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Simultaneous Prediction of Morphologies of a Critical Nucleus and an Equilibrium Precipitate in Solids

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Abstract. We investigate the critical nucleus and equilibrium morphologies during precipitation of a second-phase particle in a solid. We show that a combination of diffuse-interface description and a constrained string method is able to predict both the critical nucleus and equilibrium precipitate morphologies simultaneously without *a priori* assumptions. Using the cubic to cubic transformation as an example, it is demonstrated that the maximum composition within a critical nucleus can be either higher or lower than that of equilibrium precipitate while the morphology of an equilibrium precipitate may exhibit lower symmetry than the critical nucleus resulted from elastic interactions.

AMS subject classifications: 74G15, 74B20

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1 Introduction

Precipitation is a common, natural process which takes place in a supersaturated solid or liquid solution, e.g., during isothermal annealing of a quenched homogeneous alloy within a two-phase field of a phase diagram. It is the basic process that underlies the development of many advanced materials such as high-temperature superalloys and ultralight aluminum and magnesium alloys. The precipitate microstructure (the number density, volume fraction, and morphology) is the dominant factor that determines

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the mechanical properties of a solid. One of the main challenges in predicting precipitate microstructures in solids has been the determination of precipitate particle morphology because of the presence of both interfacial energy anisotropy and anisotropic elastic interactions. As the majority of precipitation reactions in solids take place through a nucleation-and-growth mechanism followed by particle coarsening, there are two thermodynamically well-defined morphologies: the morphology of a critical nucleus and the equilibrium morphology of a precipitate particle.

In classical nucleation models, a critical nucleus is usually assumed to be spherical and critical radius is determined by a competition between a bulk free energy decrease which is proportional to volume and an interfacial energy increase which is proportional to interfacial area. In a diffuse-interface description, a critical nucleus is defined as the composition or order parameter fluctuation having the minimum free energy increase among all fluctuations which lead to nucleation, i.e., the saddle point configuration along the minimum energy path (MEP) between the metastable initial phase represented by a local minimum in the free energy landscape and the equilibrium phase represented by the global minimum. Therefore, nucleation of new precipitate particles requires overcoming a thermodynamic barrier. The magnitude of the nucleation barrier, and thus the nucleation rate, or the resulted precipitate particle density, is strongly dependent on the morphology of critical nuclei. On the other hand, following nucleation and growth, the morphology and volume fraction of precipitate particles during coarsening are generally close to equilibrium. The particle morphology and volume fraction during coarsening together with the particle density predicted from nucleation provide all the information that is needed for predicting the strength of a solid in mechanistic models.

There have been extensive studies, particularly numerical simulations, of equilibrium shapes of a precipitate particle in solids using both sharp- and diffuse-interface approaches [5, 7, 8, 11–13]. Attempts have also been made to predict the morphology of a critical nucleus in solids by taking into account both interfacial energy anisotropy and anisotropic elastic interactions [9, 10, 14–16]. For example, we showed that one can predict the morphology of a critical nucleus in a system going through a phase transition [14–16] using a combination of the diffuse-interface (phase-field) description and the minimax algorithm based on the mountain pass theorem. The main objective of this letter is to report a first attempt to predict the morphology of a critical nucleus as well as the equilibrium morphology of a precipitate simultaneously within the same physical model and mathematical formulation. A concentration field that conserves the average concentration is considered as an illustration. We extend the string method [3, 4] to systems with constraints through a novel augmented Lagrange multiplier formulation. This leads to an effective constrained string method which may be useful in the study of many constrained barrier crossing problems in physics, chemistry and biology. In this work, we demonstrate that a combination of diffuse-interface description and the constrained string method can simultaneously predict the morphologies of a critical nucleus and an equilibrium precipitate which can be dramatically different.