A More Accurate Two-Dimensional Grain Growth Algorithm

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We describe a method for evolving two-dimensional polycrystalline microstructures via mean curvature flow that satisfies the von Neumann-Mullins relation with an absolute error $O(\Delta t^2)$. This is a significant improvement over a different method currently used that has an absolute error $O(\Delta t)$. We describe the implementation of this method and show that while both approaches lead to indistinguishable evolution when the spatial discretization is very fine, the differences can be substantial when the discretization is left unrefined. We demonstrate that this new front-tracking approach can be pushed to the limit in which the only mesh nodes are those coincident with triple-junctions. This reduces the method to a vertex model that is consistent with the exact kinetic law for grain growth. We briefly discuss the extension of the method to higher spatial dimensions.

INTRODUCTION

Over the last quarter century, numerous methods have been developed to study grain growth in two and three dimensions, including Monte Carlo Potts models [1, 2], cellular automata [3, 4], phase field models [5, 6], vertex models [7, 8], front tracking models [9], and finite element models [10]. Each approach has advantages and disadvantages. The Monte Carlo Potts model is both simple, easily implementable and extendable to a wide range of grain growth phenomena. Phase field models, like the Potts model, are based upon well-founded microscopic physics but have the advantage of being formulated in terms of continuum descriptions. Vertex models have the most compact data sets and, arguably, are based on the most fundamental objects in the microstructure – triple-junctions. Front tracking models have the advantage of well-defined equations of motion for boundary elements. Finite element methods naturally carry all material point information. In all cases, a discretization of the microstructure is involved, which necessarily compromises our ability to model the requisite grain growth physics in full fidelity.

The fundamental equation which governs normal grain growth in isotropic polycrystalline materials is the von Neumann-Mullins relation [11, 12], which describes the area evolution of individual grains in a two-dimensional polycrystal:

$$\frac{dA}{dt} = -2\pi M\gamma\left(1 - \frac{n}{6}\right), \tag{1}$$

where n denotes the number of grains that are in contact with the grain of interest, and M and γ are constants describing the grain boundary mobility and grain boundary energy, respectively. This result is exact for normal grain growth in an isotropic polycrystalline material where the velocity v at each point along the grain boundary is $v = M\gamma\kappa$, where κ is the curvature at that point.

A widely used numerical scheme for tracking microstructural evolution, including grain growth, is the front tracking method as realized in the robust and versatile program, Surface Evolver, developed by Brakke [13]. This program can track the evolution of grain boundaries moving via mean curvature motion in any number of dimensions. Several papers report grain growth simulation results based upon this method [14–16]. In this paper, we develop a new approach for simulating grain growth that is based on front tracking ideas and that satisfies the exact von Neumann-Mullins relation at all times, regardless of discretization. This approach may be easily extended to an arbitrary number of dimensions. As an example, we implement the new grain growth method in two dimensions on the Surface Evolver platform.

ALGORITHM

In most front tracking codes, nodes are distributed along a surface and moved according to a discretized equation of motion. Each node is "connected" by edges to neighboring nodes to represent a surface. New nodes are added when neighboring ones move too far apart; likewise, nodes are removed when neighboring ones become too close. A central issue in modeling normal grain growth in an isotropic polycrystalline system is a description of what happens where grain boundaries meet. In two dimensions, three grain boundaries meet at a point (i.e., a vertex, or *triple-junction*), and assuming that all boundaries have equal energy, the angle between them is $2\pi/3$. The key feature of normal grain growth is that these angles are fixed; i.e., we must view them as boundary conditions on the vertices (in three dimensions, the two-dimensional grain boundaries meet along triple-lines, also at fixed angles $2\pi/3$). If the angles are "only approximately" fixed, then the grain growth model will, at best, be "only approximately" correct. We note that when a topology change (e.g., grain switching) occurs,

triple-junction angles necessarily change. These changes are very brief and are limited only by the discreteness of the atomic structure. As described below, this is a time scale much smaller than the time step in any continuum simulation. It is important to ensure that the rate of these angle changes are not dictated by the details of the numerical method or the length scale of the observation in an experiment.

Consider a two-dimensional continuum system where three boundaries meet at a point where all of the internal angles are $2\pi/3$ (see Fig. 1). If we construct a discretized version of this system in which a node is placed at a triple-junction and additional nodes are placed on the three boundaries a short distance away from the triple-junction, then the internal angles where the connecting edges meet are not necessarily $2\pi/3$. As the spatial discretization is refined, the internal angles approach $2\pi/3$. Therefore, in the discrete model, the triple-junction angles depend on the discretization, while for the continuum, they are always fixed at $2\pi/3$. The point is that the angles only asymptotically converge to the continuum value with refinement of the discretization. Although the grain growth method proposed here is inherently discrete, it implicitly enforces the asymptotic angle condition at the triple-junctions by moving the nodes *as if* the angles in microstructure were fixed at $2\pi/3$.

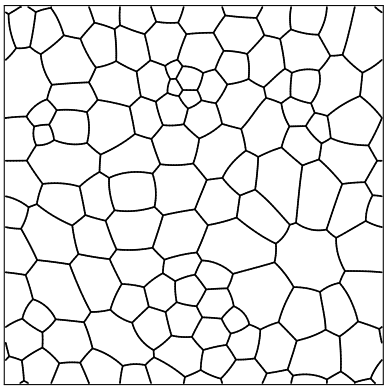


FIG. 1. An example two-dimensional polycrystalline microstructure where three boundaries meet at $2\pi/3$ angles at each triple-junction.

