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A multiple level set method for modeling grain boundary evolution of polycrystalline materials

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Abstract. In this paper, we model grain boundary evolution based on a multiple level set method. Grain boundary migration under a curvature-induced driving force is considered and the level set method is employed to deal with the resulting topological changes of grain structures. The complexity of using a level set method for modeling grain structure evolution is due to its N-phase nature and the associated geometry compatibility constraint. We employ a multiple level set method with a predictor-multicorrectors approach to reduce the gaps in the triple junctions down to the grid resolution level. A ghost cell approach for imposing periodic boundary conditions is introduced without solving a constrained problem with a Lagrange multiplier method or a penalty method. Numerical results for both uniform and random grain structures evolution are presented and the results are compared with the solutions based on a front tracking approach (Chen and Kotta *et al.* 2004b).

Keywords: level set method; multiple level set; grain boundary migration; microstructure evolution.

1. Introduction

Polycrystalline materials are aggregates of many small grains with different crystallographic orientations. Grain boundaries migrate and the microstructures evolve in response to the grain boundary driving forces. Grain boundary migration is one of the dominant processes of microstructure evolution during grain growth and recrystallization in heat treatment (Chadwick and Smith 1976, Gottstein and Shvindlerman 1999, Humphreys and Hatherly 1995). One of the most important driving forces triggering grain boundary migration is the capillary force induced due to the curvatures of the grain boundaries. As the grain boundaries migrate, the corresponding grain structure changes influence the material's mechanical properties, such as strength, toughness, corrosion resistance, electrical conductivity, magnetic susceptibility, etc. For example, it has been observed that the yield strength of a polycrystalline material increases with the decrease of grain size (Chiang 1985). The grain boundaries act as strong obstacles to the dislocation motion as demonstrated in the Hall-Petch relation (Hall 1951, Anderson 1984). The creep behavior such as the Coble diffusion creep (Coble 1963) and the Nabarro-Herring diffusion creep (Herring 1950) are also grain size dependent. Accurate prediction of grain boundary migration processes is essential to

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the understanding of fundamental material properties.

In recent years the evolution processes of grain boundary migration and grain growth have been studied extensively through computer simulations. Direct computer simulations of the grain structure and topological changes can be further classified into probabilistic and deterministic approaches. Probabilistic models include the Potts model (Anderson *et al.* 1984, Sahni *et al.* 1983) and kinetic lattice Monte Carlo methods (Huang *et al.* 1998, Huang and Gilmer 2002). Generally, these are of Monte-Carlo type and have their basis in the classical spin models of statistical physics. In deterministic models a precise description of the motion of the grain boundaries is needed. It is assumed that the grain boundary migration velocity is proportional to the driving force. Front tracking methods (Chen *et al.* 2004b, Frost *et al.* 1990, Kuprat 2000, Rojek and Onate 2008) and phase field models (Fan and Chen 1997, Krill and Chen 2002, Lusk 1999, Warren *et al.* 2000) use this assumption. Front tracking methods adopt an explicit representation of surfaces during the simulation, and phase field and level set methods use an implicit representation of the geometry. In front tracking (also called vertex models), the grain boundaries are discretized and tracked explicitly by piece-wise linear or curved segments. The model which uses straight boundaries is simple to implement but it does not satisfy the equilibrium requirement at the triple junction. The model that uses curved grain boundaries requires some rearrangement or relaxation of microstructure in order to satisfy the equilibrium requirement at triple junctions. When a driving force due to the gradient of the strain energy density in the grain structure is considered, discretization of the grain interior is also required. This yields a significant complexity in the remeshing process due to the evolution of grain boundaries and grain structure topological changes. Chen *et al.* (2001, 2002a, 2002b, 2004a, 2004b) introduced a double grid method, in which the meshfree method is introduced in the discretization and approximation of grain deformation, while a finite element method is employed in discretization and approximation of the grain boundary kinematics. Nevertheless, finite element remeshing on the grain boundary is still required in modeling the topology changes in the grain structures. In general, front tracking methods have difficulties in handling topology changes, such as the merging and breaking of surfaces, and these difficulties are substantially magnified in three dimensions.

Phase field models require that an asymptotic analysis is performed to obtain a mapping between the parameters of the phase field equations and the sharp interface equations. The asymptotics involve expanding the phase field equations in small parameter proportional to the interface width. As a result, the phase field model only reproduces the dynamics of the sharp interface equations in the limit where the expansion parameter is sufficiently small. Also a refined grid is needed to resolve the interface scale (Merriman *et al.* 1994).

The level set method avoids the aforementioned limitations of front tracking methods and phase field models. The level set method was first proposed by Osher and Sethian (1998) for front propagation with curvature dependent speed. Since then, it has been extended to numerous applications with moving interfaces in fluid mechanics, combustion, computer animation, image processing, among others, see (Osher and Fedkiw 2001, 2002). In the level set method the interface is represented as the zero contour of a level set function which satisfies an evolution equation. The physics which governs the motion of the interface motion is included naturally in this model. The front tracking method is a Lagrangian description of the interface motion, whereas the level set approach is an Eulerian description of the interface motion. The numerical solution of the level set function can be solved with a standard Eulerian finite difference or finite element methods. Thus topological changes, such as merging and breaking of the interfaces can be numerically described with ease, and the extension of the method to higher dimensions is straightforward. It has been

shown that for curvature induced boundary motion, the level set method yields the same results as those obtained from the phase field reaction diffusion equation (Roosen and Carter 1998). A superfluous stiffness is required in phase field methods due to a singular perturbation leading to incorrect solutions without the use of adaptive grids (Merriman *et al.* 1994). This is not an issue in the level set method.

The standard level set method is typically applied to problems with two phases. Methods have been proposed to extend the approach to multiple phase problems. An attempt has been made to apply the level set method to triple junctions in grain structures (Merriman *et al.* 1994), where a separate level set function is assigned to each grain, and each grain boundary moves independently according to the given interface speed. Voids and overlaps developed due to independent grain boundary motions are corrected by a reassignment step which modifies each level set function by a coupling function. In Zhao *et al.* (1996), a variational approach with Lagrange multiplier method is employed to couple the multiple level set functions at triple junction through local and/or global constraints. However, this approach encounters computational complexity and stability issues (LBB condition, Babuska 1973). A binary level set method (Chan and Vese 2001) has been proposed to track the evolution of multiple interfaces. For a N-phase problem, $log\ {}^{N}_{2}$ level set functions are used in this method. With proper partitioning of problem domain and with adequate assignment of multiple level set functions associated with the domain partitioning, triple junctions and topological changes can be represented without any voids and overlaps. However, the interface velocity can be incorrect in this approach for the problems we discuss here. A novel projection algorithm based on the particle level set method has been proposed in Losasso *et al.* (2006) to study the multiple liquids (and gases) interacting with each other. This approach allows interactions between liquids or gases with distinct viscosities, densities, and viscoelastic properties. This is achieved by using separate level sets for different regions, and each level set evolves independently. When independent level set evolutions contradict another, a level set "dictionary" is used to translate between the discrepancies in the various level sets. Smith *et al.* (2002) also proposed a more rigorous projection method by introducing a symmetric projection from N level sets to an N-1 dimensional manifold without any corrections.

