MM 53: Microstructure and Phase Transformations II

Time: Thursday 11:45–13:00 Location: H39

MM 53.1 Thu 11:45 H39

Phase Transformation in Alloyed Nanowires — •Manuel Roussel, Martin Schellenberger, Tim Lehmann, and Guido Schmitz — Institute for Materials Science, Stuttgart, Germany

Since the discovery of giant magnetoresistance, for which Albert Fert and Peter Grünberg have been awarded the 2007 Nobel Prize, thin magnetic films have attracted much interest. More particularly, multi-layered nanowires consisting of magnetic and nonmagnetic layers (FeNi/Cu, Ni/Cu, Fe/Cr, Co/Cu...) have been proven to exhibit outstanding properties which have straightforward applications: M-RAM (magnetic random access memories), nano-sensors, data storage... Most of the time, the bottle neck for the usage of such nanostructures is that their synthesis is not reliable, especially when it comes to producing very small wires, in the range of a few tens of nanometers diameter. We are exploring alternative synthesis routes in order to find a new self-ordering way of producing multilayered or core-shell nanowires which would be only based on diffusion processes and phase separation. Simply put, we would like to create a plain alloyed nanowire and provoke the formation of layers just by a well-designed heat treatment. We will first present our approach to grow alloyed metallic nanowires of various compositions. In order to do so, we adopted a process based on electro-deposition in porous membranes. Later on we will focus on the influence of the nanowire geometry on phase transformation during annealing.

MM 53.2 Thu 12:00 H39

Core-shell structure of precipitates in the Al-Sc-Zr system — •Yulia Buranova[1], Ankit Gupta[2], Vladislav Kulitckii[3], Tilmann Hickel[2], Sergiy V. Divinski[1], and Gerhard Wilde[1] — [1]Institut für Materialphysik, Westfälische Wilhelms-Universität Münster, Wilhelm-Klemm-Str.10, 48149 Münster, Germany — [2]Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf 40237, Germany — [3]Laboratory of Mechanical Properties of Nanoscale Materials and Superalloys, Belgorod State University, Pobeda 85, Belgorod 308015, Russia

Aluminum alloys containing scandium show excellent mechanical properties due to the presence of Al3Sc precipitates, which control the dislocation and grain boundary motion during the recrystallization processes. An addition of Zr can further improve the properties due to the formation of Al3(Sc,Zr) dispersoids, which are more stable at elevated temperatures. In this work we investigate a commercial aluminum alloy AA5024, containing Sc, Zr, Ti and Mg additions. The particles size, chemistry and distribution were investigated by analytical transmission electron microscopy and geometric phase analysis was applied to map local strains. It is found that the Al(Sc,Zr,Ti)-precipitates reveal complex core-shell structures which are strongly affected by mechanical deformation and heat treatment. The experimental findings are compared with predictions based on DFT calculations, which indicate the existence of a critical size for the appearance of ternary Al3(Sc,Zr) shells. The financial support of DFG within SPP 1713 is gratefully acknowledged.

MM 53.3 Thu 12:15 H39

Mechanical behaviour and deformation mechanisms of a Zn-Al-Cu-Mg alloy — •Zhicheng Wu, Stefanie Sandlöbes, Günter Gottstein, and Sandra Korte-Kerzel — Institut für Metallkunde und Metallphysik, RWTH Aachen, D-52056 Aachen, Germany

The microstructure, mechanical properties and deformation behaviour of a gravity-cast alloy ZnAl4Cu1Mg0.3 (wt.%) was studied at different temperatures and strain rates using ex-situ and in-situ tensile tests in conjunction with scanning electron microscopy, electron backscatter diffraction, transmission electron microscopy and atom probe tomography. The alloy revealed two distinct deformation regimes, i.e. work hardening and brittle fracture at room temperature and/or elevated strain rates, and work softening and ductile fracture at elevated temperatures and/or low strain rates. Further, we identified precipitates of a non-equilibrium Zn_xAl_{1-x} ($x \geq 0.7$) transition phase or Guinier-Preston zone which partly dissolved during deformation at elevated temperatures. The partial dissolution of these precipitates is assumed to partially account for the observed increase in ductility at elevated temperatures, but might also contribute to the long-term softening of Zn-Al alloys that currently poses one of the major drawbacks to their application.

MM 53.4 Thu 12:30 H39

Zener ordering of interstitials in a bcc host lattice: Interplay between short- and long-range interactions — •Xie Zhang[1], Tilmann Hickel[1], Jutta Rogal[2], and Jörg Neugebauer[1] — [1]Max-Planck-Institut für Eisenforschung GmbH, 40237 Düessldorf, Germany — [2]Interdisciplinary Centre for Advanced Materials Simulation, Ruhr-Universität Bochum, 44780 Bochum, Germany

The octahedral interstitial sites in a bcc lattice can be categorized into three sublattices that can be occupied with interstitials and that are characterized by the corresponding tetragonal deformation variants ([100], [010] and [001]). Even in an external stress-free system, the interstitials energetically prefer to occupy only one of the three sublattices below a critical temperature. This preference is triggered by the interactions between the interstitials and termed Zener ordering. Although it was proposed by Zener more than half a century ago, direct proofs from atomistic simulations have been, however, rarely reported so far, which even resulted in a debate on the validity of such ordering recently. Hence, in this work, we employ atomistic simulations to directly investigate the interplay between long-range strain induced and short-range chemical interactions. It is found that a homogenized distribution of interstitials within one octahedral sublattice is crucial, and ensures that the short- and long-range interactions are minimized simultaneously. These insights help to understand self-induced collective ordering of interstitials within a bcc host lattice which is a key mechanism to harden steels.

MM 53.5 Thu 12:45 H39

Multi-scale modeling of phase transitions around dislocations — •Gerard Paul Leyson, Blazej Grabowski, and Jörg Neugebauer — Max Planck Institute for Iron Research, Max-Planck-Straße 1, 40237 Düsseldorf

Classic nucleation theory does not take into account local stress gradients present in the material. In particular, the stress field around a dislocation is large and can provide a strong driving force for phase transition and stabilize phases that would otherwise be unstable in the unstressed bulk material. To describe the impact of dislocation strain on nucleation we have developed a multi-scale framework. First, classic nucleation theory is generalized to include the effects of external stress gradients. As input the dislocation stress field is determined using a semi-empirical embedded atom (EAM) method. Second, the change in formation energy due to the phase transformation is calculated using ab-initio calculations. Using this approach we identify conditions that lead to a quasi-one-dimensional defect that is stable against coarsening. The mechanism identified here is general and applies e.g. to the recently found linear complexions in Fe-Mn alloys [1] or the formation of nano-hydrides at dislocations [2].

[1] Kuzima M, Herbig M, Ponge D, Sandlöbes S and Raabe D. Science 2015; 349: 1080-1083. [2] Leyson GP, Grabowski B and Neugebauer J. Acta Materialia 2015; 89:50-59