MM 63: Computational Materials Modelling - Phase Stability IV

Time: Thursday 17:15–19:00 Location: H24

MM 63.1 Thu 17:15 H24

A thermodynamic consistent multi-phase-field model base on the maximal entropy production principle — •haifeng wang and herlach d.m. — Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt (DLR), 51170 Köln, Germany

The maximal entropy production principle (MEPP) based on which the additional constrains can be incorporated conveniently by the Lagrange method is applied to propose a new multi-phase-field model. The phase-field and diffusion equations follow the classical Onsanger reciprocal law which means that the present work is thermodynamic consistent with the classical irreversible thermodynamics. The bulk and interface contributions can be separated completely both at equilibrium condition and highly non-equilibrium condition where complete solute trapping happens. For medium growth velocities, the interaction between the bulk and interface contributions can be suppressed by increasing the order of a new interpolation function, which makes a quantitative modeling of rapid solidifications possible. For the one-sided growth model, the driving force for the phase field is not the grand potential but the model with solute drag as is in the classical sharp interface model. This means that the grand potential function which does not incorporate the additional constrains rightly is not thermodynamics consistent. Application to rapid solidification Si-9at.%As alloy shows that a good agreement between the model prediction and experimental results can be found.

MM 63.2 Thu 17:30 H24

Real-time observation of Ostwald ripening by synchrotron tomography — •Thomas Werz[1], Michael Heinze[2], Lukas Helfen[3], Mario Scheel[4], Stefan Odenbach[2], and Carl E. Krill III[1] — [1]Institute of Micro and Nanomaterials, Ulm University, Germany — [2]Institute of Fluid Mechanics, TU Dresden, Germany — [3]ESRF ID19, Grenoble, France — [4]ESRF ID15A, Grenoble, France

Synchrotron tomography is an ideal tool for the time-resolved, three-dimensional observation of coarsening phenomena like Ostwald ripening. In contrast to classical grain growth, in which grain boundaries migrate in a single-phase material, Ostwald ripening entails particle growth and shrinkage in the presence of at least two phases, and the evolution of the microstructure depends sensitively on the volume fraction of the coarsening phase, V_V. In the present study we focus on capturing the coarsening behavior at such high values of V_V that the system might manifest signs of a transition between Ostwald ripening and grain growth ($V_V = 1$). For this purpose, we designed a sample furnace that is compatible with the optical constraints of x-ray tomography, enabling precise control over V_V in a two-phase AlCu alloy by adjusting the temperature. After applying various image processing and segmentation steps to the reconstructed tomographic data, we extract both local and global features of the microstructure and follow their evolution with time.

MM 63.3 Thu 17:45 H24

Relaxor behavior of ferroelectric Ca0.22Sr0.12Ba0.66Nb2O6 single crystals — •Chandra Shekhar Pandey[1], Jürgen Schreuer[1], Manfred Burianek[2], and Manfred Mühlberg[2] — [1]Institute of Geology, Mineralogy and Geophysics, Ruhr-Universität Bochum, Universitaetsstrasse 150, 44801-Bochum, Germany — [2]Institute of Crystallography, Greinstrasse 6, 50939-Cologne, Germany

The relaxor behavior of tetragonal tungsten bronze uniaxial relaxor ferroelectric calcium strontium barium niobate (Ca0.22Sr0.12Ba0.66Nb2O6 or CSBN22) single crystal was studied by measuring elastic constants and thermal expansion with the aid of resonant ultrasound spectroscopy and dilatometry respectively, in the temperature range 300 K upto 1503 K. Thermal expansion yields evidence of the Burns temperature TB, and the intermediate characteristic temperature T*, which was also supported by the temperature evolutions of the elastic constants cij. CSBN22 was found to be about 2-3 % elastically stiffer than CBN28. The presented results open the perspective to understand the relaxor behavior in CSBN.

MM 63.4 Thu 18:00 H24

Acoustic emission during the martensitic transformation of a Ni-Mn-Ga single crystal under compressive stress — •Robert Niemann[1,2], Jordi Baró[3], Oleg Heczko[4], Ludwig Schultz[1,2], Sebastian Fähler[1,2], Eduard Vives[3], Lluis Mañosa[3], and Antoni Planes[3] — [1]IFW Dresden, P.O. Box 270116, 01171 Dresden, Germany — [2]Department of Physics, Institute for Solid State Physics, Dresden University of Technology, 01062 Dresden, Germany — [3]Departament d'Estructura i Constituents de la Matèria, Facultat de Física, Universitat de Barcelona. Diagonal 647, 08028 Barcelona, Catalonia, Spain — [4]Institute of Physics, Academy of Science of the Czech Republic, Na Slovance 2, 182 02 Prague, Czech Republic

The propagation of a phase front during a thermally induced martensitic transition is discontinuous due to pinning at various defects, an effect which results in acoustic emission. Here we analyze the consequences of an applied compressive stress exemplarily on a Ni-Mn-Ga single crystal. Our experiments show that the distribution of the energies of the acoustic emission events follows a power law for more than 3 decades. This indicates that the transition exhibits avalanche criticality. The exponent characterizing the distribution of energies depends on the applied stress and decreases from 1.9 at zero stress to 1.5 at stress above 3 MPa. This decrease could be attributed to the reduced multiplicity of variants possible under uniaxial compression.

