different transition temperatures will be analysed as a function of stoichiometry in order to improve the understanding of their interconnection.

MM 33.2 Wed 15:00 IFW B

Crystallization kinetics in materials for PCRAM — •Andreas Kaldenbach, Martin Salinga, Carl Schlockermann, and Matthias Wuttig — I. Institute of Physics (IA), RWTH Aachen University, 52056 Aachen, Germany

Phase-Change RAM is one of the most promising candidates for next generation electrical memory devices. One of its key features is the non-volatility of the stored data, which is due to a permanent structural rearrangement in the used phase change materials: the switching between a highly resistive amorphous state and a low resistance crystalline one. Although already utilized in memory applications, the fundamental mechanism of crystallization kinetics in these materials is still not fully understood. A continuous investigation of the temperature dependence of crystal nucleation and growth is very challenging, since crystallization speed of phase change materials is extremely fast at temperatures between glass transition temperature and the melting point. Until now, this difficulty has been bypassed by extrapolating data taken near the glass transition temperature or close to the melting point, where crystallization is rather slow.

The described experimental gap will be closed by a currently developed setup combining optical and electrical measurements to investigate the crystallization kinetics on a nanosecond timescale. It uses a pulsed laser to thermally induce the switching and a probe laser to measure the changing reflectivity during the switching process. Experimental results from the new setup will be compared with existing theories.

MM 33.3 Wed 15:15 IFW B

High energy photoemission of Heusler shape memory compounds Ni2MnGa and Mn2NiGa — •Catherine A. Jenkins[1,2], Andrei Gloskovskii[2], Jürgen Winterlik[2], Hidefumi Maeda[3], Claudia Felser[2], and Gerhard H. Fecher[2] — [1]UC Berkeley, USA — [2]University Mainz, Germany — [3]Ryukoku University, Japan

High energy photoemission [1] is demonstrated as a tool for observing the structural and magnetic phase transition in magnetic shape memory compounds based on the Heusler structure. Ni2MnGa has been known for more than a decade as a ferromagnetic shape memory compound able to undergo transitions of up to 10% strain in properly oriented crystals. Ferrimagnetic Mn2NiGa [2] has recently been found to undergo up to 20% magnetic field assisted strain in the bulk. Recent work at SPring8 in Japan in bulk single and polycrystals of Ni2MnGa and Mn2NiGa show clear transformations in the valence band. Comparison of the measured spectra to Wien2k calculations are discussed.

[1] G.H. Fecher et al, J. Electron. Spectrosc. Relat. Phenom. 156-8 (2007) 97-101. [2] Barman and Chakrabarti, PRB April 2008.

MM 33.4 Wed 15:30 IFW B

Near-surface microstructure of Ni-rich Ni-Pt — •Markus Engelke[1], Bernd Schönfeld[1], and Philip Willmott[2] — [1]LMPT, Department of Materials, ETH Zurich — [2]SLS, Paul Scherrer Institut, Villigen

While the surface structure and the local atomic arrangement in the bulk of Ni-Pt alloys have been repeatedly studied, not much is known about the intermediate regime accessible by grazing incidence diffraction. Here, Ni-23.2 at.% Pt (110) was investigated at 923 K under UHV using synchrotron radiation at an angle of incidence of 0.75 times the critical angle of total reflection. Diffuse scattering shows maxima of about 5 Laue units at 100 positions. From the diffuse scattering registered at positions in-plane and out-of-plane, Warren-Cowley short-range order parameters were recovered. The assumption of a cubic as well as a tetragonal structure for data evaluation results in similar features; dominant values for nearest and next-nearest neighbors and signs of the parameters as expected for $L1_2$ type of local order.

MM 33.5 Wed 15:45 IFW B

Keine Hinweise auf die adaptive Überstruktur $NiPt_7$ — •Bernd Schönfeld[1], Markus Engelke[1] und Andrei Ruban[2] — [1]LMPT, Departement Materialwissenschaften, ETH Zürich — [2]KTH Stockholm, Schweden

Die diffuse Streuung einer einkristallinen Ni-87,8 at.% Pt Probe wurde mit Röntgenstrahlung ausgemessen. Die Probe wurde bei 603 K ausgelagert, um einen thermischen Gleichgewichtszustand einzustellen. Aus der diffusen Streuung wurde der Beitrag der Nahordnung separiert, der schwache Maxima von etwa 2 Laue-Einheiten an 100-Positionen zeigt. Effektive Paarwechselwirkungen wurden mit der inversen Monte-Carlo-Methode bestimmt. In Monte-Carlo-Simulationen kann damit bei tiefen Temperaturen die vorgeschlagene adaptive Überstruktur $NiPt_7$ nicht eingestellt werden. Vielmehr zeigen die Simulationen eine Phasenseparation in $NiPt_3$ und eine Pt-reiche Matrix. Das Auftreten von $NiPt_3$ mit $L1_2$ Struktur konnte zudem anhand von Überstrukturreflexen einer Probe mit niedrigerer Pt-Konzentration experimentell bestätigt werden. Weiterhin ergeben Elektronenstrukturberechnungen keine Hinweise auf $NiPt_7$.

MM 33.6 Wed 16:00 IFW B

An atomistic study of low-C tetragonal Fe-C states — •Alexander Udyansky, Johann von Pezold, Martin Friák, and Jörg Neugebauer — Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Strasse 1, 402 37, Düsseldorf, Germany

The tetragonal states of interstitial Fe-C solid solutions are known as martensite, a metastable product obtained by quenching high-temperature austenitic *fcc* solutions with high C content. Along such a processing route, the tetragonality is proposed to be due to Bain's *fcc–bcc* diffusionless transformation. It has been long speculated that the tendency towards tetragonal distortions is an inherent property of the Fe matrix, i.e., it should manifest itself also at low C concentrations, independently on the processing route. To address this issue we calculated the chemical contributions of the interatomic interactions using EAM-potentials [1] and the strain-induced long-range interactions within the microscopic elasticity theory. Our study predicts tetragonal states to be preferred also at low C concentrations due to thermodynamically driven [2] orientational ordering of carbon interstitials. These states are found stable only below their order-disorder transition temperature. Above this temperature the loss of the orientational ordering results in the experimentally observed cubic ferritic phase.

1. T.T. Lau, C.J. Först, et al., PRL 98, 215501 (2007).
2. M.S. Blanter, A.G. Khachaturyan, Phys. Stat. Sol. A 51 291 (1979).

MM 33.7 Wed 16:15 IFW B

Fluence dependence of ultrafast transitions in Arsenic and Antimony — •Nils Huntemann, Eeuwe S. Zijlstra, and Martin E. Garcia — Theoretische Physik, Universität Kassel, Heinrich-Plett-Str. 40, 34132 Kassel, Germany

We extend a previous theoretical study [E. Zijlstra et al., New J. Phys. **10**, 033010 (2008)], in which we have predicted that a solid-solid phase transition from the A7 to the simple cubic phase can be induced by a laser in arsenic under pressure, to higher fluences up to 23 mJ/cm^2. This leads to a considerably decrease in the pressure that needs to be applied, namely from 23.8 GPa to 4.0 GPa, and for this reason reduces the experimental effort required for a confirmation.

We further investigate the structural changes of antimony under pressure, which has the same ground-state structure as arsenic, but

undergoes transitions to different phases in interaction with femtosecond laser pulses.

The possibility of ultrafast, laser-induced melting for both materials after excitation is also discussed.