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Level-set simulation of anisotropic phase transformations via faceted growth

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ABSTRACT

Level-set method is used to simulate phase transformations with anisotropic kinetics where the transforming interface is faceted. The method overcomes previous limitation of this simulation methodology in tracking dynamic evolution of a large number of growing grains. The method is then used to simulate multi-grain phase transformations where the facets are three low-index ([1 0 0], [1 1 1], [1 1 0]) planes that yield morphologies including cube, octahedron and rhombic dodecahedron. The microstructure evolves under site-saturated nucleation and constant nucleation rate. The cube morphology undergoes fastest transformation followed by octahedron, rhombic dodecahedron and sphere. It is also shown that the Johnson-Mehl-Avrami-Kolmorgorov theory can be used to describe the kinetics of the faceted phase transformation. The resulting microstructure shows non-convex grain shapes with highly corrugated surfaces. The structures are also characterized using the average grain length along certain low index crystallographic directions, the coherent length. This measurement shows that for a cubic morphology, there is a significant difference in the coherent length for low index directions, while there is no meaningful difference in the coherent length for kinetic Wulff shapes of other anisotropies examined.

1. Introduction

Despite a long history of research on phase transformations in materials, this subject is still of interest due to its strong connection in setting the structure and hence the properties of many advanced materials. For example, novel applications for amorphous materials require them to be thermally stable against the crystallization process [1–3]. By contrast, phase change memory technology relies on fast and explicit phase switching, initiated by heat or other excitation mechanisms [4–6]. These two examples, among many other applications, underline the need to model the kinetics of microstructural evolution. Many of these phase transformations take place via the propagation of an anisotropic interface, which makes them difficult to model analytically. There are few simulation methodologies that can model anisotropic phase transformations and among them the Level-Set Method (LSM) has the ability to simulate such anisotropic transformations in experimental time and length scales [7]. Here, we present a new approach to the level-set method that simulate faceted growth of many grains or growing domains, in order to study kinetics and microstructure of anisotropic phase transformations.

The level-set method has been used in materials science to simulate phenomena such as wet etching [8], thin film growth [9,10], grain boundary evolution [11], dendritic growth [12] and other phase transformations [7,13–15]. The ability of LSM to simulate real world experiment at experimental time and length scales makes it a suitable method for investigating kinetics of new phase evolution and comparing the results with experimental measurements. However, previous LSM studies only considered the kinetics of phase transformation under isotopic growth [7,13–15]. In the isotropic case, all grains grow as sphere with the same rate and no specific orientation. Thus, all grains basically evolve by a single level-set function with straightforward numerical solution. This is unfortunate, since many transformations occur by the motion of faceted interfaces, such as ferroelectric domain switching and relaxation [16,17], crystallization from amorphous state [18–20] and cellular precipitation [21]. The simulation of anisotropic growth via LSM requires that each evolving grain has a unique level-set function in order to follow the evolution of a grain morphology and orientation. This leads to multiple level-set functions, with the attendant numerical challenges.

In this paper, we present a computationally efficient method that can be used to simulate the growth of multiple grains in the limit where the interfacial velocity is anisotropic and constant for each facet. The simulation results of multi-grain faceted phase

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transformations in three dimensions are also provided along with proper analysis.

2. Methodology

In the simulation of a moving interface via the level-set method a continuous signed distance function $\varnothing(\boldsymbol{x}, t) = 0$ gives the location of the interface (zero level-set). The level-set function then evolves through the equation of motion as shown in Eq. (1), where, $\boldsymbol{V}$ is the interface velocity. This equation can be numerically solved via forward Euler time discretization in 3D Cartesian coordination [22,23].

$$\frac{\partial \varnothing}{\partial t} + \boldsymbol{V} \cdot \nabla \varnothing = 0 \tag{1}$$

In the case that the interface velocity ($\boldsymbol{V}$) is isotropic, the growth proceeds in all directions with constant rate. However, interface velocity is more often defined as a function of various parameters including interface curvature, orientation, concentration and temperature. In this work, we consider a phase transformation via a fully faceted interface growth process. Thus, the interface velocity only depends on orientation, $\boldsymbol{V} = M(\boldsymbol{n})\boldsymbol{n}$, where $M(\boldsymbol{n})$ is the mobility function and $\boldsymbol{n}$ is the interface normal [24,25]. Since $\boldsymbol{n} = \nabla\varnothing/|\nabla\varnothing|$, Eq. (1) becomes

$$\frac{\partial \varnothing}{\partial t} + M(\boldsymbol{n})|\nabla \varnothing| = 0 \tag{2}$$

To determine $M(\boldsymbol{n})$, we employ Russo-Smereka's approach for faceted growth, which has been proven to deliver correct kinetic Wulff shape for given morphology [26]. In this approach to acquire the desire crystal morphology with specific set of facet normals ($\boldsymbol{n_F}$), interface mobility $M(\boldsymbol{n})$ defines as:

$$M(\boldsymbol{n}) = v_i + u_{i,j}\sqrt{1 - (\boldsymbol{n} \cdot \boldsymbol{n_{F_i}})^2} \tag{3}$$