In this work, the coupled level set method proposed by Merriman *et al.* (1994) is employed. Each grain is assigned an independent level set function, and they are evolved and corrected by the coupled level set approach at the grain boundaries and triple junctions. A multiple-corrector iterative process is introduced for convergence. A local level set method (Peng *et al.* 1999) is also introduced to significantly improve the computational efficiency of this multiple level set approach.

The layout of this paper is as follows. Grain boundary migration mechanisms under curvature-induced driving force are presented in Section 2. The multiple level set method and its localization are both briefly reviewed in Section 3. The coupling of multiple level set functions at triple junctions is discussed in section 4. Section 5 demonstrates the effectiveness of the proposed methods by solving several grain boundary migration problems, and the results are compared with those obtained by the front tracking method. Concluding remarks are given in Section 6.

2. Grain boundary migration mechanisms

Grain boundary migration is the dominant factor that determines the evolution of the microstructures of polycrystalline materials in the process of grain growth and recrystallization.

Consequently, the grain morphology determines their physical, mechanical, and electromagnetic properties of polycrystalline materials. Since grain boundary migration does not involve the nucleation of new grains, it is the growth of the existing grains at the geometry compensation of the other preexisting grains by geometry compatibility in the grain structure (Thompson 2000). As a result, the average size of the grains increases, which is accompanied by a reduction in the total grain boundary energy per unit volume.

2.1 Driving forces for grain boundary migration under consideration

Migration of grain boundaries is the motion of the interface between two grains caused by a wide variety of driving forces. To yield a stable configuration, the grain boundaries evolve to reduce the total free energy, which is accomplished by the reduction of the total grain boundary area. The most important driving force triggering grain boundary migration is the force proportional to the curvature of the grain boundary. The grain boundaries migrate in response to the net driving force acting on the grain boundary.

Let f be the driving force acting on the grain boundary as shown in Fig. 1. A kinetic law that relates the driving force to the migration velocity of the grain boundary is given as,

$$v = \mu f \tag{1}$$

where μ is the grain boundary mobility and is dependent on the temperature T through the relationship

$$\mu = M_0 e^{-\frac{Q}{KT}} \tag{2}$$

where Q is the activation enthalpy associated with the motion, K is the Boltzmann constant, and M_0 has a weak dependence on temperature.

The driving force due to the grain boundary curvature can be expressed as

$$f = -\gamma(\theta)\kappa \tag{3}$$

where γ is the surface tension (the boundary energy per unit area) which is a function of the miss-orientation angle θ, and κ is the curvature of the grain boundary. This driving force acts towards its center of curvature, and this grain boundary migration reduces the surface energy through the reduction of grain boundary length or area.

2.2 Grain boundary migration topology by an explicit description of geometric changes

Grain boundary migration leads to a topological reconstruction of the entire grain structure. Let N denote the number of grains, V denote the number of vertices and E denote the number of grain boundaries as shown in Fig. 1. The grain structure in two-dimensional space obeys the following Euler equation (Smith 1952):

$$N + V - E = 1 \tag{4}$$

The above geometry rule has to be checked as a convergence criterion in a front tracking method. In two-dimensions, a grain structure with more than three grain boundaries intersecting at a point is topologically unstable. Thus a topologically stable grain network will have only 3 grain boundaries

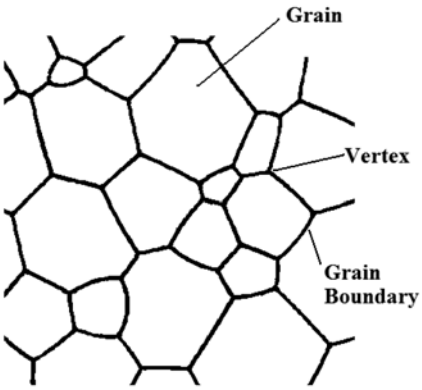


Fig. 1 2-D grain structure

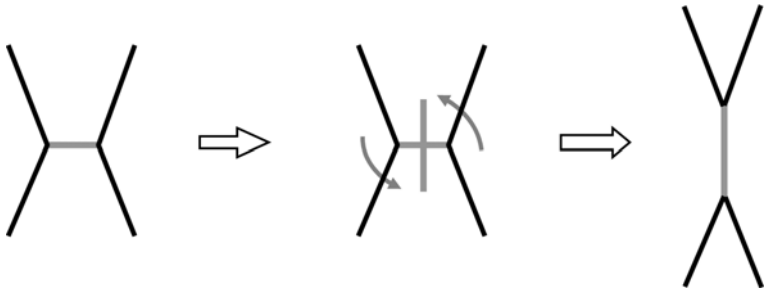


Fig. 2 Topological change of the first kind (T1) in front tracking methods

intersecting at triple junction. For explicit simulation of grain boundary migration processes via a front tracking method, it is necessary to clearly define rules governing the topological reconstruction of the grain structure. Morral and Ashby (1974) identified two types of grain topology transformations, namely the interchange of grain neighbors and the disappearance or appearance of a three sided grain. These changes were denoted as the T1 and T2 changes.

A T1 change involves the switching of the grain boundaries when two triple junctions come very close to each other. This leads to a topological instability in the grain network and results in the formation of a new grain boundary. Two grains lose an edge while two other grains gain an edge, thus maintaining the total number of edges and grains in the grain structure, as shown in Fig. 2. This transformation is called a topological change of the first kind. In numerical simulations using a front tracking method the T1 change is done by rotating the grain boundary by 90^{o} as shown in Fig. 2, with the length of the new grain boundary slightly increased such that the boundary does not undergo a T1 change immediately. This is needed for numerical stability.

A T2 change represents the topological change of a second kind where a three sided grain shrinks to a point, as shown in Fig. 3. After this happens, each neighbor of the three sided grain loses a side and the total number of grains and edges decreases. In front tracking methods this three sided grain is replaced by a triple point at the centroid of the disappearing grain, and the grain boundary connectivity is updated accordingly.

Note that these T1 change and T2 change operations are needed for numerical purposes due to the nature of discretization of grain boundaries in front tracking methods. It will be shown below that

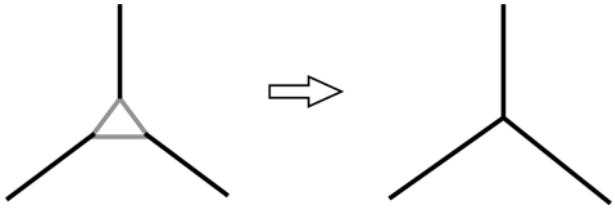


Fig. 3 Topological change of the second kind (T2) in front tracking methods

these intricate operations are eliminated in the level set approach when topology changes are naturally represented by the evolution of multiple level set functions and their interactions.

