MM 11: Growth

Time: Monday 14:45–16:15 Location: IFW D

MM 11.1 Mon 14:45 IFW D

Tales of the abnormal: nanocrystalline grain growth at low temperatures — •Heiko Paul and Carl E. Krill III — Institute of Micro and Nanomaterials, Ulm University, Ulm, Germany

Unlike in coarse-grained polycrystalline materials, which manifest grain-boundary-controlled growth kinetics, nanocrystalline specimens are presumed to exhibit a coarsening behavior that is affected by their high number density of triple junctions and quadruple points. The consequences of such microstructural features on the nature of grain growth are potentially complex and still not well understood, but most current grain-growth models predict that the rate-controlling mechanism depends on the average grain size, with the dependence extending to larger sizes at lower annealing temperatures. Using a combination of x-ray diffractometry and electron microscopy, we have investigated the low-temperature evolution of microstructure in nanocrystalline Fe prepared by ball milling. The initial stage of grain growth agrees qualitatively with models positing a transition from triple-junction-controlled boundary migration to the standard grain-boundary-controlled case, but a quantitative examination of various moments of the grain-size distribution points to a different explanation: the samples appear to coarsen abnormally at first but to resume a normal growth mode at larger average grain sizes. The striking similarity of this behavior to the room-temperature growth observed in nanocrystalline Pd [1] suggests that abnormal grain growth may not be so “abnormal” after all!

[1] M. Ames *et al., Acta mater.* **56** (2008) 4255–4266.

MM 11.2 Mon 15:00 IFW D

Potts model simulation of triple junction limited grain growth — •Dana Zöllner and Peter Streitenberger — Institut für Experimentelle Physik, Abteilung Materialphysik, Otto-von-Guericke-Universität Magdeburg, Universitätsplatz 2, D-39106 Magdeburg

The size effect observed for nanocrystalline grain growth can be attributed to a limited grain boundary junction mobility yielding a junction drag.

Two different approaches are considered in the Monte Carlo Potts model: for one an effective mobility can be introduced, which is reduced by the triple junction distance and secondly each grain feature (grain boundary, triple line and quadruple points) can be assigned an own mobility. These changes in the mobility can be implemented in the Potts model through the transition probability, which calculates the attempted orientation change.

Some results of these modified Potts model simulations will be presented especially regarding the temporal development of the mean grain size and the grain size distribution. It will be shown that for the 2D case for initially very small grains a linear grain growth kinetics is observed followed by a transient state, which in later stages becomes parabolic. Furthermore, in the linear growth regime a coarsening state is reached, where the grain size distributions are shifted to smaller relative grain sizes. The coincidence of the scaled distributions implies the existence of a temporarily universal grain size distribution, which is in agreement with theoretical results based on a grain size dependent boundary mobility.

MM 11.3 Mon 15:15 IFW D

Phase-field simulations in peritectic system — •guillaume Boussinot, efim Brener, and dmitri Temkin — IFF-th.3, Forshungszentrum Juelich, Germany

We use a multi-phase-field model, to study peritectic systems in the case of isothermal processes (where the temperature T of the sample is a given). The latter provide the limit case of directional transformations (where the sample is pulled in a temperature gradient) when the temperature gradient vanishes. When T<Tp, we have a (delta+L-> delta+gamma+L) transformation, where delta is called primary solid phase and gamma is the peritectic solid phase (and L is the liquid). When T>Tp, we obtain a (gamma+L -> delta+L) transformation occuring via a liquid film migration process.

MM 11.4 Mon 15:30 IFW D

Pattern formation during Diffusion limited Transformations in Solids — •Michael Fleck[1], Claas Hüter[1], Denis Pilipenko[1], Robert Spatschek[1,2], and Efim Brener[1] — [1]Institut für Festkörperforschung, Forschungszentrum 52425 Jülich — [2]Interdisciplinary Centre for Advanced Materials Simulation (ICAMS), Ruhr-Universität Bochum

Key feature of many metallurgical procedures to improve materials properties is the formation of very complex microstructures due to solid-solid phase transformation processes.

We develop a description of diffusion limited growth in solid-solid transformations, which are strongly influenced by elastic effects. Density differences and structural transformations provoke stresses at interfaces, which affect the phase equilibrium conditions. We formulate equations for the interface kinetics similar to dendritic growth and study the growth of a stable phase from a metastable solid in both a channel geometry and in free space. We perform sharp interface calculations based on Green’s function methods and phase field simulations, supplemented by analytical investigations.

For pure dilatational transformations we find a single growing finger with symmetry breaking at higher driving forces, whereas for shear transformations the emergence of twin structures can be favorable. We predict the steady state shapes and propagation velocities, which can be higher than in conventional dendritic growth.

MM 11.5 Mon 15:45 IFW D

Crack growth by surface diffusion in viscoelastic media — Robert Spatschek, Efim Brener, and •Denis Pilipenko — Institut für Festkörperforschung, Forschungszentrum Jülich , D-52428 Jülich

Dissipation plays a central role in fracture, since typically only a small fraction on the elastic energy is used to create the surfaces of the advancing crack. Whereas in brittle materials dissipation takes place mainly close to the crack surfaces, in materials with a more viscous behavior an extended zone of bulk dissipation can form around the crack.

We discuss steady state crack growth in the spirit of a free boundary problem. It turns out that mode I and mode III situations are very different from each other: In particular, mode III exhibits a pronounced transition towards unstable crack growth at higher driving forces, and the behavior close to the Griffith point is determined entirely through crack surface dissipation, whereas in mode I the fracture energy is renormalized due to a remaining finite viscous dissipation. Intermediate mixed-mode scenarios allow steady state crack growth with higher velocities than for pure mode I.

MM 11.6 Mon 16:00 IFW D

Theory of dendritic growth in the presence of lattice strain — Efim A. Brener, •Claas Hüter, and Denis Pilipenko — Institut für Festkörperforschung, Forschungszentrum 52425 Jülich

The need to understand the dominating phenomena during solid-solid transitions as they occur in various processes of industrial relevance is apparent.

Elastic effects as they occur due to lattice strain modify the local equilibrium condition at the solid-solid interface compared to classical dendritic growth. Both, the thermal and the elastic fields are eliminated by Green’s function techniques and a closed nonlinear integro-differential equation for the interface is derived. In the case of pure dilatation, the elastic effects lead only to a trivial shift of the transition temperature while in the case of the discussed shear transitions and superposition of these basic lattice strains, dendritic patterns are found even for isotropic surface energy. Of course, the discussed elastic effects also introduce an ”effective anisotropy“ of the system. However, the physics and structure of selection theory for the two mechanisms, anisotropy of surface energy and elastic effects, are fundamentally different. Elastic effects lead to a much more robust selection mechanism compared to tiny effects of anisotropy of surface energy. Moreover, the growth velocities for the same effective driving force can reach appreciably larger values than in the case of selection via anisotropy of surface energy.