MM 32: Microstructure and Phase Transformations

Precipitates and Grain Growth

Time: Wednesday 10:15–11:15 Location: TC 010

MM 32.1 Wed 10:15 TC 010

Multi Scale Modelling of the Size Evolution of Precipitate Clusters — •Tobias Stegmüller and Ferdinand Haider — Universität Augsburg, Institut für Physik, 86135 Augsburg

Precipitation processes in modern aluminium alloys are due to their significance for mechanical properties of great technical interest. The choice of an appropriate heat treatment, which evolves the distribution of precipitates in space, is the key that influences material parameters like strength, hardness and corrosion resistance.

The size distribution of precipitates during heat treatments is an important function for the characterisation of the temper state. In this work we will present a multi scale approach covering DFT, Cluster Expansion Monte Carlo simulations and the so-called Cluster Dynamics which directly calculates the evolution of the precipitate size distribution. The model was applied to the formation of Guinier-Preston zones in Al-Cu alloys and the results will be presented.

MM 32.2 Wed 10:30 TC 010

Investigating the size advantage of potentially abnormal grains — •Dana Zöllner[1] and Paulo R. Rios[2] — [1]B CUBE Center for Molecular Bioengineering, TU Dresden, Arnoldstr. 18, 01307 Dresden, GERMANY — [2]Escola de Engenharia Industrial Metalurgica, Universidade Federal Fluminense, Av. dos Trabalhadores, 420 Volta Redonda, RJ, 27255-125, BRASIL

The well-investigated process of curvature driven grain growth progresses by the motion of grain boundaries to the center of their curvature. In polycrystalline grain boundary networks this leads over time to a decrease in the total interfacial area and therewith also to a decreasing interfacial free energy. As a result, the grain microstructure evolves such that it has a unimodal size distribution. In contrast, abnormal grain growth proceeds in such a way that certain grains show an exaggerated growth, which leads to changes in the average growth law as well as to a bimodal size distribution. In the present work, Monte Carlo computer simulations of grain growth are employed to determine how grains showing a very large size advantage behave within a matrix of finer grains that can grow without restrictions. We demonstrate that true abnormal grain growth does not develop from those large grains. In fact, the large grains tend to decrease their size advantage over time and may eventually be *captured* by the grain size distribution of the matrix. However, another phenomenon may happen: the persistence of the size advantage of these grains may lead to pseudo-abnormal grain growth.

MM 32.3 Wed 10:45 TC 010

Evolution of the Prismatic Ultrastructure in Molluscan Shells via Hierarchical Grain Boundary Motion — •Dana Zöllner and Igor Zlotnikov — B CUBE Center for Molecular Bioengineering, TU Dresden, Arnoldstr. 18, 01307 Dresden, GERMANY

Biomineralization of complex composite architectures comprising the shells of molluscs proceeds via self-assembly in accordance with thermodynamic boundary conditions set by an organic macromolecular framework that is regulated by the organism. Hence, the formation of these ultrastructures can be reproduced using the analytical backbone of various physical theories that are commonly employed to express the growth of manmade materials. In this work, we develop an analytical framework for a quantitative study of the process of shell morphogenesis. The method is based on Monte Carlo simulations of grain boundary motion that, classically, were developed to study coarsening of polycrystalline metals. By employing this approach, we fully reconstruct the growth process of the two-level hierarchical prismatic morphology found in the shell of the mollusc Pinctada nigra. Spatial data on the latter was obtained using synchrotron-based microtomography imaging at beamline (ID19) at ESRF. The proposed framework is a fundamentally novel approach to study the structural regulation during biomineralization. It has the capacity to evaluate physical parameters, set by the organism, that are responsible for mineralized tissue morphogenesis in time and in space. Besides providing key insights into the fields of biomineralization, these parameters are pivotal to the fields of biomimicry, bio-inspiration and bottom-up materials synthesis.

MM 32.4 Wed 11:00 TC 010

Abnormal coarsening of nanoscale microstructures goes fractal — •Christian Braun[1], Raphael Zeller[2], Carl Krill[2], and Rainer Birringer[1] — [1]Experimental Physics, Saarland University, Germany — [2]Institute of Micro and Nanomaterials, Ulm University, Germany

Despite the supposed rarity implicit in its name, abnormal grain growth (AGG) appears to be a rather common mode of coarsening in nanocrystalline materials, regardless of composition or synthesis route. In inert-gas-condensed nanocrystalline Pd90Au10, thermally induced coarsening fulfills the criteria for AGG, but with an unusual twist: here, the subpopulation of abnormally growing grains sends offshoots in many directions into the surrounding matrix. The resulting irregular growth fronts manifest a fractal-like morphology characterized by a box-counting fractal dimension of 1.2 instead of the smooth interfaces observed in conventional samples. To gain insight into the nonstandard mechanisms and driving forces initiating and accordingly acting during this mode of coarsening in nanocrystalline PdAu-alloys, it is required to answer amongst others the following questions: Are there further differences in the coarsened morphology compared to conventional samples prepared by melting and solidification? What about correlations between fractality and local characteristics in microstructure? Can the fractal dimension be influenced by a variation of gold concentration, heating rate and dwell time? In this talk we will present our recent results to narrow down potential mechanisms responsible for fractal grain boundary migration in nanocrystalline metals.