3. Basic level set equations

The main idea of the level set method is to represent a moving interface $\Gamma(t)$ bounding a open region $\Omega(t)$ in R^n of co-dimension one by a Lipschitz continuous function $\phi(\mathbf{x}, t)$ which has the following properties

$$\begin{cases} \phi(\mathbf{x}, t) > 0 & \text{if } \mathbf{x} \text{ is inside } \Gamma(t) \\ \phi(\mathbf{x}, t) = 0 & \text{if } \mathbf{x} \text{ is at } \Gamma(t) \\ \phi(\mathbf{x}, t) < 0 & \text{if } \mathbf{x} \text{ is outside } \Gamma(t) \end{cases} \tag{5}$$

Since the interface $\Gamma(t)$ is represented as the zero level set of function $\phi(\mathbf{x}, t)$, the motion of $\Gamma(t)$ can be translated into an evolution equation for $\phi(\mathbf{x}, t)$ by taking the time derivative of $\phi(\mathbf{x}, t) = 0$ to yield

$$\phi_t + \mathbf{v} \cdot \nabla \phi = 0 \qquad \text{given } \phi(x, t = 0) \tag{6}$$

where $\mathbf{v}$ is the interface velocity. The initial conditions of $\phi(\mathbf{x}, t)$ are often defined to be the signed distance function to the interface, at least near the interface

$$\phi(\mathbf{x}, 0) = \begin{cases} +dist(\mathbf{x}, \Gamma(0)) & \text{if } \mathbf{x} \text{ is inside } \Gamma(0) \\ 0 & \text{if } \mathbf{x} \text{ is at } \Gamma(0) \\ -dist(\mathbf{x}, \Gamma(0)) & \text{if } \mathbf{x} \text{ is outside } \Gamma(0) \end{cases} \tag{7}$$

By projecting the velocity $\mathbf{v}$ onto the normal direction of the interface, we have

$$\phi_t + v_n |\nabla \phi| = 0 \qquad \text{given } \phi(x, t = 0) \tag{8}$$

where $\nabla \phi = (\phi_x^2 + \phi_y^2)^{1/2}$.

Typically, the interface $\Gamma(t)$ has a prescribed velocity $\mathbf{v}$ which could be a function of space variables $\mathbf{x}$, time t, the normal direction of interface, the curvature of interface, or some external physics which governs the motion of $\Gamma(t)$.

One of the advantages of the level set method is that some geometric quantities can be expressed by using derivates $\phi(\mathbf{x}, t)$. For example, the unit normal $\mathbf{n}$ and curvature κ of $\Gamma(t)$ can be

computed via the level set function $\phi(\mathbf{x}, t)$ as follows:

$$\mathbf{n} = \frac{\nabla\phi}{|\nabla\phi|} \tag{9}$$

$$\kappa = \nabla \cdot \mathbf{n} = \nabla \cdot \left(\frac{\nabla\phi}{|\nabla\phi|}\right) = \frac{\phi_{xx}\phi_y^2 - 2\phi_x\phi_y\phi_{xy} + \phi_{yy}\phi_x^2}{(\phi_x^2 + \phi_y^2)^{3/2}} \tag{10}$$

In this study we consider the curvature induced driving force as the primary driving force of grain boundary migration. The curvature of each grain boundary can be calculated by Eq. (10) (e.g. by finite differences) without the explicit discretization along the grain boundary, which is required in front tracking methods. The level set equation for grain boundary motion induced by curvature is:

$$\frac{\partial\phi}{\partial t} - \mu\gamma\nabla \cdot \left(\frac{\nabla\phi}{|\nabla\phi|}\right)|\nabla\phi| = 0 \tag{11}$$

In this work, a second-order ENO scheme is used for spatial derivative approximation of level set equation(Engquist and Osher 1980). For time derivative approximation, a simple forward Euler discretization is used.

Numerically, it is desirable to keep the level set function close to a signed distance function to the interface. However, it is generally impossible to prevent the level set function from deviating from a signed distance function. Also during time integration of the level set equation, flat or steep regions often occur near the interface, causing numerical errors and inaccurate identification of interfaces. Generally, a reinitialization procedure is needed to reset the level set function to be a signed distance function to the interface. In this work, we use the following reinitialization equation for the correction of ϕ at time t^* (Sussman *et al*. 1994):

$$\frac{\partial\phi^*}{\partial t} = S(\phi_0)(1 - |\nabla\phi^*|) \tag{12}$$

where ϕ_0 is the value of ϕ^* at the beginning of the reinitialization step. The sign function $S(\phi_0)$ is given by

$$\begin{cases} S(\phi_0) = 1 & if\ \phi_0 > 0 \\ S(\phi_0) = 0 & if\ \phi_0 = 0 \\ S(\phi_0) = -1 & if\ \phi_0 < 0 \end{cases} \tag{13}$$

For numerical purposes, a smooth sign function (Sussman *et al*. 1994) is introduced as follows.

$$S(\phi_0) = \begin{cases} -1 & if\ \phi_0 < -\varepsilon \\ \dfrac{\phi_0}{\varepsilon} + \dfrac{1}{\pi}\sin\left(\dfrac{\pi\phi_0}{\varepsilon}\right) & if\ |\phi_0| \le \varepsilon \\ 1 & if\ \phi_0 > \varepsilon \end{cases} \tag{14}$$

where ε is a regularization parameter.

4. Multiple level set method for multiphase problem

In a typical polycrystalline material, each grain has a different grain orientation and it exhibits a multiphase nature, and triple junctions in grain structure topology represent complexity in implicit geometric representation.