In this section, we describe a new method for simulating grain growth. We begin by picturing a microstructure which we discretize into a set of nodes and connecting edges. Next, we develop a method for moving nodes in a manner that ensures that the von Neumann-Mullins relation is exactly satisfied for all grains at all times. To do this, we discretize the time variable t from Eq. (1) into time steps Δt and solve for the change in grain area ΔA:

$$\Delta A = -2\pi M\gamma \left(1 - \frac{n}{6}\right) \Delta t. \tag{2}$$

For simplicity, we consider a discretization of a single isolated grain, embedded in an infinite body, as shown in Fig. 2. Moving the node σ changes the area of the shaded triangle by the same amount as it changes the area of the entire grain. This ability to localize changes of area enables us to express each side of Eq. (2) as a sum over all nodes surrounding a grain. The sum of the exterior angles around a discretized closed shape (polygon) is exactly 2π. If we ensure that the area of each triangle changes by an amount $-\alpha M\gamma\Delta t$, where α is the exterior angle at its apex, then after each time step the area of the entire polygon will change by $-2\pi M\gamma\Delta t$, with an error of the order $(\Delta t)^2$, owing to overlap between triangles associated with adjacent nodes; this error will be elaborated in detail in the next section.

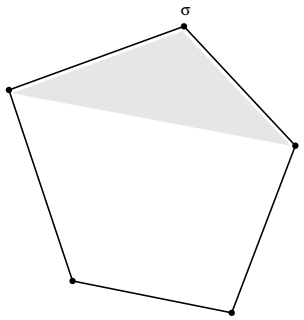


FIG. 2. An isolated grain; i.e., a grain with no triple-junctions.

We now shift attention to the more general case of a grain with n neighboring grains. Here, we move nodes as for an isolated grain with one correction. That is, we move triple-junctions in a way that changes the area of each neighboring grain by an amount $-(\alpha_i - \frac{\pi}{3})M\gamma\Delta t$. Since a body with n neighbors has n triple-junctions, the area of a body with n neighbors will change by an amount $-(2\pi - n\frac{\pi}{3})M\gamma\Delta t$, or $-2\pi M\gamma(1-\frac{n}{6})\Delta t$, which is exactly the discretized von Neumann-Mullins relation for n-sided bodies, Eq. (2).

We now provide a more precise description of the motion of each node, beginning with those that are *not* triple-junctions. Consider a node σ with edges $\mathbf{e_1}$ and $\mathbf{e_2}$, as shown in Fig. 3; the exterior angle between the two edges is α. Our goal is to move node σ by a displacement vector $\mathbf{dv}$ that will change the area of the triangle by $\Delta A = -\alpha M\gamma\Delta t$. Though we could move the node in almost any direction (with an appropriate magnitude) to achieve the desired area change, for reasons of numerical stability we move the node in the direction of $\mathbf{e_1} + \mathbf{e_2}$. If α is the exterior angle between the two edges, then to change the area of the triangle by exactly $-\alpha M\gamma\Delta t$, we let:

$$\mathbf{dv} = \alpha M\gamma\Delta t \frac{\mathbf{e_1} + \mathbf{e_2}}{|\mathbf{e_1} \times \mathbf{e_2}|}. \tag{3}$$

We next consider a triple-junction node τ (i.e., a node at which three grains meet), as shown in Fig. 4. To be

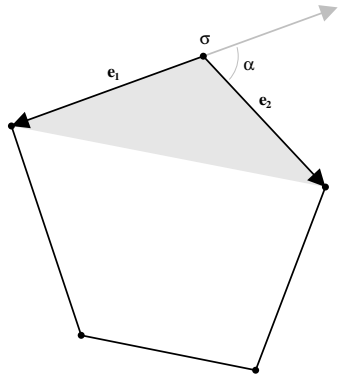


FIG. 3. A schematic of an isolated grain, emphasizing a single triangle with apex σ and directed edges $\mathbf{e_1}$ and $\mathbf{e_2}$.

consistent with the von Neumann-Mullins relation, displacement of the triple-junction must change the area of each neighboring grain by $\Delta A_i = -(\alpha_i - \frac{\pi}{3})M\gamma\Delta t$, where α_i is the exterior angle at the triple-junction with respect to grain i. Unlike boundary nodes, which have a degree of freedom in their solution, triple-junctions have exactly one solution.

If α_1 and α_2 are exterior angles at the triple junction with respect to bodies 1 and 2, as shown in Fig. 4, then:

$$\mathbf{dv} = 2M\gamma\Delta t \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} \mathbf{e_1} - \mathbf{e_2} \\ \mathbf{e_2} - \mathbf{e_3} \end{bmatrix}^{-1} \begin{bmatrix} \alpha_1 - \frac{\pi}{3} \\ \alpha_2 - \frac{\pi}{3} \end{bmatrix} \quad (4)$$

will tell us exactly how to move the triple junction node τ. Equations (3) and (4) then describe the motions of all boundary nodes and all triple-junction nodes, respectively. These equations represent the displacement vectors for each node at every time step.

