Simulations of anisotropic grain growth: Efficient algorithms and misorientation distributions

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Abstract

An accurate and efficient algorithm, closely related to the level set method, is presented for the simulation of Mullins's model of grain growth with arbitrarily prescribed surface energies. The implicit representation of interfaces allows for seamless transitions through topological changes. Well-resolved large-scale simulations are presented, beginning with over 650,000 grains in two dimensions and 64,000 grains in three dimensions. The evolution of the misorientation distribution function (MDF) is computed, starting from random and fiber crystallographic textures with Read–Shockley surface energies. Prior work had established that with random texture the MDF shows little change as the grain network coarsened whereas with fiber texture the MDF concentrates near zero misorientation. The lack of concentration about zero of the MDF in the random texture case has not been satisfactorily explained previously since this concentration would decrease the energy of the system. In this study, very-large-scale simulations confirm these previous studies. However, computations with a larger cut-off for the Read–Shockley energies and an affine surface energy show a greater tendency for the MDF to concentrate near small misorientations. This suggests that the reason the previous studies had observed little change in the MDF is kinetic in nature. In addition, patterns of similarly oriented grains are observed to form as the MDF concentrates.

Keywords: Grain growth; Computer simulations; Texture evolution; Unequal surface energies

1. Introduction

Macroscopic properties of a polycrystalline material depend on its crystallographic texture and grain boundary character. These properties can evolve under thermomechanical processing, such as heat treatment or deformation. Ignoring recrystallization, the evolution of the texture and the grain boundary character is largely determined by properties of the initial grain boundary network. The motion of this network of surfaces is often modeled as steepest descent for a weighted surface energy, where low-angle grain boundaries (formed between adjacent grains with similar orientations and said to have low misorientation) receive lower weights than high angle ones. A specific functional dependence due to Read and Shockley [22] with a standard extension for high-angle grain boundaries (see e.g. [12]) is commonly used to assign the weight to a grain boundary in terms of the orientations of the two adjacent grains.

In the anisotropic case there are two aspects to this energy minimization process. First is grain growth: as some grains grow, others must shrink, and so the total length of the grain boundaries must decrease. In fact, in the isotropic case, this is the only mode of energy reduction. However, in the anisotropic case, the energy will decrease if the grain boundary energy is reduced. This can happen when two grains with similar orientations happen to meet. Therefore, it might be expected that the distribution of misorientations in the system will also change as the grain network coarsens.

For this reason, a useful statistical descriptor of the grain boundary character is the misorientation distribution function (MDF), which measures the relative area of
interfaces in the network with a given misorientation. It is useful to note that, if the grain boundary energy is isotropic, then, as the grain network evolves, the MDF is expected to remain stationary. On the other hand, if the grain boundary energy is an increasing function of misorientation (as it is often modeled), then one would expect that, as the grain network evolves, low-misorientation grain boundaries would predominate and as a consequence the MDF would concentrate near small misorientations.

The time evolution of the MDF has attracted attention. Holm et al. [12,13] studied the evolution of the MDF via kinetic Monte Carlo (KMC) simulations of grain growth in two dimensions. In one case, orientations were chosen randomly from SO(3), and misorientations were computed with regard to cubic symmetry, resulting in an initial MDF following the well-known Mackenzie distribution [16]. They observed that the MDF evolved into a steady state quite close to the initial Mackenzie distribution, characterized by a slight enhancement of the low-misorientation boundaries. More recently, Gruber et al. [9] carried out larger KMC simulations, both in two and three dimensions, which helped remove the statistical uncertainties in some of the results of Refs. [12,13]. Their initial conditions contained over 75,000 well-resolved grains in two dimensions, and they obtained essentially the same results as found by Holm et al. [12].

These results are rather surprising in view of the discussion above. From an energetic point of view, one would expect that MDF would concentrate for small misorientations. Indeed, both Holm et al. and Gruber et al. also considered simulations with initial conditions dominated by a single-component texture. In this case, they observed that the MDF evolves in such a way that it tends to concentrate at low misorientations. In addition, the fiber texture case was studied by Holm et al. and Kinderlehrer et al. [15] (using front tracking, with a different misorientation to surface energy map). Both investigations observed the concentration of the MDF at zero misorientation.

Barmak et al. [2] went on to further suggest that the MDF converges to a Boltzmann distribution, namely

\[ g(\phi) = \frac{1}{Z_\lambda} e^{-\lambda\sigma(\phi)} \]

where \( \phi \) is the misorientation, \( \sigma(\phi) \) is the grain boundary energy associated with a misorientation \( \phi \), and \( Z_\lambda \) a normalization factor. Note that, if the surface energy is a strictly increasing function of the misorientation angle, then Eq. (1) will have a maximum value at zero misorientation. From a thermodynamic point of view, Eq. (1) is reasonable. In addition, there is a remarkable formulation to determine the thermal energy, \( \lambda \). This value of \( \lambda \) is the one that yields the fastest decrease in the relative entropy [2]. The difference between the results observed in the fiber texture and strongly textured simulations as compared to the random texture case is remarkable: in the former, concentration of the MDF about zero misorientation is clearly observed. In the latter, only a small deviation from the Mackenzie distribution is observed. The “stability” of the Mackenzie distribution is peculiar since an energetic point of view suggests that the MDF should tend to concentrate near zero.