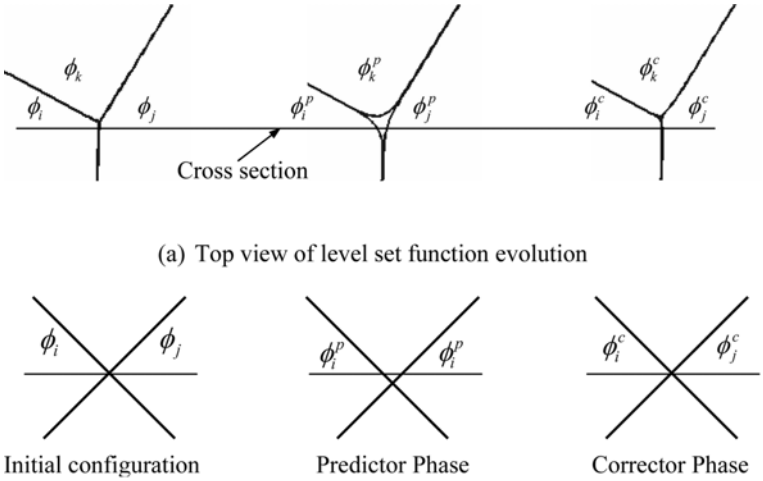


Fig. 4 Coupling of multiple level set functions around a triple junction

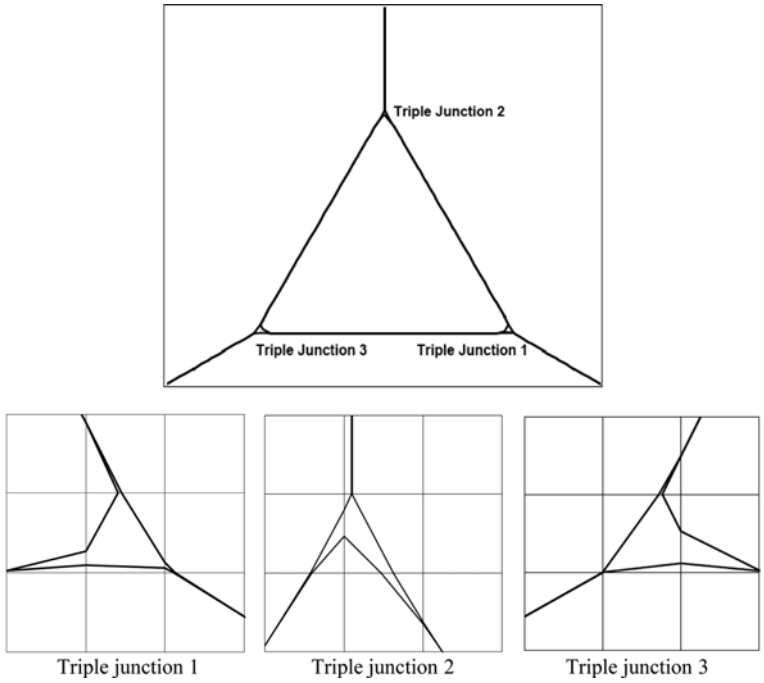


Fig. 5 A grain structure with 3 triple junctions (the background lines represent computational grid)

4.1 Coupling of multiple level set functions

Multiple level set for triple junctions has been proposed (Merriman *et al*. 1994). In this approach, each grain is assigned a level set function ϕ_i, and in the predictor phase each level set function ϕ_i is evolved independently according to Eq. (11) as a predictor ϕ_i^p. In the corrector phase, the level set functions are corrected as

$$\phi_i^c = \frac{1}{2}\left(\phi_i^p - \max_{i \neq j} \phi_j^p\right) \tag{15}$$

where ϕ_i^c is the corrector of ϕ_i^p. This predictor-corrector computational procedure is illustrated by considering a triple junction obtained from the zero level sets of 3 functions, as shown in Fig. 4. In the predictor phase each of the 3 level set functions is evolved independently as shown in Fig. 4 (a). In the corrector phase, each of the level set functions is corrected according to Eq. (15) as shown in Fig. 4 (b).

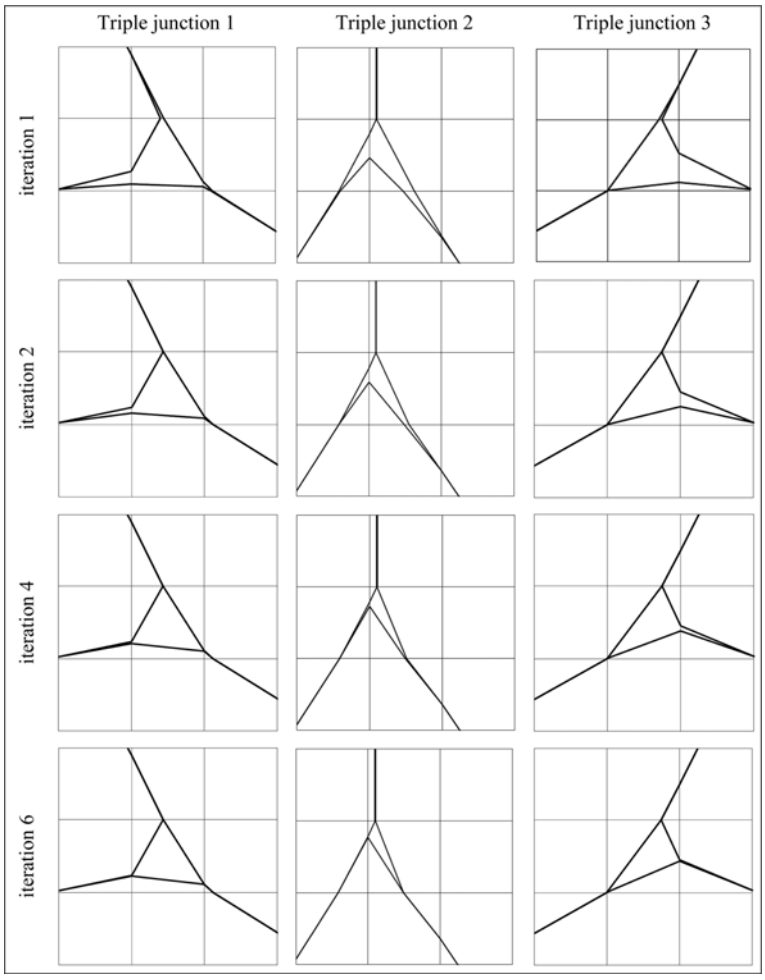


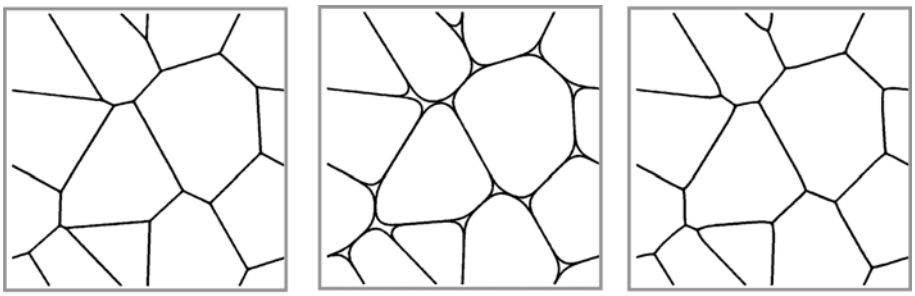
Fig. 6 The evolution of triple junctions under the iteration of predictor-corrector steps (the background lines represent computational grid)

The numerical errors associated with this predictor-corrector approach is shown in Fig. 5 where gaps exist after the corrector phase. These gaps can be reduced down to the grid resolution level by a predictor-multicorrectors iteration as shown in Fig. 6. The predictor-multicorrectors multiple level set approach for a grain network evolution is demonstrated in Fig. 7.