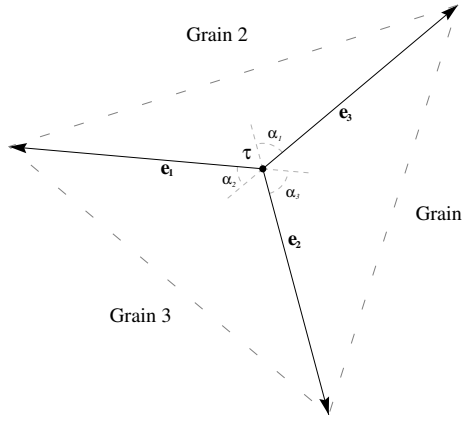


FIG. 4. A triple-junction τ where grains 1, 2, and 3 meet, where $\mathbf{e_i}$ are the vectors from the triple-junction node to the nearest nodes on each of the three boundaries.

ERROR ANALYSIS

We now evaluate the errors associated with evolving a system using the Brakke method and that proposed here. We show that the Brakke method leads to an error linear in Δt and that proposed here leads to an error linear in $(\Delta t)^2$. We define the error as follows. After one time-step, the area of an individual grain *should* change exactly:

$$\Delta A = -2\pi M\gamma \left(1 - \frac{n}{6}\right)\Delta t,$$

as given by Eq. (2). We define the error to be the difference between this exact, theoretical result and what actually happens to a grain after one time-step. If ΔA_B is the change in area of a grain after one Brakke time-step, then we define the absolute error after one Brakke time-step to be $E_B = |\Delta A - \Delta A_B|$; the relative error is $\epsilon_B = E_B/\Delta A$. Likewise, if ΔA_P is the change in area of a grain after one time-step using the proposed method, then the absolute and relative errors are $E_P = |\Delta A - \Delta A_P|$ and $\epsilon_P = E_P/\Delta A$, respectively.

We first show that the absolute numerical error involved in our method is of the order $O(\Delta t^2)$. To do so, we let a denote the area of a shape A, b denote the area of a shape B, and so forth. If we move an individual node to change an area by $-\alpha M\gamma\Delta t$ for boundary nodes or $-(\alpha_i - \frac{\pi}{3})M\gamma\Delta t$ for triple-junctions and keep all other nodes fixed, there would be no error (up to machine precision). This is because the proposed method moves the nodes in a manner that is consistent with the exact von Neumann-Mullins relation.

If we move all nodes simultaneously, errors result from "interference" between motions of neighboring nodes. Consider for example the edge segment shown in Fig. 5. If we move only node n_1 by $\mathbf{dn_1}$ and leave all other nodes fixed, the area of the body will change by exactly $-(a+b+c)$. Similarly, if we move only n_2 by a motion $\mathbf{dn_2}$, leaving all other nodes fixed, the area of the body changes by $-(c+e+f)$. When we move both nodes si-

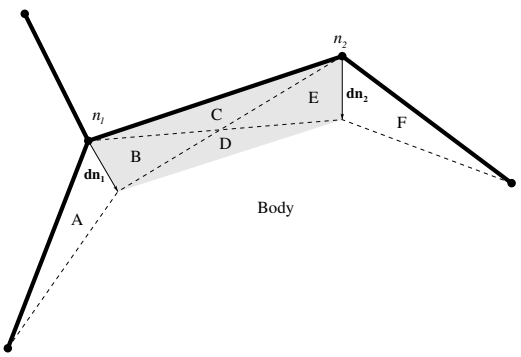


FIG. 5. Representation of part of an edge between two bodies.

multaneously, we want to change the area of the body by $a+b+2c+e+f$. However, the simultaneous motions of nodes n_1 and n_2 instead change the area of the body by $a+b+c+d+e+f$. This produces an absolute error $|d-c| = \frac{1}{2}|\mathbf{dn_1} \times \mathbf{dn_2}|$. Since each $\mathbf{dn_i}$ is linear in Δt, the cross product $\mathbf{dn_1} \times \mathbf{dn_2}$, and hence the the error resulting from the "interference" of the two motions, is linear in $(\Delta t)^2$.

Similar errors occur for all pairs of adjacent nodes moving simultaneously. Because any finite shape in our system has a finite number of these "interference" errors, the total error involved in the motion of all nodes will be $O(\Delta t)^2$. More precisely, the error is given by:

$$E_P = \frac{1}{2}\Big|\sum_{i=1}^{N} \mathbf{dn_i} \times \mathbf{dn_{i+1}}\Big|, \tag{5}$$

where the summation is around an individual grain.

In the Brakke method, the displacements of the nodes are also linear in Δt, and so it too produces "interference" errors of order $(\Delta t)^2$. However, in the Brakke case, the displacement of each node (even when all other nodes are fixed) results in errors that are $O(\Delta t)$. In summing these errors we arrive at a total error that is also $O(\Delta t)$. Though the expressions that demonstrate this are cumbersome for the general case, the validity of this statement can be shown by consideration of a regular polygon.