We propose to explore this issue with a numerical approach capable of simulating a very large number of grains over much longer periods of time. This is accomplished by introducing a new computational approach to anisotropic (unequal surface energy) grain growth, which in two dimensions can readily simulate the coarsening of approximately 670,000 grains down to less than 4000. This new algorithm allows arbitrary surface energies to be specified between any two grains in the network. It is accurate, robust, efficient and easily parallelized. It builds on the distance-function-based diffusion-generated motion (DFDGDM) approach [7], which was used in earlier work [4,5] to simulate long-time isotropic (equal surface energy) grain growth with very large numbers of grains. The initial simulations presented demonstrate that this method repeats previous results using KMC simulations [9,12,13] and front tracking [15,2]. Subsequent simulations demonstrate the importance of the surface-energy-to-misorientation map in predicting the time evolution of the MDF and suggests a framework capable of explaining the different MDFs obtained in the fiber texture and random texture cases.

2. The model

We will use Mullins’s model [11,20] of normal grain growth. Denoting the boundary between two adjacent grains \( \Sigma_j \) and \( \Sigma_k \) as \( \Gamma_{jk} \), the specific form of Mullins’s model we consider is

\[ E = \sum_{j<k} \sigma_{jk} \text{Area}(\Gamma_{jk}) \]

The constants \( \sigma_{jk} \) are known as the surface energies associated with the \( \Gamma_{jk} \). This model ignores in particular the dependence of the energy density on the boundary plane. Moreover, we assume constant mobilities for all \( \Gamma_{jk} \). Accordingly, \( \Gamma_{jk} \) moves by the normal speed

\[ v_n(\Gamma_{jk}) = \kappa_{jk} \delta_n(\Gamma_{jk}) \]

where \( \kappa_{jk} \) denotes the mean curvature of \( \Gamma_{jk} \). At a triple junction formed by the meeting of three distinct phases \( \Sigma_j, \Sigma_k \) and \( \Sigma_{\ell} \), Herring angle conditions [10] hold; they stipulate that:

\[ 0 = \sigma_{jk} n_{jk} + \sigma_{k\ell} n_{k\ell} + \sigma_{ij} n_{ij} \]

so that the angles formed by the normals \( n_{jk}, n_{k\ell} \) and \( n_{ij} \) to the three interfaces \( \Gamma_{jk}, \Gamma_{k\ell} \) and \( \Gamma_{ij} \) along the triple curve are determined by the surface energies \( \sigma_{jk}, \sigma_{k\ell} \) and \( \sigma_{ij} \).

The surface energies \( \sigma_{jk} \) will be assumed to be positive and to respect the triangle inequality

\[ \sigma_{jk} + \sigma_{k\ell} > \sigma_{ij} \] for any distinct \( j, k, \) and \( \ell \)

which turns out to be necessary to rule out wetting. Otherwise, the \( \sigma_{jk} \) are arbitrary.
3. The algorithm

This section presents our new algorithm for model (3) and (4) with arbitrarily prescribed surface energies $\sigma_{jk}$, suitable for large-scale simulations of grain networks. Our previous work [4,5] developed an efficient algorithm for the same model in the equal surface energy (i.e. $\sigma_{jk} = 1$) case, in both two and three dimensions. As in that previous work, our approach uses distance function-based diffusion-generated motion [7]. The extension described here to arbitrary surface energies from Refs. [4,5] is highly non-trivial. We start by reviewing distance function based diffusion generated motion in its most elementary form.

3.1. Distance function diffusion-generated motion

We start with the simplest setting of two-phase curvature flow: consider a single grain, $\Sigma$, surrounded by another grain of infinite extent. To evolve the boundary $\partial \Sigma$ with normal speed $v_\Sigma = \kappa$ using the level set method, one would first take a level set function $\phi$ so that $\Sigma = \{ x : \phi(x) > 0 \}$ and $\phi = 0$ on $\partial \Sigma$; then, one would evolve $\phi$ by $\partial_t \phi = \kappa |\nabla \phi|$. Among the many possible level set representations of $\Sigma$, if $\phi$ is chosen to be the signed distance function, $d$, then the level set equation greatly simplifies: $\Delta d = \kappa$ along the interface and $|\nabla d| = 1$, by which the level set equation reduces to $\partial_t \phi = \Delta \phi$. However, during this evolution, $\phi$ will not remain a signed distance function even if it starts as one; it must be reinitialized to remain as such. Therefore, alternating these two operations (namely, linear diffusion and reinitialization) repeatedly yields motion by mean curvature. The threshold dynamics scheme proposed in Refs. [18,19] and developed further in Ref. [23] for this problem applies a similar approach using the characteristic function of $\Sigma$ rather than the signed distance function.

To be more precise, let $d'(x)$ be the signed distance function at times $\Delta t$, $s = 0, 1, 2, \ldots$, where $\Delta t$ is the time step. The solution of the heat equation for one time step with $d'$ as an initial condition is $G_M * d'$, where

$$G_M = (4\pi \Delta t)^{-D/2} e^{-|x|^2/(4\Delta t)}$$

in $D$ dimensions. Finally, $d = \text{Redist}(\phi)$ is the operation that will produce a distance function from $\phi$ where both $d$ and $\phi$ have the same zero level set. The resulting algorithm is

Algorithm 1.