Solving for a level set function only in the region close to the interface reduces the operation from $O(n^2)$ to $O(\delta n)$, where δ is the width of the region surrounding the interface. This is referred to as the local level set method (Peng *et al*. 1999). Since we assign each grain an independent level set function, the standard local level set method can be applied directly.

4.2 Imposition of periodic boundary conditions

For a unit cell microstructure to be representative for the macroscopic structure, periodicity of grain structure and grain boundary migration in the unit cell needs to be considered. The initial grain structure is generated by Voronoi cells with periodic boundary conditions. The periodicity in the initial level set function requires



(a) Initial grain structure (b) Predictor phase (c) Corrector phase

Fig. 7 Coupling of multiple level set functions by a predictor-multicorrectors approach

16	*13*	*14*	*15*	*16*	*13*
4	1	2	3	4	*1*
8	5	6	7	8	*5*
12	9	10	11	12	*9*
16	13	14	15	16	*13*
4	*1*	*2*	*3*	*4*	*1*

Fig. 8 Ghost cells for the calculation of grain boundary curvature along the unit cell boundaries

$$\phi|_{\Gamma^+} = \phi|_{\Gamma^-} \tag{16}$$

where Γ^+ and Γ^- represent the opposite boundaries.

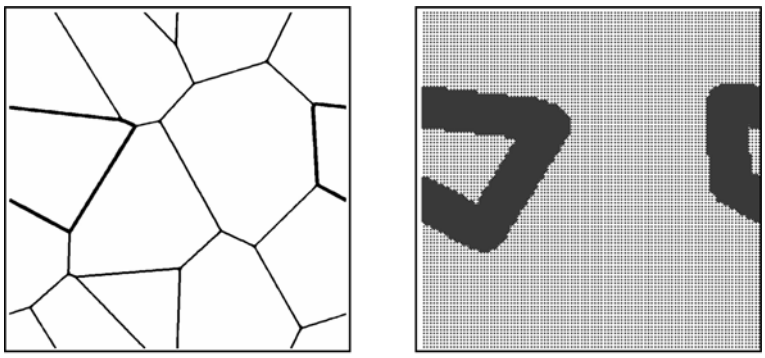
To avoid imposing periodicity as a constraint condition, we consider a layer of ghost cells along the periodic boundaries created by copying the geometry and the signed distance function of the grains on the opposite sides of the unit cell, as shown in Fig. 8. With this ghost cell approach, periodicity can also be imposed in the local calculation. Fig. 9 shows the local level set of the grains near the unit cell boundaries using this ghost cell approach.

5. Numerical examples

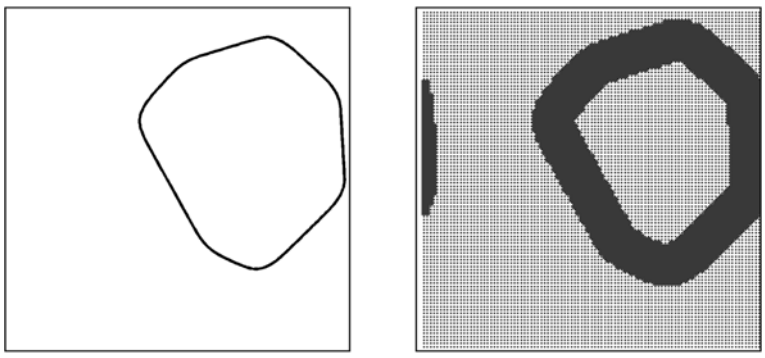
The following material parameters are used in all numerical examples: $\mu = 0.1$ μm^3/μNμs, $\gamma = 0.5$ μN/μm, box size = 1 μm × μm.

5.1 Fundamental topological changes by the multiple level set method

A grid size of 100×100 is employed in all of the following numerical examples. The grain boundary migration of the first grain structure shown in Fig. 10 is modeled by four level set