Consider an isolated grain represented by a regular polygon of m sides and radius r, as shown in Fig. 6. The area of this grain is $\frac{1}{2}mr^2 \sin\left(\frac{2\pi}{m}\right)$. After one time-

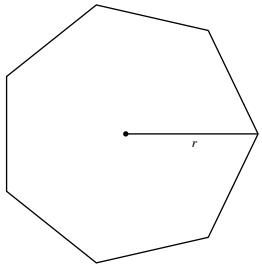


FIG. 6. Regular polygonal grain with m sides and radius r.

step, the area of this shape should change by $\Delta A = -2\pi M\gamma\Delta t$. In the Brakke scheme [1], evolution by one time-step changes the radius r of the grain by $-\frac{M\gamma\Delta t}{r\cos(\frac{\pi}{m})}$, while in the proposed method, one time-step changes the radius by $-\frac{2\pi M\gamma\Delta t}{mr\cos(\frac{2\pi}{m})}$. The corresponding changes in grain area are

$$\Delta A_B = -M\gamma\left[2m\sin(\frac{\pi}{m})\Delta t - \frac{m}{r^2}\tan(\frac{\pi}{m})(\Delta t)^2\right] \tag{6}$$

$$\Delta A_P = -M\gamma\left[2\pi\Delta t - \frac{2\pi^2(\Delta t)^2}{mr^2 sin(\frac{2\pi}{m})}\right]. \tag{7}$$

The absolute and relative errors are, therefore,

$$E_B = M\gamma\left[\left(2\pi - 2m\sin(\frac{\pi}{m})\right)\Delta t + \frac{m}{r^2}\tan(\frac{\pi}{m})(\Delta t)^2\right] \tag{8}$$

$$E_P = M\gamma\left[\frac{2\pi^2(\Delta t)^2}{mr^2 sin(\frac{2\pi}{m})}\right] \tag{9}$$

$$\epsilon_B = \left(1 - \frac{m}{\pi}\sin(\frac{\pi}{m})\right) + \frac{m}{2\pi r^2}\tan(\frac{\pi}{m})(\Delta t) \tag{10}$$

$$\epsilon_P = \frac{\pi\Delta t}{mr^2\sin(\frac{2\pi}{m})}. \tag{11}$$

The absolute error in the Brakke method has a leading order term proportional to Δt for all m; the relative error has a leading order term entirely independent of the time-step Δt! On the other hand, in the proposed method, the leading order term in the absolute and relative errors are $(\Delta t)^2$ and Δt, respectively.

To show the impact of these differences, we inserted the values of r and Δt, taken from a simulation in which the number of grains decreased from 25,000 to 20,000, into Eqs. (10) and (11) for the relative errors of the two methods and tabulate the results in Table I for several levels of discretization m. Clearly, the relative error in the proposed method is several orders of magnitude smaller than in the Brakke method.

m	ϵ_B	ϵ_P
3	17.31%	0.00919%
4	9.97%	0.00597%
5	6.46%	0.00502%
6	4.51%	0.00459%
7	3.33%	0.00436%
8	2.55%	0.00422%
9	2.02%	0.00413%
10	1.64%	0.00406%
11	1.36%	0.00401%
12	1.14%	0.00398%

TABLE I. Relative errors ϵ in the area change of a grain discretized into m pieces using the Brakke method and that proposed here; the radius is $r = 0.003989L$ and the time step size is $\Delta t = 1.21 \times 10^{-9} M\gamma L^2$.

Similar results can be obtained for grains with different numbers of neighbors. These calculations show that for both vertex and non-vertex nodes, the Brakke scheme produces an absolute error that is, to leading order, proportional to Δt, while in the proposed method the absolute error is proportional to $(\Delta t)^2$. In the Brakke method, reducing the time-step by a factor of 100 reduces the absolute error by a factor of 100, while in the proposed method, it reduced the error by a factor of 10,000.

[1] We used the `area normalization` and `effective area` options in Surface Evolver. These options are meant to approximate motion by mean curvature. With these options, resistance to motion of a node is proportional to the component of the area associated with that node which is also perpendicular to the force on the node. See [17] for more details.