1. $A = G_M * d'$
2. $d^{s+1} = \text{Redist}(A)$

Under the algorithm above, the surfaces defined implicitly via ($d' = 0$) move by an approximation to motion by mean curvature with mobility equal to one; convergence to the exact flow takes place as $\Delta t \to 0$.

In the multiphase setting, let $\Gamma_{jk}$ denote the boundary between grains $\Sigma_j$ and $\Sigma_k$, with $j,k \in \{1,2,\ldots,N\}$. Let $d'_j$ denote the signed distance function for the $j$th grain at time step $s$, i.e. $\Sigma_j^s = \{ x : d'_j(x) > 0 \}$. First, diffuse all of the distance functions $d'_j$, denoting the result $A'_j = G_M * d'_j$. Then each spatial point $x$ must be reassigned to a single grain, which is done according to the following rule: if $A'_j(x)$ is the largest among all the convolutions, then $x$ is assigned to grain $k$. Thus, the algorithm is:

Algorithm 2.

1. $A_j = G_M * d'_j$
2. $B_j = \frac{1}{2}(A_j - \max_{k \neq j} A_k)$
3. $d_{jk}^{s+1} = \text{Redist}(B_j)$

The resulting normal speed for the boundary of each grain under Algorithm 2 is $v_\Sigma = \kappa$. Furthermore, the relevant Herring angle condition is satisfied along triple curves. Algorithms 1 and 2 are due to Esedoglu et al. [7].

In Refs. [4,5], Algorithm 2 was extended by recognizing that a separate signed distance function is not needed for each individual grain: well-separated grains can be lumped into families. A single signed distance function is then computed to represent an entire family, which can contain thousands of distant grains. This partitioning is constantly updated to ensure the good separation of grains belonging to the same family, preventing unphysical interactions and mergers. In practice, as few as 18 families can be sufficient to simulate over 670,000 grains in two dimensions. This procedure will be discussed in more detail below. In Ref. [6], we further extended this algorithm to models of recrystallization. The schemes have thus proven their mettle in very-large-scale, fully resolved, accurate simulations in both two and three dimensions, handling hundreds of thousands of topological changes along the way.

3.2. Arbitrary surface energies

Extending DFDGM to the case of arbitrarily prescribed surface energies, the algorithmic meat of the present paper is based on two observations. First, Algorithm 2 for equal surface energies extends to the additive surface energy case quite easily. We call a set of surface energies $\sigma_{jk}$ additive if they arise as

$$\sigma_{jk} = \frac{1}{2} (\gamma_j + \gamma_k)$$

for $N$ arbitrarily chosen non-negative weights $\gamma_j$. Note that this is a very small subset (of dimension $N$) of all admissible surface energies (a set of dimension $N(N - 1)/2$). Nevertheless, our second observation is that any three-grain model satisfying Eqs. (3) and (5) can be expressed in terms of the additive case. The energy (2) of the system becomes
\[ E = \sum_{j=1}^{N} \gamma_j / \text{Area}(\partial \Sigma_j). \]  

This suggests the following modification to Algorithm 2:

**Algorithm 3.**

1. \( A_j = G_{r, \Delta t} * d_j^p \)
2. \( B_j = \frac{1}{3} (A_j - \max_{k \neq j} A_k) \)
3. \( d_j^{p+1} = \text{Redist}(B_j) \)

Note that the only difference between Algorithms 2 and 3 is the convolution kernel used in the first step. Here, and subsequently, the notation \( G_{r, \Delta t} \) indicates that \( \Delta t \) is replaced by \( \gamma_j \Delta t \) in Eq. (6). Under Algorithm 3, the normal speed of the grain boundary \( T_{jk} \) is \( v_n = \frac{1}{3} (\gamma_j + \gamma_k) k \). Numerical tests presented in Section 3.3 indicate that the appropriate Herring angle conditions (4) are also enforced by this modified algorithm.

One drawback of Algorithm 3 compared to Algorithm 2 is the necessity to represent and convolve each grain separately. In our original Algorithm 2, all grains are convolved with the same Gaussian kernel, allowing us to represent many well-separated grains with a single signed distance function to their union, which allows all their convolutions to be computed at once. This allows for great computational efficiency and the simulation of over 100,000 well-resolved grains in both two and three spatial dimensions. In Algorithm 3, as each grain may be associated with a different value of \( \gamma_j \), either the convolutions must be performed locally (prohibiting the use of the efficient discrete Fourier transform) or each grain must be represented in its own signed distance function. To redress this drawback of Algorithm 3, we make the following observation:

Let \( \Xi_j \) denote the union of all grains represented by \( d_j \), i.e. \( |d_j| > 0 \) = \( \Xi_j \). Next, we define \( \gamma_j(x) = \gamma_k \) for the grain \( \Sigma_k \subseteq \Xi_j \) nearest to \( x \). We can now replace \( A_j \) in the Algorithm 3 by

\[ A_j(x) = \gamma_j(x) / \gamma^* \left( G_{r, \Delta t} * d_j^p \right) + \left( 1 - \gamma_j(x) / \gamma^* \right) d_j^p \]

with \( \gamma^* = \max \gamma_j \). It can be shown that the expressions for \( A_j \) given above and in step 1 of Algorithm 3 agree with \( O(\Delta t) \) along smooth interfaces \( T_{ij} \) away from triple junctions.