(a) Periodic local level set of a grain intersects with the domain boundaries



(b) Periodic local level set of a grain near the domain boundaries

Fig. 9 Periodic boundary conditions for construction of local level set

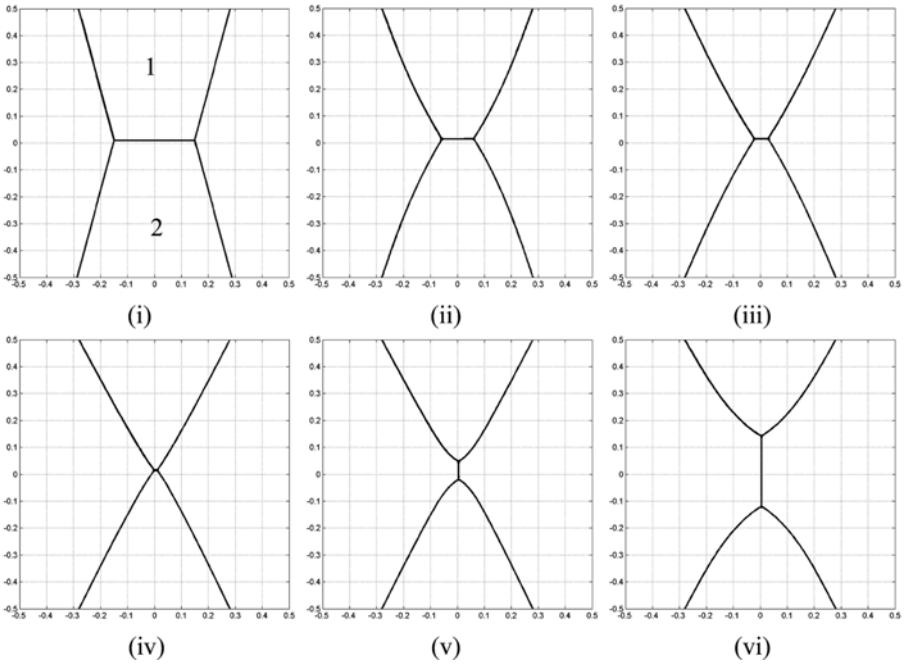


Fig. 10 Topological change of the first kind (T1) by multiple level set method

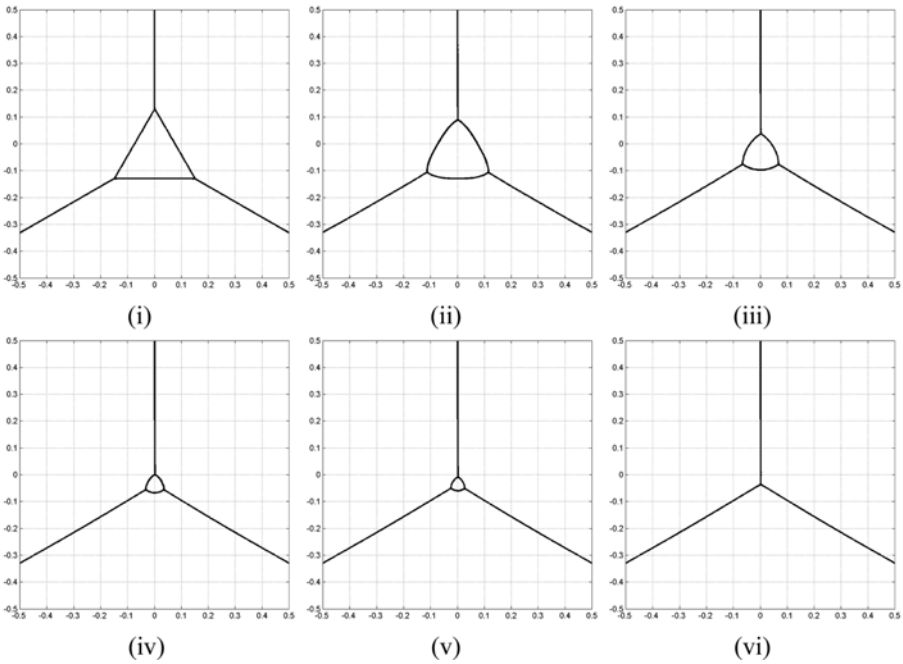


Fig. 11 Topological change of the second kind (T2) by multiple level set method

functions. The grain boundaries migrate until they reach a stable configuration, where the 3 vertices at each triple junction are in a balanced 120^{o} angle. In the second grain structure shown in Fig. 11,

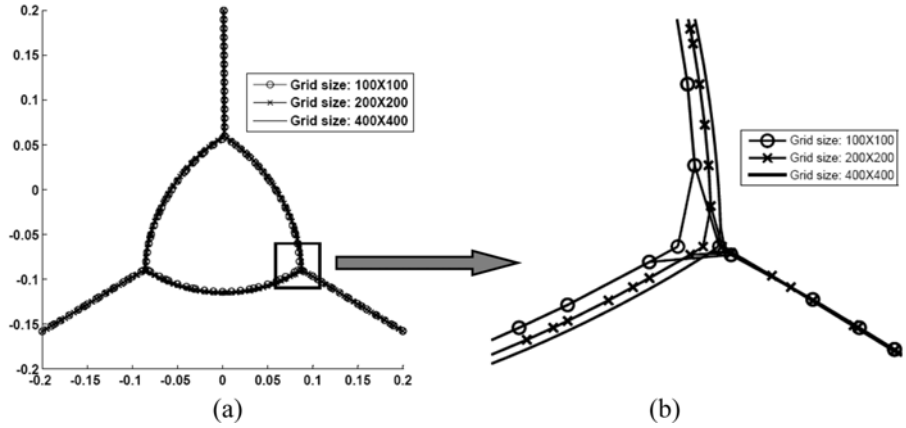


Fig. 12 Convergence study of T2 change by multiple level set method

four level set functions are again employed. According to the initial grain configuration, the resultant driving forces at the three triple junctions act toward the centroid of the center grain. As such, the center grain shrinks to a point, and the vertices at the triple junction are in the balanced 120^o angle. The T1 and T2 topology changes in this example are again naturally represented by the interaction of level set functions. The numerical convergence study using three grid refinements is also investigated for T2 change as shown in Fig. 12. It can be seen clearly that the evolution of grain boundaries converges around a triple junction as shown in Fig. 12(b).

5.2 Grain growth in a uniform grain network with geometric imperfection and a random grain network

In the first case, abnormal grain growth is studied by introducing a geometric imperfection in an otherwise perfect grain structure of uniform hexagonal grains, as shown in Fig. 13(i). The imperfection is created by introducing two eight sided grains, two seven sided grains and six five sided grains in the uniform hexagonal grain structure. The presence of geometrical imperfections in the grain structure triggers the evolution of the grain boundaries. A grid size of 200×200 is employed, and numerical stability requires a time step restriction of $\Delta t\left(\frac{2\mu\gamma}{\Delta x^2}+\frac{2\mu\gamma}{\Delta y^2}\right) < 1$ for a forward Euler time approximation, where Δx and Δy are the grid sizes, μ is the grain boundary mobility, and γ is the surface tension. The progressive evolution of grain boundaries is shown in Fig. 13. The grains with less than six edges generate larger driving forces towards the center of the grains, compared to that of the adjacent grains with more than six edges. Thus the grains with less than six edges continue to shrink while the ones with more than six edges continue to grow. The level set approach effectively model grain boundary migration and topological changes as shown in Fig. 13.

In the second case, the growth of a random grain structure with 100 grains is modeled as shown in Fig. 14. As shown in Fig. 14 (ii), the grains with fewer than six edges in the initial configuration continue to shrink while the ones with more than six edges continue to grow due to the curvature effects. Any front tracking method would require remeshing and adaptivity in response to the grain structure topology changes, consuming considerable computational effort. Note that the curved grain

