MM 13: Growth

Time: Monday 14:45–16:15 Location: H 0111

MM 13.1 Mon 14:45 H 0111

Triple junction controlled room temperature grain growth revealed by X-ray measurements of nanocrystalline palladium — •Markus Ames, Jürgen Markmann, and Rainer Birringer — Universität des Saarlandes

X-ray measurements at room temperature of nanocrystalline, pure palladium prepared by inert-gas condensation reveal a very fast grain growth from 10 nm up to the instrumental limit of about 60 nm within several hours. Two grain growth regimes have been observed, showing quite different growth kinetics, an intermediate regime in the first 12 h after synthesis which is dominated by an overall decrease of microstrain and only minor grain growth followed by a regime of about 8 h duration that shows linear grain growth kinetics. The latter can neither be explained by a boundary-curvature-driven growth mechanism nor by a vacancy drag model, but in our case by a triple junction controlled grain growth.

MM 13.2 Mon 15:00 H 0111

Monte Carlo simulation and mean-field theory of nanocrystalline grain growth — •Dana Zöllner and Peter Streitenberger — Institut für Experimentelle Physik, Abteilung Materialphysik, Otto-von-Guericke-Universität Magdeburg, Universitätsplatz 2, D-39106 Magdeburg

Nanocrystalline grain growth in polycrystals is modelled under the assumption that the mobility of grain boundaries is limited at small grain sizes. In particular, following the works of Gottstein, Shvindlerman, Novikov and others, it is assumed that the grain boundary mobility depends, for two-dimensional grain growth, on the triple junction distance.

Based on this assumption a modified Monte Carlo Potts model algorithm is presented allowing the simulation of grain growth controlled by size effects. For initially very small grains linear grain growth kinetics is observed, which is associated with an approximately quasi-stationary self-similar grain size distribution shifted to smaller relative grain sizes. This linear growth regime can adequately be described by a statistical mean-field theory yielding an analytical grain size distribution function that is in good agreement with the simulation results.

MM 13.3 Mon 15:15 H 0111

Kinetics of grain growth in nanocrystalline Fe at low annealing temperatures — •Heiko Paul and Carl E. Krill III — Institut für Mikro- und Nanomaterialien, Universität Ulm, Albert-Einstein-Allee 47, D-89081 Ulm

The migration rates of curved grain boundaries (GB) and triple junctions (TJ) manifest different dependencies on the average grain size $\langle R\rangle$, implying that there may be a critical grain size $\langle R\rangle_c$ below which the overall growth kinetics are controlled by TJ migration. If the activation enthalpy for TJ migration is significantly higher than that for GB migration, then a linear growth law is expected when $\langle R\rangle < \langle R\rangle_c$, whereas the well-known parabolic growth behavior should still obtain when $\langle R\rangle > \langle R\rangle_c$. To test this hypothesis, we carried out long-term *in situ* annealing experiments on highly pure samples of nanocrystalline Fe. Grain growth was measured in a laboratory x-ray diffractometer (XRD) equipped with a heating stage and a position-sensitive detector. By fitting linear and parabolic growth models to isothermal grain-growth curves recorded at temperatures between 409°C and 482°C, we were able to extract activation enthalpies for initial and late-stage coarsening, observing a decrease suggestive of a transition between TJ-controlled and GB-controlled growth. Additional microstructural analysis was performed to verify the average grain-size values calculated from the XRD measurements.

MM 13.4 Mon 15:30 H 0111

On the role of elastic strains in the precipitation of second phases — •Volker Mohles, Emmanuel Jannot, and Günter Gottstein — Institut für Metallkunde und Metallphysik, RWTH Aachen

The use of Green functions allows the efficient resolution of elasticity problems. However, previous attempts to use this methodology to derive the stored elastic energy in a solid solution haven't been fully successful. For example, the one atom thick plate morphology of GP zones in Al-Cu alloys can't be reproduced using the theory developed by Khachaturyan. The present work provides an explanation for this discrepancy. An improved version of the Microscopic Elasticity theory will be presented. Calculations indicate that this improvement reduces the error generated by the use of Green functions to less than 2% compared to Molecular Statics relaxations. Consequently, the role of elastic strains for the precipitation of second phases can be evaluated more precisely. Simulations for model materials revealed that elastic strains should be first considered as a positive driving force for nucleation. For example, the energy gain offered by the concentration of point defects like solute atoms explains the stability of second phases up to the melting point of aluminum for solute atoms having a 10% lattice mismatch. Using the improved theory, new insight on the factors explaining the precipitate morphology is provided. This work confirms the importance to consider elastic anisotropy.

MM 13.5 Mon 15:45 H 0111

Optical-image-furnace growth and characterisation of transition metal Heusler compounds — •Andreas Neubauer, Christian Franz, and Christian Pfleiderer — Physik-Department E21, Technische Universität München, D-85747 Garching, Germany

Both full (X_2YZ) and half (XYZ) Heusler compounds offer a huge variety of electronic and magnetic phenomena [1], e.g., half-metallic ferromagnetism, the magnetic shape memory effect, heavy-fermion behavior and unusual antiferromagnetic states. To gain further information about the physical properties of Heusler compounds detailed studies on high quality single crystals are essential. In recent years it has been found that optical as opposed to RF heated floating zone crystal growth produces very high quality single crystals [2]. Minimizing sample contamination (e.g. oxygen) is thereby a key prerequisite for high quality crystals. Going beyond present day technology [2], we set up a commercial image furnace for use with ultra-high vacuum and ultra-pure inert gas atmosphere by converting it to all metal-sealing. The furnace may be baked out to reduce any residual contamination by the system. To prepare polycrystalline feed rods for single-crystal growth we also set up a RF heated high-purity casting assembly employing a Hukin-type cold-crucible. Single crystals of the Heusler compounds Mn_3Si and Fe_2TiSn were grown and characterised. We present a structural analysis as well as transport and thermodynamic bulk properties. [1] for a review see e.g., I. Galanakis et al, cond-mat/0709.4183v2 (2007). [2] G. Behr, W. Löser, Recent Res. Devel. Crystal Growth **4**, 129 (2005).

MM 13.6 Mon 16:00 H 0111

Influence of Strain on Kinetics of Nonisothermal Solid-Solid Phase transitions — •Michael Fleck, Efim Brener, Robert Spatschek, and Guillaume Boussinot — Institut für Festkörperforschung, Forschungszentrum 52425 Jülich

Structural phase transitions in solids involve a discontinuous change in the lattice structure, leading to the presence of elastic deformations. In some cases, these effects are of minor influence and can be ignored, but nevertheless for many applications the elastic strain causes qualitatively new and observable effects.

A motion of the interface due to first order phase transitions is a source of latent heat due to the finite entropy difference of the two phases. This heat has to be transported away from the interface before further phase transformations can take place. From solidification or melting processes it is known, that these kinds of thermal effects can cause interface instabilities leading to dendritic growth, which is very important for many metallurgical applications.

We derive a thermodynamically consistent phase field model for non-isothermal solid-solid phase transitions, to be able to investigate the coupled influence of elastic and thermal effects on the kinetics of solid-solid phase transitions. We show results from simulations with different geometries and boundary conditions. In particular, we investigate the steady state growth in a narrow channel, and compare the results to analytical predictions for the region far behind the tip.