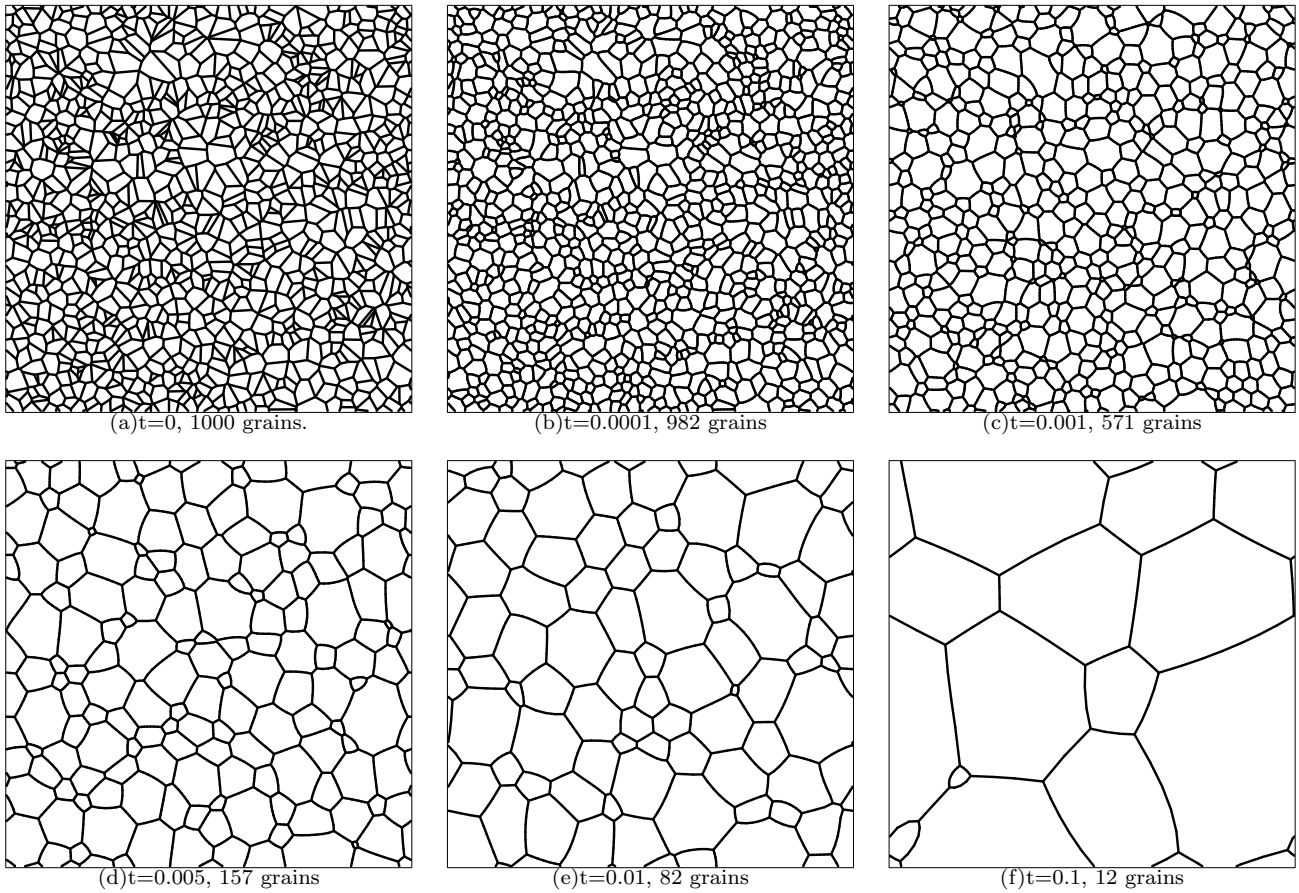


FIG. 7. Temporal evolution of a microstructure based upon the proposed method for $M\gamma L^2 = 1$. This microstructure was initialized as a Voronoi tessellation of the unit square into 1000 grains.

Examination of Eqs. (8)-(11) shows that both methods lead to identical errors in the very fine mesh limit (i.e., the number of sides m tends to infinity).

MICROSTRUCTURE EVOLUTION

The evolution of a typical microstructure using the proposed method is shown in Fig. 7; the microstructure began as a Voronoi tessellation of the space based upon 1000 randomly distributed points. The initial microstructure has grains with straight edges and triple-junctions where three boundaries do not generally meet at $2\pi/3$. However, after a short time, the triple-junction angles become very close to $2\pi/3$ and many of the boundaries are curved. The structure coarsens over time resulting in fewer grains and a larger average grain size. Figure 8 shows a comparison of two microstructures, starting from the same Voronoi initial condition state, where one has been evolved using the method developed by Brakke and the other has been evolved using the method proposed here. While the microstructures appear similar, a grain-by-grain comparison shows that they are microscopically quite different. This does not prove that one method is correct and the other erroneous since small numerical differences between the two methods can lead to differences in the microstructures that increase over

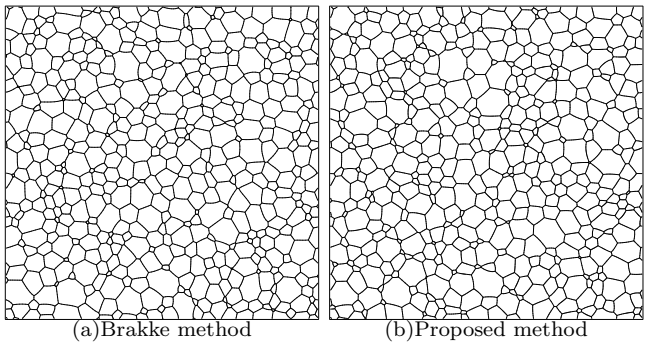


FIG. 8. Microstructures evolved from a single Voronoi tessellation of 1000 grains after half of the grains have been consumed, using (a) the Brakke method and (b) the proposed method.

time. In the following sections, we will offer more quantitative descriptions of these systems that highlight the differences between the two evolution methods.

GRAIN SIZE EVOLUTION

While the microstructure generated using the Brakke method and that generated using the method proposed here appear similar, the comparison presented above is not quantitative. In this section we look at how the average grain size changes over time using these two approaches. To this end, we simulate the evolution of four different microstructures using the two approaches, each initialized by Voronoi tessellations based on random distributions of 25,000 points. For each method we considered two cases: a refined system, where each grain boundary is described by approximately 5 line segments (i.e., placing 4 nodes between each triple-junction) and an unrefined system, where nodes are placed only at the triple-junctions. We evolved these system until 1000 grains remained.

