

Summary

In the early 2000's Elder et al. have managed to formulate the phase-field crystal (PFC) model, which is a one-mode approximation to the well-established classical density functional theory (CDFT), for the study of the solid-liquid phase transition. While CDFT is considered to be accurate, it also suffers from a large computational cost when time-dependent numerical solutions are required. In addition to being computationally less demanding than CDFT, the PFC model has many benefits over the more coarse-grained phase-field models, as it incorporates the crystal symmetries of the solid phase. This leads to the natural coupling of elastic effects to thermodynamics, without the use of ad hoc auxiliary fields.

Within the PFC framework, I analyse the structural signatures of solid clusters, that develop in quenched liquids, prior to the appearance of BCC crystals. For local structure identification, I use the first neighbor averaged bond orientational order parameters of Lechner and Dellago. I analyse the medium range crystalline order (MRCO) recognized by Tan et al., in terms of these bond order parameters. For a more coarse-grained analysis, I compare the radial distribution functions (RDFs) of the amorphous clusters to molecular dynamics (MD) simulations of BCC metal nanoparticles, conducted by Hoang and Shibuta et al. In summary, dynamical mean field theories, such as the PFC model are not limited by the assumptions of CNT and predict the non-direct appearance of the thermodynamically most stable solid phase at large undercoolings via an amorphous solid structure.

The interaction of nucleation and the growth front plays the determining role in the structure of polycrystalline growth forms, such as disordered dendrites and spherulites. The mechanism behind the creation of these complex polycrystalline growth forms, has been identified as growth front nucleation (GFN). It describes the formation of grains of new orientation at the propagating solid-liquid interface, the growth front. While this approach, relying on a coarse-grained orientation field proved to be quite successful in capturing rather complex solidification patterns, the microscopic kinetics of the GFN phenomenon remained largely hidden in such coarse-grained models. Due to the fact, that in the HPFC model I observe a change in growth forms with changing undercooling, it seems promising to study the microscopic origins of GFN in the HPFC model. I find mechanisms, which are not present in the DPFC model and manage to gain insight, under what conditions a single crystal develops into a polycrystalline growth form.

I also make progress in the understanding of defect formation during strained epitaxial growth. I study the growth process under various circumstances in the two-dimensional DPFC model, in the section perpendicular to the substrate-epilayer interface. I show, that the critical thickness (h_c) increases with decreasing strain. This is in qualitative agreement with experiments, static energy-balance based approaches, such as the van der Merwe (VDM), the Matthews-Blakeslee (MB) and People-Bean (PB) models. However, I find large discrepancies when the simulation data from the h_c vs. strain relationship is analyzed in terms of the theoretical results from the VDM, MB and PB models. For the resolution of this issue, I investigate the reasons behind defect formation from the kinetic perspective, based on the Asaro-Tiller-Grinfeld (ATG) instability. I finally conclude, that the dynamic theory of the ATG instability is a more appropriate approach to the study of the formation of misfit dislocations during growth, than the previous, energy-balance based static approaches.