Let Algorithm 4 denote the modification of Algorithm 3 that replaces its step 1 with Eq. (9). The major resultant gain is the use of a single convolution kernel, which allows the simultaneous computation of the convolutions of many grains with a single fast Fourier transform (FFT) and an inverse FFT pair.

Next, observe that, in the three-phase case, arbitrary surface energies \( \sigma_{12}, \sigma_{13} \) and \( \sigma_{23} \) can be mapped to \( \gamma_1, \gamma_2 \) and \( \gamma_3 \) so that \( \gamma_{12} = (\gamma_1 + \gamma_2)/2 \), etc., by the mapping

\[
\begin{pmatrix}
\gamma_1 \\
\gamma_2 \\
\gamma_3
\end{pmatrix} =
\begin{pmatrix}
1 & 1 & -1 \\
1 & -1 & 1 \\
-1 & 1 & 1
\end{pmatrix}
\begin{pmatrix}
\sigma_{12} \\
\sigma_{13} \\
\sigma_{23}
\end{pmatrix}
\]

where the triangle inequality for \( \sigma_{jk} \) implies that \( \gamma_j \) are positive. This observation has recently been made independently by Matsutani et al. [17]. Thus, Algorithm 3 is sufficient to generate three-phase motion with arbitrarily chosen surface energies. For \( N \)-phase motion, we note that there is, in general, no assignment of surface energies \( \gamma_j \) so that the arbitrary \( \sigma_{jk} \) can be written as \( \sigma_{jk} = (\gamma_j + \gamma_k)/2 \).

Algorithm 3 or 4, together with Eq. (10), can be used to update grain boundaries \( T_{jk} \), including at and around triple curves. Note that quadruple junctions are common at all times on the face of three-dimensional grains as the meeting place of triple curves, and higher multiplicity junctions arise, e.g. during topological transitions. We now explain how four and higher multiplicity junctions are handled.

Our approach is related to the weighted averages used in Ref. [23] for handling junctions of high multiplicity. In our version, for a phase \( j \) present at the junction, we calculate convolution values for each of the triple junctions it can form with any two of the remaining phases at the same junction, and take a weighted average of how it would have been updated had it been at a triple junction with them. Consider the case of a quadruple junction. First, compute \( A_j \) as given in Eq. (9) for the \( \gamma_j \) computed by Eq. (10) for each of the three possible triplets that phase \( j \) can participate in, and denote those values \( \psi_{jkl} \). For example, for \( j = 1 \), we apply Eqs. (10) and (9) to compute \( \psi_{123}, \psi_{134} \) and \( \psi_{124} \). Next, we compute the quantity

\[ T_1(x) = \frac{1}{3} (\psi_{123} + \psi_{134} + \psi_{124}) \]

Analogous quantities \( T_2, T_3 \) and \( T_4 \) are also computed.

An important observation is that if \( x \) is well inside \( \Sigma_j \), then \( A_j(x) > K \) and if \( x \) is well outside \( \Sigma_j \), then \( A_j(x) < -K \)

where \( K = 2.5 \sqrt{\Delta t \log(1/(4\pi \Delta t))} \). By “well inside (outside)” we mean that a single step of Algorithm 4 will not bring \( x \) out of (into) set \( \Sigma_j \). It therefore follows that if \( x \) is well inside grain \( \Sigma_1 \), then \( T_1(x) > K \), and if \( x \) is well outside grain \( \Sigma_1 \), then \( T_1(x) < -K \). This leads us to define the following weight function

\[ w_j(x) = \begin{cases} 1, & T_j(x) < K \\ e + (1 - e) \left( \frac{1 + T_j(x)}{2} \right), & |T_j(x)| < K \\ e, & T_j(x) > K \end{cases} \]

Therefore, if \( w_j(x) = 1 \), then we are in grain \( \Sigma_j \), and if \( w_j(x) = e \), we are not in grain \( \Sigma_j \), \( w_2(x) \) and \( w_3(x) \) and \( w_4(x) \) are also computed.

To understand the third step, consider the quantity \( w_j w_k \) for \( j \neq k \) and let the values \( T_{jk} \) and \( k \) be \( j \) and \( k \), respectively, which maximize it. Then grains \( j \) and \( k \) are interacting most strongly with grain \( \Sigma_1 \). This would suggest that we might replace \( A_1 \) by \( \psi_{1jk} \). In practice, we do something smoother, namely
\[ A_t(x) = \frac{\sum_{j,k=2}^{N} w_j w_k \psi_{1,jk}}{\sum_{j,k=2}^{N} w_j w_k} \]

In a similar way, we compute \( A_2, A_3 \) and \( A_4 \). The above procedure now replaces step 1 of Algorithm 3 or 4.

The general algorithm is now stated.

**Algorithm 5. Full algorithm for arbitrary surface energies**

Fix \( \Delta t, \varepsilon \) and \( K > 0 \). Define \( \gamma_{jk} \) to be the weight \( \gamma_j \) obtained from solving (10) with inputs \( \sigma_{jk}, \sigma_{kj} \) and \( \psi(x, d_j^r, \sigma_j) \) to be the right-hand side of Eq. (9). Define \( M \leq N \) collections \( \Xi_j \) of disjoint grains so that \( \bigcup_{j=1}^{M} \Xi_j = \bigcup_{j=1}^{N} \Xi_j \). Maintain \( M \) signed distance functions \( d_j(x) \), giving the signed distance to the collection \( \Xi_j \), with \( d_j(x) > 0 \) for \( x \in \Xi_j \). The signed distance functions are updated by the following: For \( s = 0, \ldots, \frac{\pi_{\text{max}}}{C_15} \) and \( j = 1, \ldots, M \), perform steps 1–4.

