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Growth and form of spherulites: A phase field study.

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Polycrystalline patterns termed spherulites are present in a broad variety of systems including metal alloys, polymers, minerals, and have biological relevance as well (see e.g. semi-crystalline amyloid spherulites and spherultic kidney stones). The fact that similar polycrystalline patterns are observed in systems of very different nature suggests that a minimal model based on coarse-grained fields, which neglects the details of molecular interactions, might be appropriate. Although such a field-theoretic approach disregards most of the molecular scale details of formation, some features such as crystal symmetries can be incorporated via the anisotropies of the model parameters. The rationale for developing such coarse-grained models is the current inability of fully molecular models to address the formation of large scale morphologies. A phase field theory of polycrystalline growth, we developed recently, is applied for describing spherulitic solidification in two and three dimensions. Our model consists of several mechanisms for nucleating new grains at the perimeter of the crystallites, including homogeneous (trapping of orientational disorder and branching in certain crystallographic directions) and heterogeneous (particle-induced nucleation) processes. It will be shown that the diversity of spherulitic growth morphologies arises from a competition between the ordering effect of discrete local crystallographic symmetries and the randomization of the local crystallographic orientation that accompanies crystal grain nucleation at the growth front. This randomization in the crystal orientation accounts for the isotropy of spherulitic growth at large length-scales and long times. We find the entire range of observed spherulite morphologies can be reproduced by this generalized phase field model of polycrystalline growth.