MM 63.5 Thu 18:15 H24

Inverse magnetocaloric effect of epitaxial Ni-Mn-based films — •Anett Diestel[1], Robert Niemann[1,2], Maximilian Uhlmann[1,2], Ludwig Schultz[1,2], and Sebastian Fähler[1] — [1]IFW Dresden, Institute for Metallic Materials, P.O. Box 270116, 01171 Dresden, Germany — [2]Dresden University of Technology, Institute of Materials Science, 01062 Dresden, Germany

The Heusler alloys Ni-Mn-X (X = Ga, In, Sn, Sb) have been identified as versatile functional materials. Due to the diffusionless phase transformation from austenite to martensite, which can be induced by magnetic field, the materials show the (inverse) magnetocaloric effect (MCE). They are promising materials for magnetocaloric cooling devices at room temperature application. Due to the high surface-to-volume ratio of thin films a fast heat exchange and a higher cycle frequency is possible. Therefore higher cooling efficiency can be achieved using less material compared to bulk. We prepared epitaxial Ni-Co-Mn-In [1] and Ni-Mn-Ga-Co films by magnetron sputter deposition on single crystalline MgO(100). For both materials we proved epitaxial growth and the reversible transformation from ferromagnetic austenite to modulated, non-ferromagnetic martensite. For Ni-Co-Mn-In an inverse MCE with an entropy change of 8.8 J/(kgK) at 9 T near room temperature was achieved.[1] By adding Co the martensitic transformation and the Curie temperatures can be shifted to maximize the inverse MCE at room temperature. The results show that epitaxial Ni-Mn-based films are promising materials for efficient magnetocaloric cooling devices. [1] R. Niemann et al. Appl. Phys. Lett. 97, 2010

MM 63.6 Thu 18:30 H24

Ion-Irradiation-Assisted Phase Selection in Single Crystalline Fe7Pd3 Ferromagnetic Shape Memory Alloy Thin Films: From fcc to bcc along the Nishiyama-Wassermann Path — •Ariyan Arabi-Hashemi[1] and Stefan G. Mayr[1,2,3] — [1]Leibniz-Institut für Oberflächenmodifizierung e.V., Leipzig, Germany — [2]Translationszentrum für Regenerative Medizin, Universität Leipzig, Germany — [3]Fakultät für Physik und Geowissenschaften, Universität Leipzig, Germany

Fe7Pd3 exhibits four different metastable phases: the austenite fcc phase and three martensite phases (fct, bct, and bcc). Our work aims at exploring the influence of generalized internal stresses due to (i) point defects and (ii) deviations from equilibrium short-range order. While the former are stresses in a strict mechanical sense, the latter are the conjugate variable of the short-range order parameter. In a given sample, manipulation of both, (i) and (ii) can conveniently be achieved by means of irradiation with energetic ions. 500 nm thick single crystalline Fe7Pd3 films were deposited at 850°C on MgO (001) single crystalline substrates. The unirradiated samples exhibit prevalently the austenite fcc phase. These thin films were ion-irradiated with 1.8 MeV Kr+ -ions. Fluency dependant T2T-measurements show that ion-irradiation-assisted phase selection along the whole transformation path ranging from fcc->bcc is possible. Fluency dependant pole figure measurements describe the fcc->fct and the transformation

into the bcc phase in detail. An orientation relationship according to Nishiyama-Wassermann for the fcc->bcc transformation is observed.

MM 63.7 Thu 18:45 H24

Study of RGS (Ribbon Growth on Substrate) microstructure development — •Pierre Yves Pichon[1,2], Dieter Herlach[1], Schönecker Axel[2], Dirk Holland-Moritz[1], and Matthias Kolbe[1] — [1]DLR, Institut für Materialphysik im Weltraum, Linder Höhe 51170 Köln — [2]RGS Development B.V. Bijlestaal 54 A 1721 PW Broek op Langedijk The Netherlands

Silicon wafer for solar cell applications can be produced at high speed and in one step by the RGS technique. Textured substrates at initial temperature below the melting point of silicon are moved at a constant speed under a silicon bath, providing the driving force for nucleation and crystal growth. Heat extraction is perpendicular to the wafer transport; therefore production rate is decoupled from crystallization velocity. The development of the microstructure is strongly influenced by the thermal-mechanical contact interface between the wafer and the substrate: the summits of the substrate surface texture make discrete contact points with the wafer. It was found that a better contact leads to higher growth velocity, smaller grain size and higher dislocation density. The important parameters influencing the formation of the interface were studied during casting experiments and by bringing silicon droplets in contact with the substrate. It was found that the initial temperature of the substrate is strongly influencing the formation of the thermal contact. Under certain conditions it was found that the crystallization front can form twinned dendritic crystals. This was attributed to a higher driving force for crystal growth than the driving force for nucleation on the substrate.