1. **Update**: For each grid location \( x \), define \( R(x) = \{i: d_i(x) > -\varepsilon\} \), and let \( r(x) = \#R(x) \).
   
   (a) If \( R(x) = \{j\} \), set \( A_j(x) = d_j'(x) \).
   
   (b) If \( R(x) = \{j,k\} \), set \( A_j(x) = \psi(x; d_j', \gamma_{jk}) \), and \( A_k(x) = \psi(x; d_k', \gamma_{kj}) \).
   
   (c) If \( R(x) = \{j,k,\ell\} \), set \( A_j(x) = \psi(x; d_j', \gamma_{jk}, \gamma_{j\ell}) \), \( A_k(x) = \psi(x; d_k', \gamma_{kj}, \gamma_{k\ell}) \), and \( A_\ell(x) = \psi(x; d_\ell', \gamma_{j\ell}, \gamma_{k\ell}) \).
   
   (d) If \( r(x) > 3 \),
   
   • For each \( i \in R \), compute
     \[ T_i(x) = \frac{1}{r(x)-1} \sum_{j,k \neq i} \psi(x; d_j', \gamma_{jk}) \]
     
   • Next compute \( w_j(x) \) by (11).
   
   • Set
     \[ A_j(x) = \frac{\sum_{j,k \neq i} w_j w_k \psi(x; d_j', \gamma_{jk})}{\sum_{j,k \neq i} w_j w_k} \]

2. **Redistribute**: Construct

   \[ B_j(x) = \frac{1}{2}(A_j(x) - \max_{k \neq j} A_k(x)) \]

   to remove overlaps and vacuums from the previous step.

3. **Redistance**: Set \( C_j(x) \) to be the signed distance function to the zero-level set of \( B_j(x) \).

4. **Swap**: As necessary, swap appropriate grains between signed distance functions \( C_j \) to ensure a minimum separation between grains associated with the same signed distance function. Redistance around swapped grains and denote the resulting signed distance functions as \( d_j^{r+1}(x) \).

This algorithm has computational complexity \( O(M \log P) \), where \( P \) is the total number of grid points \( (P = p^D \) for a cubic grid with \( p \) points in each of \( D \) spatial dimensions). The large-scale simulations described in Section 4 make use of \( M = 18 \) (48) signed distance functions in two (three) spatial dimensions. This complexity is the same as in the original DFDGM algorithm. The extension presented here differs from the original algorithm only in the first step. This step has computational complexity \( O(P \log P + r_i(x)) \), as the convolution is computed just once for each of \( M \) signed distance functions, then \( O(r_i(x)) \) linear combinations are formed at each grid location. However, high-order junctions (corresponding to large \( r_i(x) \) ) are expected to be very rare and highly unstable. In our simulations, we observe that \( r_i(x) \leq 6 \) at each spatial location and each time; so \( r_i(x) \) may be bounded by a constant.

Tests in Ref. [4] suggest that evolutions beginning with average grain width on the order of 10 grid points match very well visually with more resolved calculations away from topological changes. The vast majority of topological changes agree with those observed at greater resolution, though a single difference in the choice made by the algorithm at a topological change may lead to a very different microstructure at later times. No statistically significant change was observed in the statistics of the evolution under increased resolution in these tests.

### 3.3 Validation

In this section we provide numerical results demonstrating the accuracy of Algorithms 3, 4 and 5. The first two examples are three-phase evolutions: a generalized version of the well-known “Grim Reaper” exact solution, and an initial set of conditions devoid of symmetry which we compare with front tracking. We then investigate the ability of Algorithm 5 to preserve stable quadruple junctions, the existence of and conditions for which have been previously studied by Cahn [3].

#### 3.3.1. “Grim Reaper” profile

A derivation for a constantly transported profile in the axially symmetric case \( \sigma_{12} = \sigma_{13} \), commonly referred to as the “Grim Reaper”, is given in the Appendix of Ref. [8]. We straightforwardly extend this calculation to the more general case where all surface energies may be chosen independently of each other. The derivation is omitted but follows that in Ref. [8] closely. We choose \( \sigma_{12} = 1 \), \( \sigma_{13} = 0.8 \) and \( \sigma_{23} = 1.2 \). The simulation was performed using Algorithms 3, 4 and 5. All results are in good qualitative agreement.

We measure the interfacial velocity by interpolating to find the location of the interfaces corresponding to \( \mu_{12}(x) \) and \( \mu_{13}(x) \) at \( t = 0 \) and \( t = 3/128 \). The \( L^2 \) error in interfacial velocity converges approximately linearly. The maximal error occurs near the triple junctions and appears to be converging at a sublinear rate. These results agree with analysis performed on the basic, isotropic algorithm in Ref. [7].
3.3.2. Comparison with front tracking

To verify that the numerics of the previous experiment are not influenced by the axial symmetry or the vertical interface of the “Grim Reaper” profile, we also study a three-phase evolution with asymmetric curved interfaces. In this case, an exact solution is not known, so we compare with a very-high-resolution front-tracking simulation containing over 4800 points instead. The results obtained are displayed in Fig. 1a. The evolving front-tracking solution was periodically reparameterized to maintain approximately constant spacing between the discretized points. The surface energies were chosen as \( \sigma_{12} = 1, \sigma_{13} = 2/3 \) and \( \sigma_{23} = 4/3 \); here, the first phase is the upper interior region, the second phase is the “background” and the third phase is the lower interior region. The numerical solutions generated by Algorithms 3, 4 and 5 were compared with the reference solution generated by the front-tracking code. Due to the very close agreement between Algorithms 3 and 4, only the results obtained from Algorithms 4 and 5 are displayed in Fig. 1. Due to the excellent agreement between the various algorithms, we use Algorithm 5, which allows for the full generality of Eq. (3), in all subsequent simulations.

