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An Efficient Rescaling Algorithm for Simulating the Evolution of Multiple Elastically Stressed Precipitates

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Abstract. In this paper, we propose a space-time rescaling scheme for computing the long time evolution of multiple precipitates in an elastically stressed medium. The algorithm is second order accurate in time, spectrally accurate in space and enables one to simulate the evolution of precipitates in a fraction of the time normally used by fixed-frame algorithms. In particular, we extend the algorithm recently developed for single particle by Li et al. (Li, Lowengrub and Leo, J. Comput. Phys., 335 (2007), 554) to the multiple particle case, which involves key differences in the method. Our results show that without elasticity there are successive tip splitting phenomena accompanied by the formation of narrow channels between the precipitates. In presence of applied elastic field, the precipitates form dendrite-like structures with the primary arms aligned in the principal directions of the elastic field. We demonstrate that when the far-field flux decreases with the effective radius of the system, tip-splitting and dendrite formation can be suppressed, as in the one particle case. Depending on the initial position of the precipitates, we further observe that some precipitates grow while others may shrink, even when a positive far field flux is applied.

AMS subject classifications: 74N25, 74B15
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1 Introduction

The growth of precipitates in an elastic matrix is an important problem in the metal industry. One example is the production of alloys (e.g. [Al-Ni]) by solid/solid phase

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transformations, in which the metal mixture is suddenly driven out of its initial equilibrium state by lowering the temperature. As a consequence, precipitates nucleate within the bulk material and forms a new dispersed (precipitate) phase with different material properties. The precipitates undergo diffusional growth until a new thermodynamic equilibrium state between the precipitates and matrix is reached.

Since the features of the microscopic precipitates determine the macroscopic properties of the material (e.g., stiffness, strength and toughness), there have been many computational investigations of phase transformations in metallic alloys (e.g., [1,2,6,15,17,18, 21,27,30,33,38,39,41–43,46,48]). Under appropriate assumptions, the diffusional growth system can be posed as a moving boundary problem. From an analytical perspective, Mullins and Sekerka proposed a linear stability theory to address the evolution of a single, slightly perturbed spherical precipitate [32], which was later generalized to consider elastic stresses [15, 20, 22]. As perturbations grow, nonlinearity becomes important and the precipitate develops complex dendritic, or ramified, morphologies. Computer simulations have then been used to study this nonlinear phenomenon.

Boundary integral methods are one of the most accurate numerical techniques for simulating free boundary problems. Such methods can be made very efficient through the use of fast solvers, such as the fast multipole method (e.g., [8, 13, 19, 49]) or tree algorithms (e.g., [10,28,35,47]) among others and the fact that the dimension of the problem is reduced by one. Other methods for simulating microstructure dynamics include level-set and phase-field methods, which have their own advantages and disadvantages. See for example the reviews [5, 16, 18, 23, 34, 37, 43].

Following S. Mikhlin's approach [31], Greenbaum et al. developed an efficient boundary integral method for solving the quasi-steady diffusion problem in a multiply connected domain and evaluated the Dirichlet Neumann mapping [11]. This approach was later used in [4, 14] and [15, 21] to perform simulations of precipitate dynamics with and without elastic stresses in two dimensions, respectively. Other boundary integral methods have also been used to study two dimensional precipitate evolution, see e.g., [1, 38–42, 44, 45] among others. Three dimensional boundary integral simulations of precipitate dynamics can be found in [9, 27].

There are numerous difficulties associated with simulating the long-time evolution of single and multiple precipitates. First, the morphologies tend to be complex. Second, the precipitates grow in size, which together with the complex morphologies, increases the range of scales that need to be resolved. Third, although the precipitates are growing, their rate of growth slows as time increases. This makes long-time simulations of precipitate growth expensive. We address these issues by extending a space-time rescaling scheme, originally developed for single particles [3, 26] to the multiple particle case. The extension involves key differences in the algorithm. The idea is to rescale time and space such that the precipitate evolves exponentially fast in the rescaled frame and does not change size in the rescaled frame. We demonstrate that the algorithm, which is second order accurate in time and spectrally accurate in space, is able to simulate the evolution of precipitates in a fraction of the time normally used by fixed-frame algorithms.