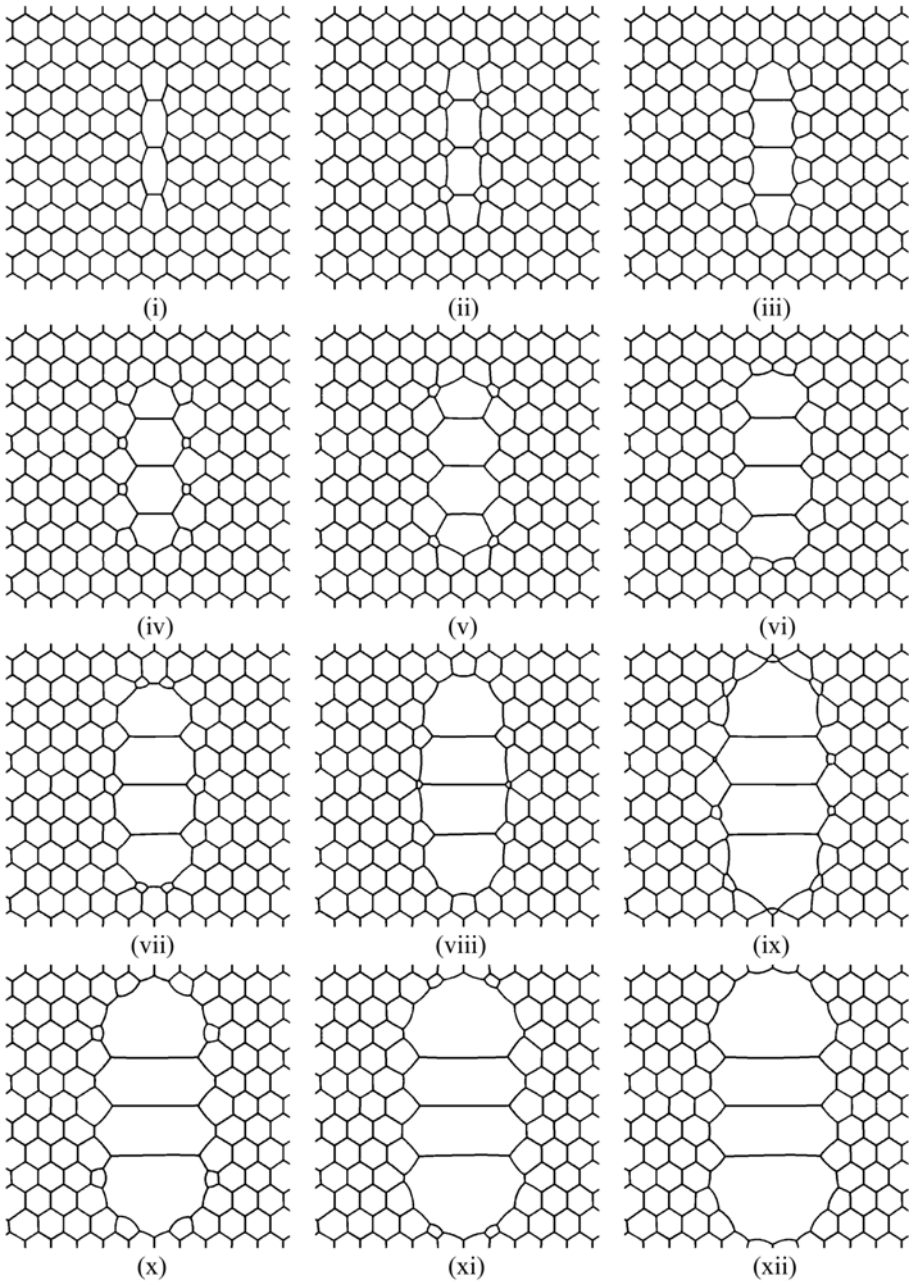


Fig. 13 Evolution of a uniform grain structure with geometric imperfection

boundaries are naturally represented by the level set approach, whereas in a front tracking approach, higher order approximation functions are required for the representation of grain boundary kinematic variables and grain boundary geometries.

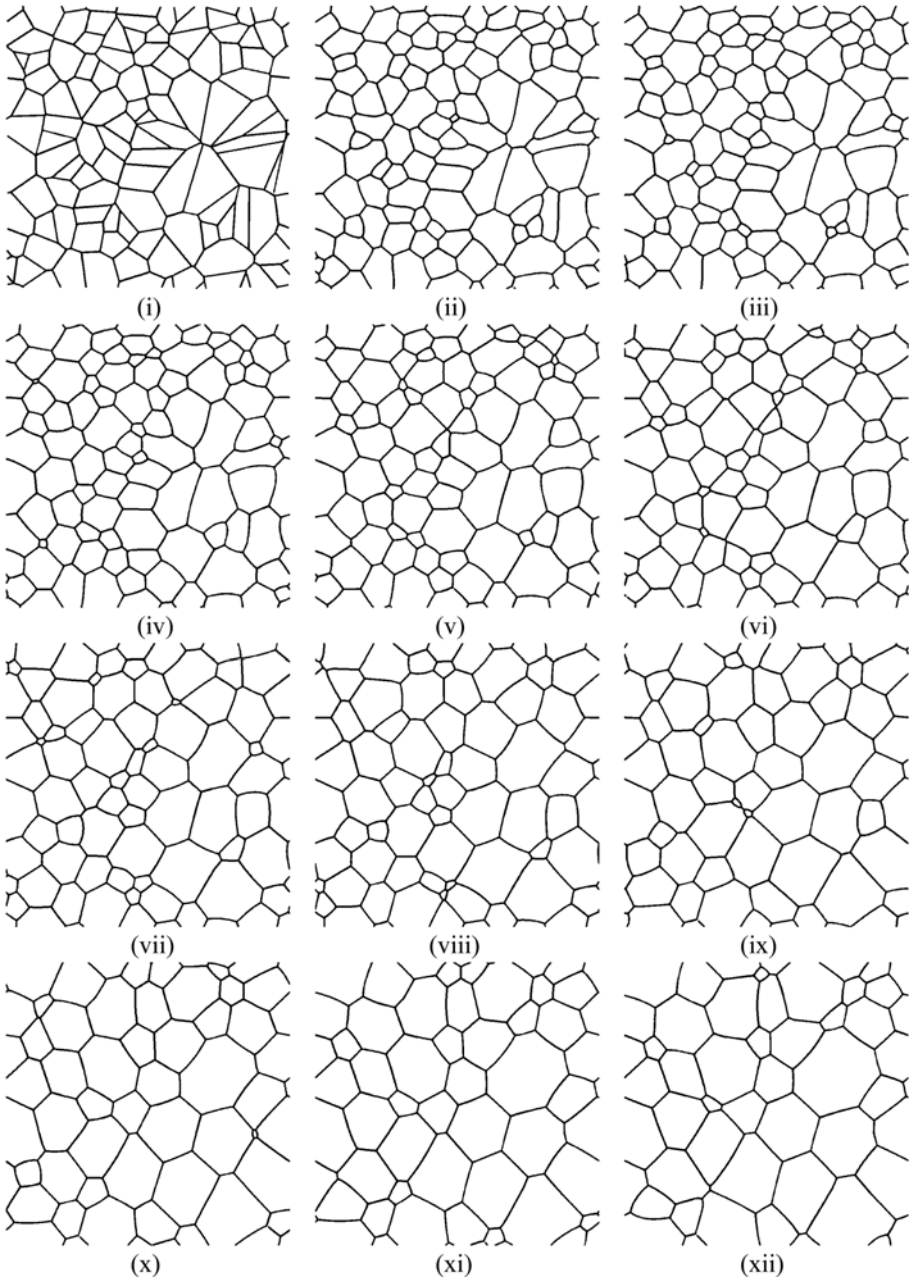


Fig. 14 Evolution of a random grain structure

5.3 Comparison with front tracking method

In this section, we compared simulation results obtained by the proposed multiple level set method and the front tacking method (Chen *et al*. 2002a, Chen *et al*. 2002b). Although similar results are obtained with the two methods in the uniform grain with imperfection, as shown in Fig.