3.3.3. Stable quadruple junctions

With equal surface energies, quadruple junctions are unstable under multiphase curvature motion in the plane. Cahn [3] investigated the stability of quadruple junctions in the case where there are two “types” of phases, which he denotes type \( a \) and type \( b \). Let \( q_{ab\beta\gamma} \) describe a quadruple junction with the \( a \) and \( \gamma \) phases opposite each other. The condition

\[
\sigma_{ax}^2 + \sigma_{b\beta}^2 \geq 4\sigma_{ab}^2
\]

is shown to be necessary and sufficient condition for a \( q_{ab\beta\gamma} \) quadruple junction to be stable over a range of opening angles. Denote the opening angle of the \( a \) phases to be \( \Phi_a \) and the opening angle of the \( b \) phases to be \( \Phi_b \). As long as \( \Phi_a \) is larger than the angle \( \theta_a \) arising from the Herring angle condition (4) for the \( \tau_{ab} \) triple junction and \( \Phi_b \) is larger than the angle \( \theta_b \) for the \( t_{b\gamma} \) triple junction, the quadruple junction remains stable.

In our tests, we consider phases \( \Sigma_1 \) and \( \Sigma_3 \) to be of type \( a \) (see Fig. 2) and phases \( \Sigma_2 \) and \( \Sigma_4 \) to be of type \( b \). In the first simulation, we choose \( \sigma_{ax} = \sigma_{b\beta} = 1.85 \) and \( \sigma_{ab} = 1 \). The \( q_{ab\beta\gamma} \) junction should be stable as long as both \( \Phi_a \) and \( \Phi_b \) are greater than \( \Phi^* = \arccos (0.71125) \approx 44.66^\circ \). \( \Phi_b = \Phi^* \) is marked in dashed lines on Fig. 2. Numerically, the quadruple junction persists (appearing as two triple junctions separated by a \( \Gamma_{13} \) interface, which has length \( O(\Delta x) \)) until \( \Phi_b \) passes through the critical angle.

4. Large-scale simulations

In this section, we use Algorithm 5 to study the evolution of large networks of grains starting from random and fiber textured initial data, as discussed in the introduction. Simulations are performed in both two and three spatial dimensions. Computational requirements allow for the two-dimensional simulations to be initialized with over 650,000 well-resolved grains. In three dimensions, we take an initial condition with approximately 64,000 well-resolved grains. We focus primarily on the results from the simulations performed in two spatial dimensions,
as the results are more statistically reliable due to the larger number of grains; however, qualitatively similar results are observed in three spatial dimensions. The results seen in these simulations will be seen to confirm the observations of the prior numerical work [1,2,9,12,13].

4.1. Two spatial dimensions

As discussed in the introduction, two significantly different types of simulation results have been seen in the literature. For randomly textured initial conditions, KMC simulations [9,12,13] show only slight evolution from the initial MDF, which is a Mackenzie distribution. In contrast, the strong single component textured and fiber textured simulations [12,13,15] demonstrate sharpening of the MDF about zero misorientation from an initially uniform MDF. We perform a number of very-large-scale, well-resolved simulations in two spatial dimensions to (i) confirm the results of these other much smaller simulations and (ii) to give an explanation for the dissimilar character of these results.

4.1.1. Effect of texture

We begin by comparing two simulations with different initial orientation distributions. In the first simulation, fiber-textured grain orientations are assigned, so only the angle in the axis–angle description of grain orientation varies, and are chosen uniformly at random. In the second simulation, fully random orientations from $SO(3)$ are assigned to each grain.

The simulations were initialized with same microstructure of 671,088 well-resolved grains, chosen as the approximate Voronoi diagram to points placed uniformly at random in the simulation domain. The simulations were run until $t = 1.22 \times 10^{-5}$, when less than 4000 grains remain in each case. To make the computation on this long time scale computationally feasible, the simulation begin on a $8192 \times 8192$ grid discretizing $[0,1)^2$, and is downsampled onto a $2048 \times 2048$ grid at $t = 7.15 \times 10^{-5}$, when less than 40,000 grains remain in each simulation. The time step is also commensurately increased at this time. The total wall time of each simulation was between 9 and 12 days, running on 18 Intel Nehalem i7 processors.