Here, v is the magnitude of normal velocity and u is the magnitude of the tangential velocity of the interface. Eq. (3) defines mobility for every point of the interface in a way that yields faceted growth with a given set of crystallographic planes. For instance, in a cubic kinetic Wulff shape the evolution is due to the motion of a set of six facets with normals ($\boldsymbol{n_{F_1}}$ to $\boldsymbol{n_{F_6}}$) that are defined along the $\langle 1\,0\,0\rangle$ directions with a specific normal velocity (v). After formation of the fully faceted morphology, every facet grows with its normal velocity (first term in Eq. (3)). However, tangential term still becomes active at the corner in order to impose sharp edge formation and ensures fully faceted evolution of the grain. The tangential velocity between facet i and its adjacent (j) is given by,

$$u_{i,j} = \frac{v_j - v_i Cos\,\theta}{Sin\,\theta} \tag{4}$$

where θ is the internal angle between facet i and j. This approach with standard re-initialization method for level-set simulation [22,23] can generate a fully faceted morphology, evolving over the time with sharp edges. Fig. 1 depicts temporal evolution of a Cube Octahedron, with 8 triangular {1 1 1} facets and 6 square {1 0 0} facets.

While this approach delivers correct kinetic Wulff shape for single grain evolution, extending it to multiple grains evolution leads to the challenge of designating each grain within the level-set formulation, especially when large number of grains are involved. Usually the approach is to grow each grain by its own level-set function, which means multiple level-set functions have to be solved simultaneously in computational domain. When large number of grains needs to be considered, solving all these functions becomes very expensive both in terms of computational time and memory. Although implementing narrow bond algorithm and allocating memory dynamically [10] can enhance the performance, but still simulating large number of grains associated with real microstructure requires relatively large computational power [26,27].

For particular case of anisotropic interface kinetics-limited faceted growth, we introduced an alternative method, which not only results in significant improvement in computational power and time, but also has no practical limitation on the number of grains. In this method, the entire temporal and spatial information of a single grain interface evolution via the level-set method is recorded at every time step in order to build a master grain morphology database. Since the level-set method simulation is being done for only one grain, it is not computationally intensive. Therefore, highest precision can be achieved by re-initializing the level-set function into the signed distance function in every time step over the course of simulation. Using this database, it is possible to model a multiple grain phase transformation by calling the database for each grain, according to the nucleation mechanisms and the interface growth rate. The orientation of the growing nuclei are set by Euler angles, as shown in Fig. 2. Since the transformation is limited by interfacial kinetics, there is no long-range diffusional interactions between grains, thus the growth process of a single grain can be used for every grain in the system, appropriately transformed for its size and orientation.

Like the actual transformation, the simulation begins from nucleation. Nucleation mechanisms are commonly categorized as Site-Saturated Nucleation (SSN), which requires one time simultaneous nucleation at the beginning of the transformation and Constant Nucleation Rate (CNR), which follows continuous nucleation with constant rate over the entire transformation. For the sake of simplicity, site-saturated nucleation is considered for step-by-step description of the simulation procedure, which implies that nucleation occurs at the beginning of the transformation. Nucleation can take place either homogenously or heterogeneously. The first one requires a random spatial distributed for the grains, while the later demands preferential location such as surfaces, grain boundaries or inclusions. Once the location of each nucleus is set, the orientation for each growing grain is assigned according to Euler angles, which are associating with rotation around x, y and z axes by α, β and δ degrees, respectively (Fig. 2).

The orientation assignment also can be done randomly or based on desired texture. As shown in Fig. 3, next step is to apply rotation transformation on the interface data (called from repository). This task must be carried out for all nuclei based on their own α, β and δ values. Eq. (5), illustrates rotational transformation matrixes in 3D spaces for given Euler angles.

$$\mathcal{R}(\alpha) = \begin{bmatrix} 1 & 0 & 0 \\ 0 & \cos\alpha & -\sin\alpha \\ 0 & \sin\alpha & \cos\alpha \end{bmatrix}$$

$$\mathcal{R}(\beta) = \begin{bmatrix} \cos\beta & 0 & \sin\beta \\ 0 & 1 & 0 \\ -\sin\beta & 0 & \cos\beta \end{bmatrix} \tag{5}$$

$$\mathcal{R}(\delta) = \begin{bmatrix} \cos\delta & -\sin\delta & 0 \\ \sin\delta & \cos\delta & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

The interface location is then used to determine the next configuration of evolved phases, considering the local rotated coordinates of a grain. This yields the configuration of the multi-grain system at the next time step.

Each grain grows until it meets another grain and forms a grain boundary (Fig. 4a). When the two interfaces are within one mesh