MM 16: Phase transitions II

Time: Tuesday 11:45–12:45 Location: H4

MM 16.1 Tue 11:45 H4

Metadynamics Simulations of Phase Transitions in Solids — •Jörg Behler[1], Davide Donadio[1], Roman Martoňák[2], and Michele Parrinello[1] — [1]ETH Zurich, Department of Chemistry and Applied Biosciences, USI Campus, Lugano, Switzerland — [2]Comenius University, Department of Experimental Physics, Bratislava, Slovakia

The theoretical prediction of crystal structures for a given pressure and temperature based only on the chemical composition is still a challenging task. We present a combination of the metadynamics approach, which uses the edges of the simulation cell as collective variables to drive the system away from the local minimum towards a new crystal structure, and an efficient generalized neural network potential representation, which provides the energy and forces as a function of all atomic positions in a system of arbitrary size. This potential is several orders of magnitude faster than the underlying density-functional theory (DFT) calculations while the accuracy of DFT is essentially maintained. The capability of the method is demonstrated for a silicon model system and the results obtained are in excellent agreement with experiment.

MM 16.2 Tue 12:00 H4

The contribution of elastic strain onto the early stage of decomposition in a Cu1,7at%Fe alloy — •Thomas Rademacher, Talaat Al-Kassab, and Reiner Kirchheim — Institut für Materialphysik, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

The early stage of decomposition of supersaturated Cu Fe alloys has been previously intensely studied in the course of classical homogeneous phase separation. Up to now contributions of the strain energy to the decomposition process and its influence on the early stage has been neglected in this system.

In a former study Heinrich et al. (Mat. Sci. Eng. A353 (2003) 92-98) showed that decomposition at low temperatures of supersaturated Cu Co alloys is mainly controlled by strain energy. Hence, cluster's size and morphology are biased and the formation of chains of precipitates in the elastic soft <100> directions of the Cu-matrix is promoted.

In the current study, these phenomena will be investigated for Cu1,7at%Fe after a heat treatment at 722 K for times ranging from 1 to 48 hours. Analyses are performed by utilizing the Tomographic Atom Probe (TAP) and the newly developed computer assisted Field Ion Image Tomography (CFIIT). Amongst others, a chain like formation of precipitates can be observed in our results as well. By means of computer based methodical analyses the directions and distances of alignments of precipitates can be ascertained. The consistency of the results with calculations established by Miyasaki and Yamauchi/ De Fontaine in terms of linear anisotropic elasticity theory will be presented and discussed.

MM 16.3 Tue 12:15 H4

Simulationsrechnungen zu Positronenannihilationssignale von Frühstadien der Ausscheidungsbildung in AlCu-Legierungen — •Björn Korff und Torsten Staab — Helmholtz-Institut für Strahlen und Kernphysik der Rheinischen Friedrich-Wilhelms-Universität Bonn, Nußallee 14-16, D-53115 Bonn, Germany

Messungen mit Positronen stellen ein wichtiges Hilfsmittel bei der Untersuchung von Gitterfehlern und Ausscheidungen in Metallen dar. Leider lässt sich aus den Messdaten in Form von Positronen-Lebensdauer und Dopplerspektrum der Annihilationsstrahlung nicht direkt auf die Gitterstruktur des Materials schliessen. Durch Simulationsrechnungen für das Positron lassen sich jedoch Lebensdauer und Dopplerspektrum in einem hypothetischen Gitter berechnen. Ein Vergleich der berechneten und gemessenen Werte lässt dann eine Prüfung der Hypothese zu. Auf diese Weise wollen wir die atomare Struktur von Cu-Ausscheidungen in Aluminium im Frühstadium (1-5 Cu Atome) charakterisieren. Die Ausscheidungen wurden mit und ohne Leerstellen mit Hilfe des ab-initio Codes von SIESTA relaxiert.

MM 16.4 Tue 12:30 H4

Simulation of plate shaped second phase particles — •Emmanuel Jannot[1], Volker Mohles[1], Günter Gottstein[1], and Barend Thijsse[2] — [1]Institut für Mtellkunde und Metallphysik, RWTH Aachen, Aachen, Germany — [2]TU Delft, the Netherlands

In several metallurgical systems, plate shaped precipitates are observed. The most well-known example are the GP zones in AlCu alloys, composed of layers of pure copper in the [1 0 0] plane. This morphology is usually attributed to the conjugate effect of a size mismatch between the solute and the matrix atoms and an elastic anisotropy of the fcc lattice, the <1 0 0> direction being the soft and the <1 1 0> the hard direction. The object of this work is to assess the validity of this assertion. For this purpose a MonteCarlo approach is used where the Metropolis algorithm allows finding stable atomic configurations. The configuration energy is evaluated by Molecular Statics. The input parameters of this study are the potentials describing the atomic interactions. At first, harmonic potentials are employed. Using them, a condition for the stability of the plate morphology is found. This result is confirmed using various kinds of pair potentials (Lennard-Jones*). Moreover the Matrix-Solute interaction can be designed to reproduce the precipitate thermal stability. An interfacial energy of 0.08 J/m2 is derived for GP zones in AlCu alloys. Eventually, the influence of dislocations is studied. Simulation results are compared with TEM observations and a mechanism for heterogeneous precipitation in AlCu alloys is proposed.