Figure 9 shows the change of the average grain area over time, averaged over four runs, for each of the four cases described above: Brakke method-refined, Brakke method-unrefined, proposed method-refined, and proposed method-unrefined. In all four cases, the average

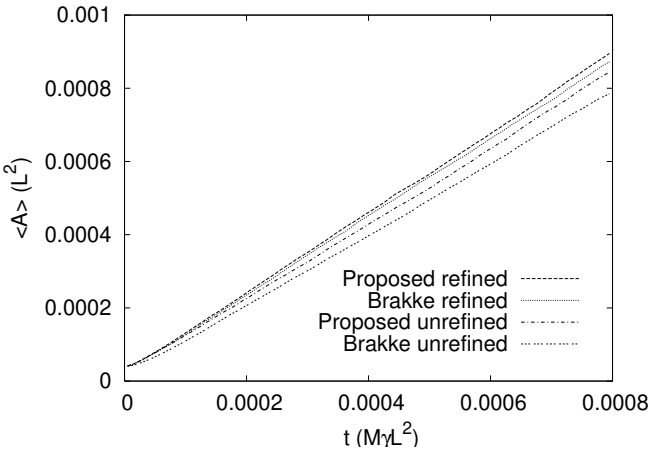


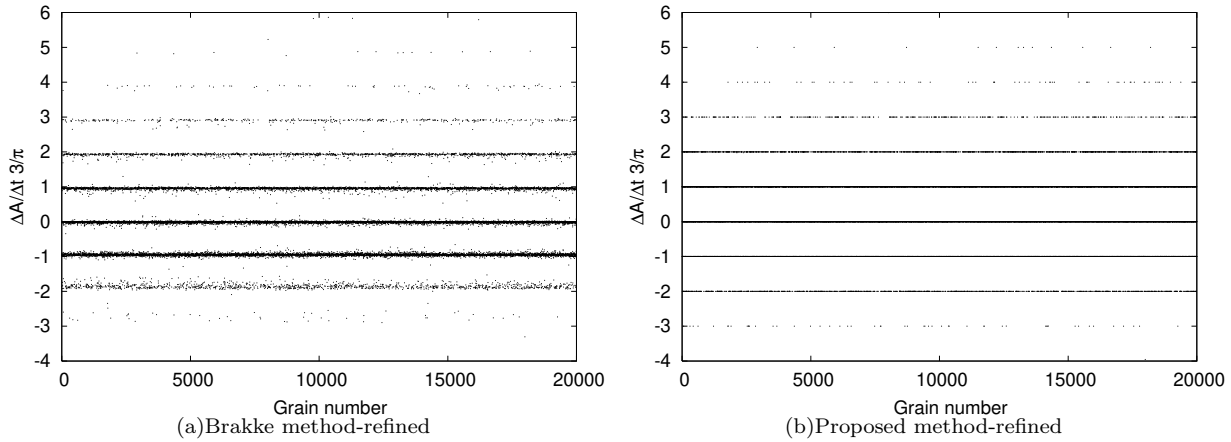
FIG. 9. The temporal evolution of the average grain area $\langle A \rangle$ for the four cases described above; four samples were run for each case and the averages are plotted. Each system began with 25,000 grains; when $t = 0.0008$, there remain slightly more than 1000 grains. The typical error is about two or three times the size of the dots; the errors are not shown for the sake of clarity.

grain size appears to grow linearly with time, albeit at slightly different rates. These rates are very similar with the exception of the Brakke method-unrefined. This discrepancy should not be surprising since the unrefined discretization implies that the triple-junction angles are not fixed at $2\pi/3$, a condition necessary for the Brakke method to accurately describe the evolution. The proposed method implemented with the unrefined discretization yields results consistent with the refined simulation because deviations from the triple-junction angle are accounted for within this method. For the refined cases shown in Fig. 9, the slopes of the curves are 1.067 and 1.092 for the Brakke and proposed simulations, respectively. While these slopes are close to unity, we know of no rigorous analytical results that predict them; both are close to the 1.12 ± 0.04 reported in Ref. [18]. See also Ref. [19] which obtains slopes ranging from 0.5 to 20 using various simulations methods.

While these results show the evolution behavior of entire systems, the exact von Neumann-Mullins relation (Eq. (1)) describes how each individual grain evolves; i.e., at a constant rate that depends only on its number of sides. Figure 10 shows the area growth rates at a single time step for each of the 20,000 grains in a system that was evolved from a 25,000 grain Voronoi microstructure using the Brakke and proposed methods together with a refined discretization. When $M\gamma = 1$, these figures should show sharp, horizontal lines at integer values of $\frac{3\Delta A}{\pi \Delta t}$, where each line corresponds to a different number of grain neighbors n. Figure 10(b) is an excellent description of the results for the proposed method. However, there is discernible scatter in the data for the Brakke method results, Fig. 10(a). Furthermore, the average values of $\frac{3\Delta A}{\pi \Delta t}$ differ slightly from the von Neumann-Mullins prediction that these should all be integers.