The surface energy $\sigma_{jk}$ is determined based on the following modified Read–Shockley relationship [22]:

$$\sigma_{jk} = \left\{ \begin{array}{ll}
\sigma_{\text{min}} + (1 - \sigma_{\text{min}}) \frac{|\phi_{jk}|}{\phi_{\text{max}}} \left[ 1 - \log \left( \frac{\phi_{jk}}{\phi_{\text{max}}} \right) \right] & \text{if } |\phi_{jk}| \leq \phi_{\text{max}} \\
1 & \text{if } |\phi_{jk}| > \phi_{\text{max}}
\end{array} \right. \quad (16)$$

where $\phi_{jk}$ is the misorientation angle between the $j$th and $k$th grains. The value $\sigma_{\text{min}}$ is chosen to be 1/10 to prevent numerical artifacts related to stationary interfaces. For these simulations, we choose $\phi_{\text{max}} = 30^\circ$ to agree with simulations performed in Refs. [9,12] and to lie within the experimentally observed range [24].

The results for the fiber texture case and the random texture case are shown in Fig. 3. The evolution of the MDF for each case is shown in Fig. 3b and e. The initial MDF (thin red bars) is approximately uniform in the fiber texture case. The MDF is seen to rapidly sharpen around zero misorientation, consistent with prior investigations [12,13,15]. For random texture, the MDF is initially the Mackenzie distribution. Our simulations show that the MDF evolves very slowly in time, revealing only a slight preference for low-misorientation grain boundaries at the expense of high-misorientation grain boundaries. These results are also consistent with the KMC simulations of Refs. [9,12].

Let us now examine the grain microstructure. In the fiber texture case, the crystallographic orientation is determined by a single angle. This means that its orientation can be easily represented by a color scale. The entire microstructure is displayed at time $t = 1.15 \times 10^{-3}$ (Fig. 3a). We observe that grains of similar orientations tend to form connected domains, a phenomenon we refer to as grain clustering. The interfaces between grains of similar orientations have very small surface energies associated with them, so have lower velocities and contribute much less to the energy of the system than the interfaces between grains of very different orientations; as such, it is reasonable that these interfaces disappear much more slowly than high-misorientation interfaces. At the end of the simulation, the remaining high-energy interfaces (interfaces between grains of very different orientations) tend to be quite straight. Badmos et al. [1] also reported the phenomenon of grain clustering, though on much a smaller scale, using front tracking.

We point out that the formation of grain clusters should be expected from general considerations. The orientation distribution of the grains is not expected to change as the grain network coarsens. However, it is energetically favorable for grains with similar orientations to be next to each other. Therefore, over time, one might expect clusters of grains to form. Since the orientation distribution does not change significantly as the grain network evolves, this clustering phenomenon can be rather complex.

For the random texture case, we make use of a coloring scheme designed by Patala et al. [21] which maps the fundamental zone for cubic symmetry (432-misorientation space) onto the hue saturation value (HSV) color space in such a way that low misorientations are represented by lighter colors and high misorientations are represented by darker colors. Following Patala et al.’s work, we select a reference grain randomly among those surviving until the end of the simulation, and color all grains by their misorientation with respect to this particular grain. Snapshots of the microstructure when 4000 grains remain are shown in Fig. 3d. In contrast to the fiber texture case, there appears to be no significant grain clustering. While consistent with the result that the MDF did not change much from the initial Mackenzie distribution, it is surprising that clusters seem to be unable to form.

To gain some insight into this, we introduce the distribution of surface energies and define the histogram of area-weighted grain boundaries as a function of surface energy
to be the surface energy distribution function (SEDF). It is customary in both experiment and simulation to study the MDF rather than the SEDF. From an experimental viewpoint, it is much easier to measure grain orientations than it is to measure surface energies. The former can be measured, for example, by electron backscatter diffraction techniques. In contrast, the latter is indirectly measured using a variety of techniques (for example, by measuring triple junction angles and applying them to Eq. (4)). However, no such barrier exists in our numerical simulations. Indeed, a functional form for surface energy as a function of misorientation is assumed and thus the surface energy of any interface can be determined directly from the simulation results.

In the Read–Shockley case, the SEDF is initially very sharply peaked about the maximum surface energy (Fig. 3f). Very few interfaces interact with any other surface energy, so there is little opportunity for the system to form low-misorientation interfaces. In contrast, the fiber texture case has an initial SEDF that is less sharply peaked at the maximum surface energy (Fig. 3c; note the different scale) and has a significant fraction of low-energy grain boundaries. As a consequence, more interfaces feel a sub-maximal surface energy, allowing the grain network to lower its total energy more quickly. As the MDF concentrates near zero, grain clustering occurs.

4.1.2. Effect of surface energy

In order to more fully explain the differences in results of the fiber texture and the random texture simulations presented previously, the role played by the surface energies must be more fully appreciated. To this end, we perform two additional simulations. In these simulations, we take the same randomly textured initial microstructure as before, but assign different forms of the surface energy. We choose an affine surface energy function,

\[ \sigma_{jk} = \sigma_{\min} + (1 - \sigma_{\min}) \frac{\phi_{jk}}{\phi_{\max}} \]  

and also again consider the Read–Shockley surface energy. In these cases, we again choose \( \sigma_{\min} = 1/10 \), but now choose \( \phi_{\max} \) to be the maximum possible misorientation, \( \approx 62.8^\circ \). These forms both satisfy the triangle inequality (5).
Fig. 4 shows the microstructure of these new simulations when 4000 grains remain, and the time evolution of the MDF and SEDF, with the Read–Shockley surface energy in the top row and the affine surface energy below. Both simulations initially have the Mackenzie distribution as the initial MDF; however, in both cases the time evolution of the MDF is noticeably different from the Read–Shockley case with \( \phi_{\text{max}} = 30^\circ \). This difference is most pronounced in the affine case. The differences in each of these three cases can be understood by the corresponding initial SEDFs. If we compare the SEDF for the Read–Shockley case with \( \phi_{\text{max}} = 62.8^\circ \) with the one for \( \phi_{\text{max}} = 30^\circ \), we see that it is less concentrated at the maximum surface energy; and compared with the affine case, the SEDF is dramatically different – there is no concentration at the highest surface energy.

