Phase field modeling of polycrystalline solidification in two and three dimensions

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Recent results on the application of the phase field theory for crystal nucleation and polycrystalline growth will be reviewed. In two dimensions a single orientation field is applied to describe the crystallographic orientation of the crystallites [1], while in three dimensions quaternion fields are used [2]. Our model incorporates various nucleation modes including heterogeneous and homogeneous mechanisms for primary nucleation of growth centers and secondary nucleation of new grains at the growth front. We address the formation of various complex polycrystalline morphologies such as polydendritic structures, “dizzy” (or disordered) dendrites, crystal sheaves, and other spherulitic forms [3-5]. A transition between “symmetric” single crystal dendrites and isotropic “seaweed” structures is observed when increasing the number of foreign particles that perturb crystal growth. A similar morphological transition is seen if one reduces the orientational mobility, which leads to the formation of orientational defects at the growth front that induce new grains at the perimeter. It will be demonstrated that a broad variety of polycrystalline structures can be recovered by changing only a few model parameters such as crystal anisotropy, branching angle, and orientational mobility.

This is a joint work with T. Pusztai, G. Bortel, and G. Tegze.

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