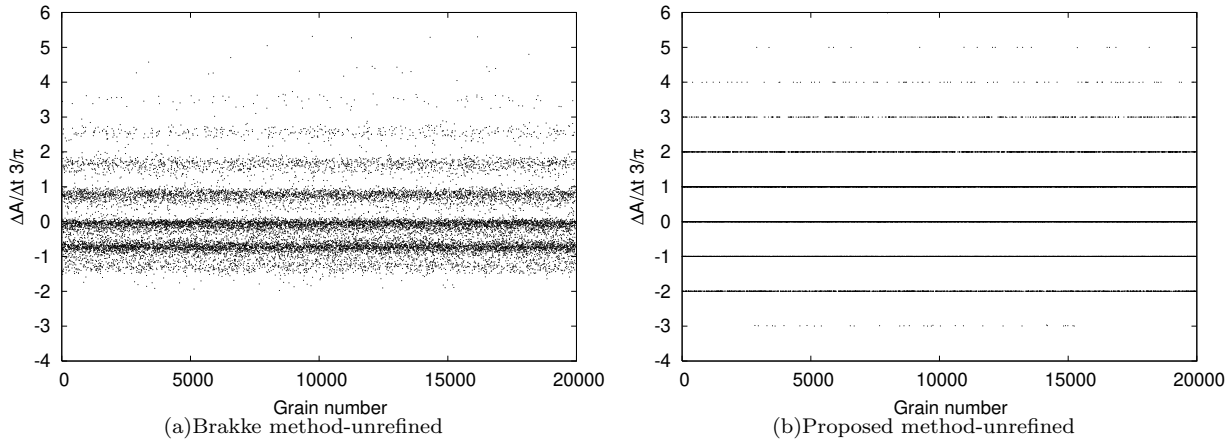
Figure 11 shows results similar to those shown in Fig. 10, but for the unrefined discretization (i.e., nodes placed only at triple-junctions). The proposed method shows results that accurately match the von Neumann-Mullins relation even in this unrefined discretization. However, the scatter in the results from the Brakke calculations is very much increased compared with that for the refined discretization. Even more problematic is that the mean position of each set of horizontal lines in Fig. 11(a) is in strong disagreement with the prediction of the von Neuman-Mullins exact relation. This again emphasizes the necessity for maintaining a sufficiently refined discretization in the Brakke calculations. The robustness of the proposed method for any discretization is one of its main advantages.

The data in Figs. 11(a) and 11(b) can be summarized in a plot of $\Delta A/\Delta t$ versus n. See Fig. 12 where we collect data from a microstructure beginning with 10,000 grains and evolving until 5000 grains remain, using both refined and unrefined discretizations. The best fit line through each set of data is $\frac{3\Delta A}{\pi t} = 0.99997n - 5.9998$. The errors here, provided by comparing this equation with Eq. (2), are several orders of magnitude smaller than the $1 - 3\%$ errors reported in Refs. [18, 20]. That the results are so accurate even for the unrefined microstructure demonstrates another strength of the proposed method.



(a)Brakke method-refined (b)Proposed method-refined

FIG. 10. Area growth rates $\Delta A_i/\Delta t$ for each grain in a 20,000 grain system for one time step using a refined discretization using (a) the Brakke method and (b) the proposed method. We assign a random number to each grain. In this simulation $M\gamma = 1$.



(a)Brakke method-unrefined (b)Proposed method-unrefined

FIG. 11. Area growth rates $\Delta A_i/\Delta t$ for each grain in a 20,000 grain system for one time step using an unrefined discretization using (a) the Brakke method and (b) the proposed method. We assign a random number to each grain. In this simulation $M\gamma = 1$.

DISTRIBUTIONS

We also examine the topological (number of sides) and area distributions for the different systems. The graphs in Figs. 13 and 14 show these distributions after the systems have evolved from 25,000 grains until only 5000 grains remain. Examination of the topology distributions (see Fig. 13) shows that the Brakke and proposed methods yield nearly identical results when refined, but easily distinguishable distributions when unrefined. In particular, when unrefined, the Brakke method yields more small n and large n grains than does the proposed method. Results very similar to those of the unrefined Brakke method were obtained in Ref. [7] using a vertex model; a refined version of this model [18] produces results more similar to those of the proposed method. Since refining the discretization generally increases the accuracy of a simulation, this suggests that the distribution of the proposed method is indeed the more accurate.

Examination of the grain area distributions (see Fig. 14) shows that the Brakke and proposed methods yield very similar results when refined; the proposed method produces nearly identical results when refined and unrefined, which is not the case for the Brakke method. In particular, the Brakke method, when unrefined, produces too many very small grains.

The observation that simulations that produce too many grains of small areas also produce too many grains

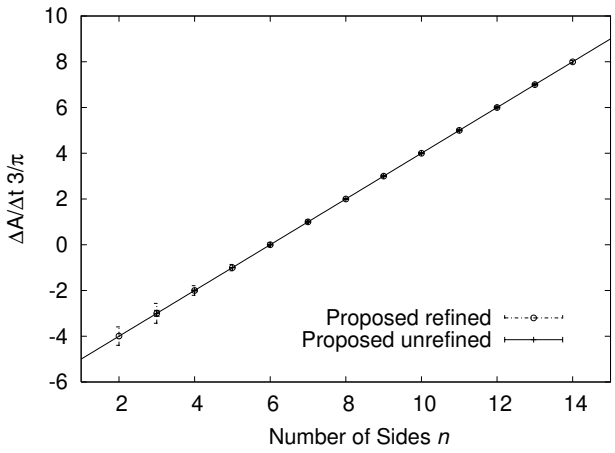


FIG. 12. Validation of the von Neumann-Mullins relation from data obtained using the proposed simulation method with both a refined and an unrefined discretization; $M\gamma$ is set to 1. The von Neumann-Mullins relation predicts that the points will fall on the line shown. The points here represent data averaged over all grains and time steps in simulations that began with 10,000 grains and ended with 5000. The error bars here show the standard deviations magnified by a factor of 100.