When the SEDF is heavily concentrated at the highest surface energy, very few interfaces feel any other surface energy, so there is little opportunity for the system to form low-misorientation interfaces. In contrast, the affine surface energy gives an initial SEDF that is shaped like the Mackenzie distribution. This means that many more interfaces have a sub-maximal surface energy in this case and are thus energetically preferred to survive. The lower misorientation interfaces are even more preferred, and the MDF evolves to reflect this. This effect can be controlled by the value of \( \phi_{\text{max}} \). As \( \phi_{\text{max}} \to 0 \), the surface energy function becomes uniform and the SEDF is completely concentrated at its maximal value. Since the network is independent of the grain orientations in this case, we expect the MDF to remain exactly a Mackenzie distribution. Following this logic, we speculate that the reason why the MDF stays close to the Mackenzie distribution for non-zero values of \( \phi_{\text{max}} \) is that the energy pathway for minimization is kinetically limited.

Finally, we remark that in these two cases we see some evidence of grain clustering, though it is not as prominent as in the fiber texture case. This is consistent with the evolution of the MDF. In both of these cases the MDF was only enhanced at low misorientations, whereas in the fiber texture case a strong concentration of the MDF at zero misfit was observed. Therefore it is reasonable to expect more grain clustering in the fiber texture case than in the random texture case.

4.2. Three spatial dimensions

In three dimensions, the simulation is performed on a \( 400 \times 400 \times 400 \) grid discretizing \([0,1)^3\). The initial microstructure contains 64,000 grains. Orientations are assigned uniformly at random. Three simulations are run until \( t = 8.50 \times 10^{-3} \). At this time, fewer than 1050 grains remain in each simulation. The total wall time of each simulation was between 4 and 5 days, running on 48 Intel Nehalem i7 processors. The first simulation, with microstructure and MDF shown in Fig. 5, takes the
Read–Shockley surface energy with $\phi_{\text{max}} = 30^\circ$. The simulation is repeated, as before, with the same initial microstructure and orientations, but with the Read–Shockley surface energy and affine surface energy with $\phi_{\text{max}} = 62.8^\circ$. Too few grains remain at the end of the simulation to make statistical inferences about the evolution of the MDF, though the evolution of the MDFs and SEDFs, shown in Fig. 6, is in qualitative agreement with the results in two spatial dimensions. In this case, the simulation was not large enough to observe the presence or absence of any grain clustering.

5. Summary

We have introduced an algorithm for simulating multiphase curvature motion with arbitrary surface energies. The algorithm represents interfaces implicitly and, much like a level set method, allows for automatic handling of topological changes. In addition, this method is unconditionally stable and achieves good accuracy on uniform grids. We have demonstrated that this algorithm is useful for simulations of normal grain growth—a problem important in computational materials science. The algorithm can be extended to include other physical effects; for example, the addition of bulk energy terms for modeling recrystallization can be incorporated using the approach proposed by Elsey et al. [6]. Further generalizations, for example to anisotropic surface energies, are currently under investigation.

The numerical simulations described here show good agreement with the results of prior simulations [9,12,13,15] but allow for the accurate evolution of much larger grain boundary networks. These simulations show that the MDF evolves quite differently in the fiber texture and random texture cases. In particular, the MDF concentrates at zero misorientation for the fiber texture case whereas in the random texture case the MDF remains close to its initial Mackenzie distribution. Our large-scale simulations reveal that different microstructures arise in these two cases. In the fiber texture case, grains of similar orientation cluster together whereas in the random texture case this does not appear to occur. We argue that while clustering would further decrease the energy in the random texture case, the rarity of low-misorientation interfaces makes clustering difficult to achieve by grain growth kinetics.

Our simulations suggest that the difference in the evolution of the grain network between the fiber texture and random texture cases is kinetic in nature and is tied to the properties of the initial conditions. In the random texture case far fewer grains have low misorientation compared to the fiber texture case. For example, with fiber texture crystallography, 22% of interfaces initially can be expected to have a misorientation of less than $10^\circ$. On the other hand, for the random texture case, less than 0.7% of
randomly selected interfaces are expected to have such a low misorientation and over 80% of randomly selected interfaces have a misorientation greater than 30°. Using the Read–Shockley surface energy (16) with \( \phi_{\max} = 30° \), this means that the vast majority of interfaces will have the maximal surface energy. Such a simulation has only a small proportion of interfaces with lower surface energy, so it must be expected that the evolution of the MDF in this regime will be dramatically slower. Indeed, our simulations using the Read–Shockley surface energy with \( \phi_{\max} = 30° \) show little change in the MDF, whereas using the Read–Shockley surface energy with \( \phi_{\max} = 62.8° \) and the affine surface energy sees the MDF evolving quite far from a Mackenzie distribution. We observe similar behavior in three-dimensional simulations as well. Finally, we should mention that this work seems to suggest that, as the MDF concentrates for low misorientations, clusters of grains with similar orientation must occur.

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