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A more accurate three-dimensional grain growth algorithm

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Abstract

In a previous paper, the authors described a simulation method for the evolution of two-dimensional cellular structures by curvature flow that satisfied the von Neumann–Mullins relation with high accuracy. In the current paper, we extend this method to three-dimensional systems. This is a substantial improvement over prior simulations for two reasons. First, this method satisfies the MacPherson–Srolovitz relation with high accuracy, a constraint that has not previously been explicitly implemented. Second, our front-tracking method allows us to investigate topological properties of the systems more naturally than other methods, including Potts models, phase-field methods, cellular automata, and even other front-tracking methods. We demonstrate this method to be feasible in simulating large systems with as many as 100,000 grains, large enough to collect significant statistics well after the systems have reached steady state.

Keywords: Modelling; Grain growth; Three dimensions; Front-tracking method

1. Introduction

Current knowledge of grain growth in polycrystalline materials relies on a combination of experimental observations of grain growth microstructures, developments in kinetic theory, and more recently, simulations of microstructural evolution. This understanding is limited by the difficulty of experimentally accessing the details of a three-dimensional microstructure, by the anisotropy of properties that govern grain boundary motion (e.g. grain boundary energy and mobility), and by impurities and inhomogeneities in real materials (i.e. the presence of a solute species or crystalline defects). Hence, despite recent advances in three-dimensional microscopy [1,2], in characterizing the anisotropy of grain boundary energies and mobilities [3,4], and in analyzing the effects of impurities [5,6], the importance of theory and simulations developed for simplified and idealized microstructures cannot be overstated. Indeed, a model that assumes material isotropy, a grain boundary motion governed only by interfacial thermodynamics (the Gibbs–Thomson relation), and the absence of impurities provides fertile ground for investigating basic features of the complicated process of grain growth. As an example, these idealizations have permitted an exact solution for the rate of growth of any given grain within a microstructure. This was done first in two dimensions by von Neumann [7] and Mullins [8], and more recently in three and higher dimensions by MacPherson and Srolovitz [9].

Nonetheless, even with this idealized model and the accompanying exact solutions, our understanding of the properties of the evolving microstructure remains rudimentary. Difficulties with developing a theory of the broader microstructure arise principally in understanding the interactions between grains and from the many degrees of freedom of a grain boundary network in three dimensions. As an alternative, simulations have provided important insights into the mechanisms and energetics of grain growth [10,11], but contemporary simulation methods do not rigorously adhere to the same assumptions of isotropy

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and curvature-driven grain boundary motion that have proven instrumental in developing the theory for individual grains. In this paper, we present a new method for simulating grain growth in an idealized microstructure that is consistent with these assumptions. This new method for three-dimensional grain growth obeys the exact relation for the rate of growth of every grain, is more accurate and more efficient than prior simulations, and is capable of investigating microstructural properties previously overlooked. An example of a simulated three-dimensional microstructure is illustrated in Fig. 1.

One of the most frequently used simulation methods is a Monte Carlo Potts model [12–14], which represents grains as ensembles of lattice points sharing the same label. Evolution of the structure is performed by allowing the label of a lattice point to change probabilistically based on an energy that is a function of the labels of neighboring points. The implementation of this method is relatively straightforward, without the need to explicitly distinguish between the interior of grains and the grain boundaries or explicitly implement topological changes in the grain boundary network. While this approach has been used to simulate polycrystalline systems with more than 2,000,000 grains [15], certain questions remain. The discretization of the structure into volume elements limits the resolution of the simulation and often introduces spurious anisotropy (e.g. facet formation on surfaces commensurate with the lattice) [12,16]. Furthermore, the resulting microstructures do not rigorously maintain the angles along grain boundary junctions as demanded by thermodynamics. Finally, the discretization inherent to this method introduces to the microstructure a length scale associated with the underlying numerical lattice (unrelated to the atomic lattice length scale), and makes measuring topological and geometrical quantities difficult [17].

A closely related approach is the cellular automata model [18,19]. This model inherits the simplicity of the Potts model's discrete lattice structure and labeling system, but allows a wider range of energetic conditions to be introduced into the switching probabilities of the labels. Recent work has been able to simulate systems with roughly 30,000 grains [20]. Cellular automata models have many of the same limitations as the Potts model though, including the possibility of faceting and lattice pinning due to the lattice-based discretization of the microstructure.

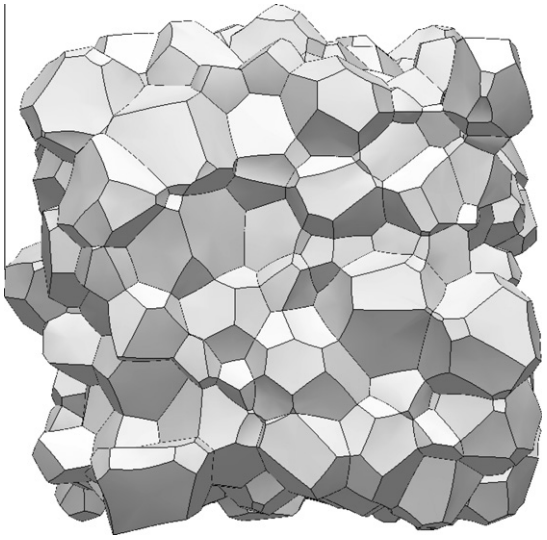

Fig. 1. A system of 250 grains.

Another approach developed for three-dimensional systems is the phase-field method [21,22], where a smoothly varying order parameter is defined for every grain orientation. A given grain occupies the region where the corresponding order parameter is 1 and all other order parameters vanish. The energy of the system depends on the values and gradients of all the order parameters, and the system is evolved using a non-conserved Ginzburg–Landau equation [23]. While this procedure allows for the incorporation of sophisticated energetics, a large number of coupled nonlinear differential equations must be numerically solved at every time step [24]. Furthermore, this method requires a finite grain boundary width (rather than the sharp boundaries for the Potts and cellular automata models), implying that the thermodynamic constraint on the angles at which grain boundaries meet is relaxed. This finite width is a result of the requirement that gradients of the order parameters be small, and the consequent requirement for a very fine discretization of the microstructure [25]. The resulting demands for computational resources currently limit phase-field methods to systems containing 30,000 grains [26].

The final primary approach to simulate three-dimensional grain growth are various front-tracking methods in which two-dimensional grain boundaries are explicitly represented. Most front-tracking simulations are either "vertex models", which follow the motion of only the quadruple points (where four boundaries meet) [27], or are only slightly more refined, and allow for nonplanarity of the faces by introducing a further node in the center of a face [28–30]. These methods provide only coarse discretizations of the grain boundary network and cannot adequately capture the curvature of the interfaces. A more severe limitation of these models is their inability to represent two-edged faces and three-faced grains, entities that certainly arise in physical systems [31,32].

Apart from vertex models, several other implementations of front-tracking methods exist. A recent simulation [33] uses Brakke's Surface Evolver [34] to construct and evolve grain boundaries with a finer discretization that is more able to reflect the boundary curvature, an essential feature of grain growth. While Surface Evolver is able to handle many of the topological transitions that arise in the grain boundary network, it is currently unable to describe others that routinely occur during normal grain growth. When such transitions occur, the microstructure must be manually readjusted to account for the change. A separate front-tracking approach [35] uses finite-element methods to provide an elegant, accurate discretization of