Diffusion-Limited Cluster Growth During Nucleation

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Abstract

Nucleation of clusters of a stable phase from a metastable phase is the initial stage of numerous phase transformations. Nucleation is often modeled by classical nucleation theory (CNT), but CNT is only applicable when growth of nucleating clusters is collision (or interface) limited. Therefore, CNT has recently been adapted by Slezov for growth limited by long-range diffusion [Slezov, V. V., Kinetics of First Order Phase Transitions, Wiley, 2009]. Slezov's model describes, e.g., precipitation of oxygen in silicon, and, more generally, crystallization in alloys. However, Slezov's model is applicable only in 3D due to its reliance on quasistatic growth, which does not occur in lower dimensions. Generalizing the model requires relaxing the quasistatic assumption, but this is difficult because the growth rate has no general analytic solution. Specific solutions are available only for fixed density of the source phase at the cluster surface. However, this situation does not arise in real systems. Instead, the surface density varies with the cluster's size through capillarity. In this case, growth rates can only be computed numerically. Nevertheless, if growth rates of clusters with fixed surface density are close to those of real clusters, solutions for the former may be used as simple approximations of the latter. We therefore numerically obtain real growth rates in COMSOL Multiphysics® simulation software for comparison with predictions by the models with simplifying assumptions. The study's results will not only help extend Slezov's model to 2D but also increase the model's accuracy for systems without quasistatic growth.

Figures used in the abstract

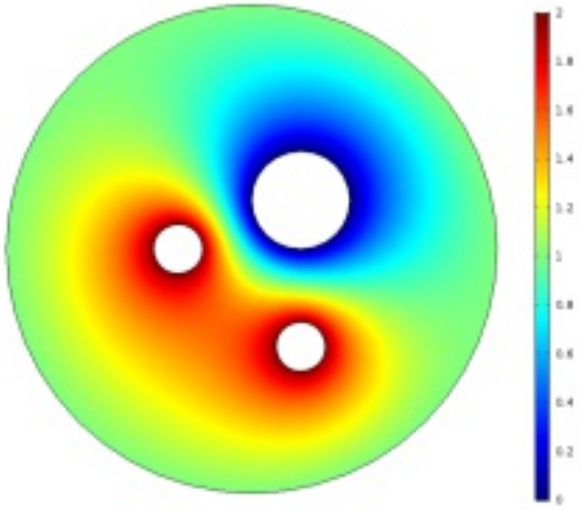

Figure 1: Spherical clusters (white) formed from solution (colored) during nucleation. Colors indicate solute density. The density at the cluster surfaces depends on cluster size due to capillarity, causing density variations through the origin phase. These variations in turn affect cluster growth rates, and thus rates of nucleation of the new phase. By computing the growth rates numerically, we can assess the validity of using simplifying approximations in modeling nucleation.