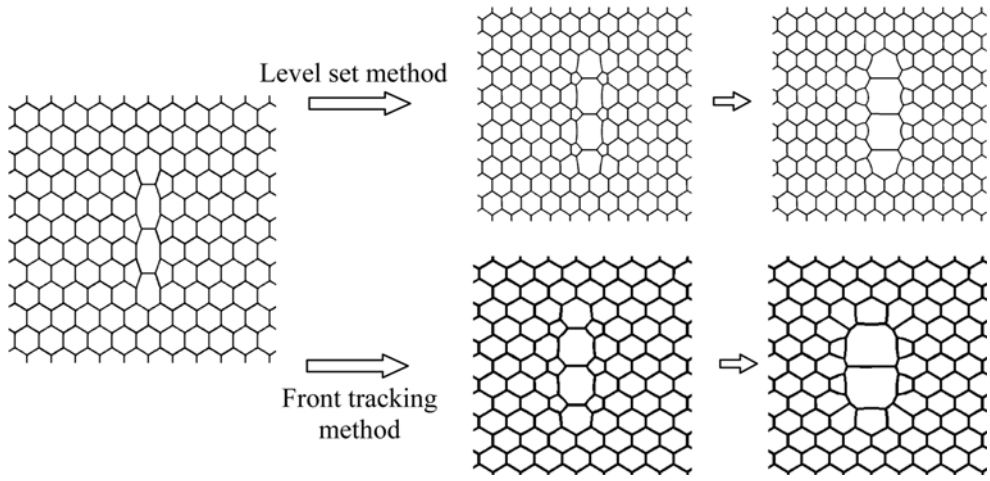


Fig. 15 Uniform grain growth modeled by multiple level set method and front tracking method

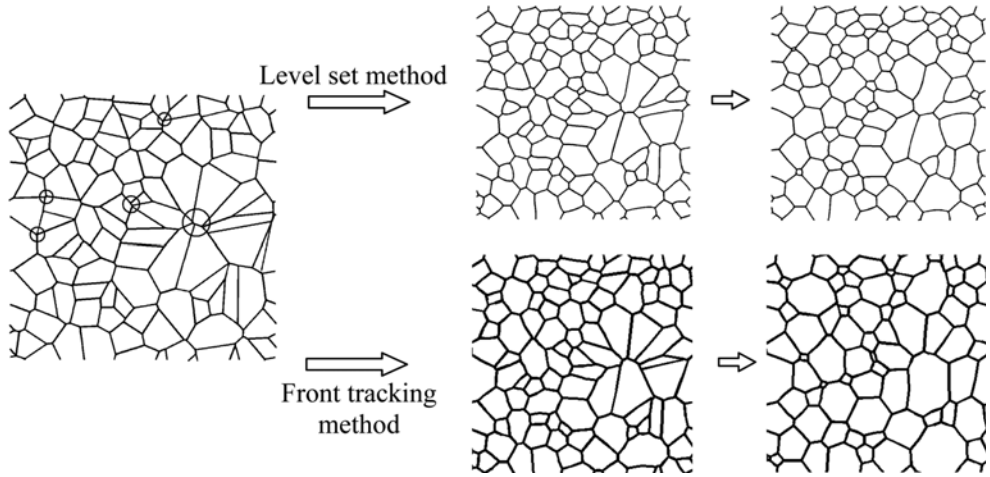


Fig. 16 Random grain growth modeled by multiple level set method and front tracking method

15, some differences can be seen in the random grain structure evolution case as shown in Fig. 16. For a precise comparison of simulation results, the evolution of five triple junctions as shown Fig. 17 are followed closely. In the front tracking method, a couple of T1 changes, one inside the circle domain and two inside the square domain, are triggered as shown in Fig. 18 due to the ad hoc rules of topological changes and the piecewise linear approximation on the grain boundaries. For multiple level set method, the T1 changes in the circle domain in Fig. 17(b) yield the similar configuration as shown in front tracking method. However, a significant difference can be observed in the square domain in Fig. 17(b), where errors due to topological changes ad hoc rules and the piecewise linear approximation are avoided in the level set method. Similar situations can be observed in the regions with circle markers displayed in Fig. 16. In the random grain network case, comparable CPU time of 216 minutes in the multiple level set method is achieved compared to 181 minutes in the front tracking method.

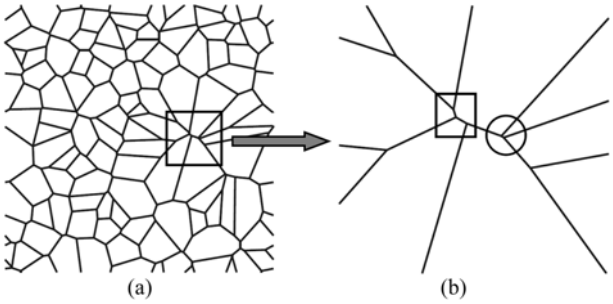


Fig. 17 A local grain structure with five triple junctions

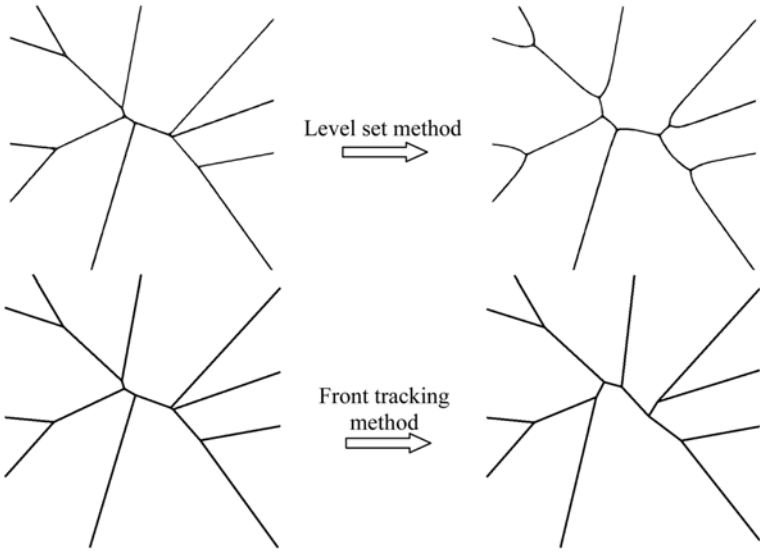


Fig. 18 A local grain structure with T1 changes modeled by multiple level set method and front tracking method

6. Conclusions

In this work, a multiple level set method for modeling grain boundary migration in polycrystalline materials has been presented. A predictor-multicorrectors approach has been introduced in the evolution of level set functions near triple junctions. The numerical results show that this iterative approach reduces the gaps in the triple junctions down to the grid resolution level. For grain boundary migration under curvature induced driving forces, it is shown that the topological changes are properly modeled by the multiple level set method without the need of the ad hoc geometric rules that are required in the front tracking methods. We also show that the curved grain boundaries can be naturally represented with the level set method, whereas higher order approximation functions are required in the approximation of grain kinematics variables and grain boundary geometry using front tracking methods. A ghost cell approach for imposing periodic boundary conditions has been introduced without solving a constrained problem with a Lagrange multiplier

method or a penalty method. In order to improve the computational efficiency, a local level set method has been used. Numerical results for both uniform and random grain structures have been presented, and they compared favorably with the solutions based on front tracking method. It is also demonstrated that the errors induced due to topological changes ad hoc rules and the piecewise linear approximation in the front tracking method are avoided in the level set method. This framework can be easily extended to 3-D grain growth simulation. Additional driving forces, such as the grain boundary migration due to strain energy difference between anisotropic grains, will be included in future work.

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