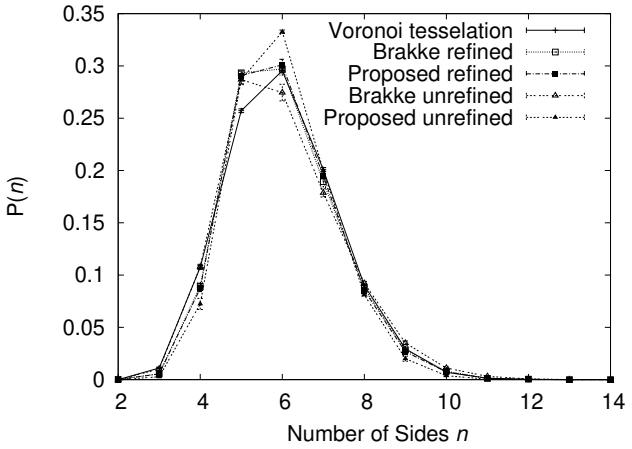


FIG. 13. Topological (number of sides, n) distributions for microstructures evolved from four Voronoi tessellations of 25,000 grains until only a fifth of the grains remain.

of few sides is not surprising in light of Lewis's Law [21], which states that the area of a grain and its number of sides are proportional. The excess of small grains in the Brakke method on an unrefined mesh can be understood by reference to Fig. 11. This figure shows that grains with few sides shrink much too slowly than they should according to the von Neumann-Mullins exact result. We also note that this figure shows that large grains grow too slowly. This is also consistent with the distributions, although this effect is weaker.

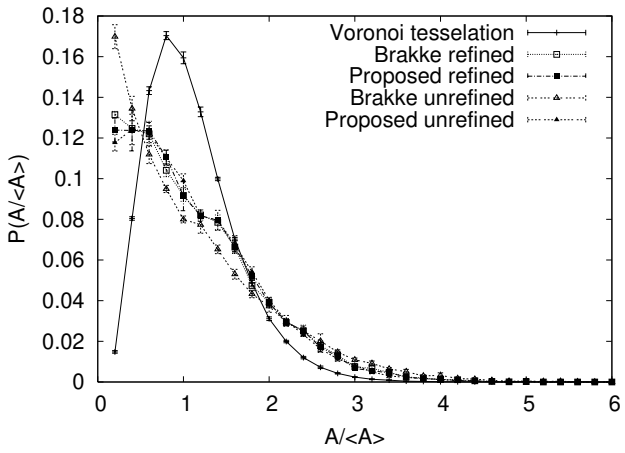


FIG. 14. Normalized grain area distributions ($A/\langle A\rangle$) for microstructures evolved from four Voronoi tessellations of 25,000 grains until only a fifth of the grains remain.

DISCUSSION AND CONCLUSIONS

The von Neumann-Mullins relation in two-dimensions provides an exact expression for the evolution of the size of every grain in a polycrystalline microstructure. We have developed a simulation method for evolving these structures in a manner consistent with this exact relation. Brakke developed the Surface Evolver program that is widely used for simulating grain growth (and other phenomena where capillarity plays an important role). We demonstrate that a new method, presented here, provides better accuracy and efficiency than the Surface Evolver method for simulating normal grain growth. The absolute errors in the Brakke method are linear in the time step, while those for the proposed algorithm are second order in the time step for the same spatial discretization. The most important advantage of the proposed method is that it allows for the maximum coarsening of the spatial discretization with little consequence to the quality of the observed microstructures, the grain size and topology distributions or the grain size kinetics. In order for Surface Evolver to provide a similar level of precision, the discretization must be very fine relative to the grain size. This is necessary to ensure that the triple-junction angles are accurately represented. In the proposed method, errors in the triple-junction angle have little effect on the evolution kinetics because the evolution of each node is always consistent with the exact kinetic relation.

Because accurate simulations in the present method are insensitive to accurate description of the triple-junction angles, it is possible to coarsen the mesh to the extent that the only nodes are those coincident with the triple-junctions. This reduces the simulation from tracking grain boundary segments to tracking triple-junctions. While others have simulated grain boundary evolution based only on tracking of triple-junctions

(so-called vertex models [7, 8]), the proposed method is higher accuracy and is based upon the mathematically exact von Neumann-Mullins relation. Since MacPherson and Srolovitz [22] recently provided an exact extension of this formula to all integer dimensions greater than one [22], it should be possible to extend the present approach to three and higher dimension much more efficiently than trying to track the motion of all grain boundary elements. In three-dimensions, this means tracking triple-junction line segments, rather than grain boundary simplices. The importance of the present efficiency gains should increase in going from two to three and higher dimensions.

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