

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. For computational efficiency a localized level set approach is used to advance each level set function associated with each grain. 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 [10].

Keywords: Level Set; Grain Boundary Migration; Polycrystalline Materials, Moving Interface, Microstructure Evolution,

1. Introduction

Polycrystalline materials are aggregates of many small grains with different crystallographic orientations. Under various driving forces acting the grain boundaries the grain boundaries migrate and the microstructure evolves 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 which occurs during heat treatment of a polycrystalline material [5, 16, 21]. One of the most important driving forces triggering grain boundary migration is due to the curvature of the grain boundary. This is also called the capillary force. As a grain boundary migrates, the corresponding change of grain size influences the material's physical and mechanical properties, such as strength, toughness, corrosion resistance, electrical conductivity, magnetic susceptibility, etc. For example, it has been shown through experiments that the yield strength of a polycrystalline material increases with a decrease of the grain size [12]. In this case, grain boundaries act as strong obstacles, as demonstrated in the Hall-Petch relation [17, 32]. The grain size dependence of creep, such as Coble diffusion creep [13] and Nabarro-Herring diffusion creep [18] are also observed in experiments. Accurate prediction of grain boundary migration processes is essential in the understanding of 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 [1, 34] and kinetic lattice Monte Carlo methods [19, 20]. Generally, these are of Monte-Carlo type and have their basis in the classical spin models of statistical physics. The advantage of a Monte-Carlo method is its simplicity and the ease of implementation in two and three-dimensional systems. However, in this method the origin of the stochastic

aspect is not clear, nor is the relation between the Monte-Carlo time step and the physical time.

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 [10, 15, 23, 33] and phase field models [14, 22, 25, 38] use this assumption. Front tracking methods adopt an explicit representation of surfaces and/or volumes 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 where 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 topological changes. Chen et al. [7, 8, 9, 10, 11, 24,] 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 problems are substantially magnified in three dimensions.

Phase field models require that an asymptotic analysis be 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 some 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 [26].

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 [29] 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 [30, 41]. 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 motion by curvature, the level set method yields the same results as those

obtained from approximation of the phase field reaction diffusion equation [29]. A superfluous stiffness is required in phase field methods due to a singular perturbation and this will lead to incorrect solutions without the use of adaptive grids [26]. This is not an issue in the level set method.

The standard level set method is applied to problems with two phases. Methods have been proposed to extend the method to multiple phase problems. An attempt has been made to apply the level set method to triple junctions in grain structures [26], 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 [39], 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 [42]). A binary level set method [6] has been proposed to track the evolution of multiple interfaces. For a N -phase problem, \log_2^N level set functions are used in this method. With proper partitioning of problem domain and adequately assigning 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.

In this work, the coupled level set method proposed by [26] 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 local level set method [31] 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 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 use of 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 [37]. 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. A kinetic law that relates the driving force to the migration velocity of the grain boundary is given as,

$$v = \mu f \quad (1)$$

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

$$\mu = M_0 e^{-\frac{Q}{KT}} \quad (2)$$

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

$$f = -\gamma(\theta)\kappa \quad (3)$$

where γ is the surface tension (the boundary energy per unit area) which is a function of the mis-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. Here N represents the number of grains, V represents the number of vertices and E represents the number of grain boundaries as shown in Fig. 1. The grain structure in two-dimensional space obeys the following Euler equation [35]:

$$N + V - E = 1 \quad (4)$$

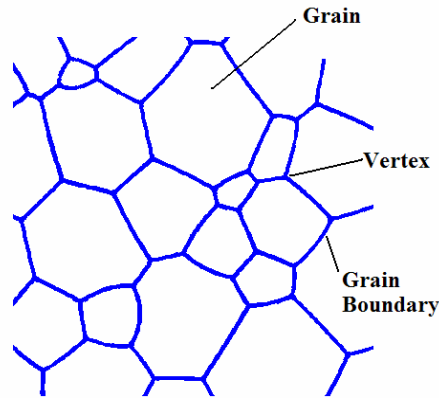


Figure 1. 2-D grain structure

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 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 [27] 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° 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.

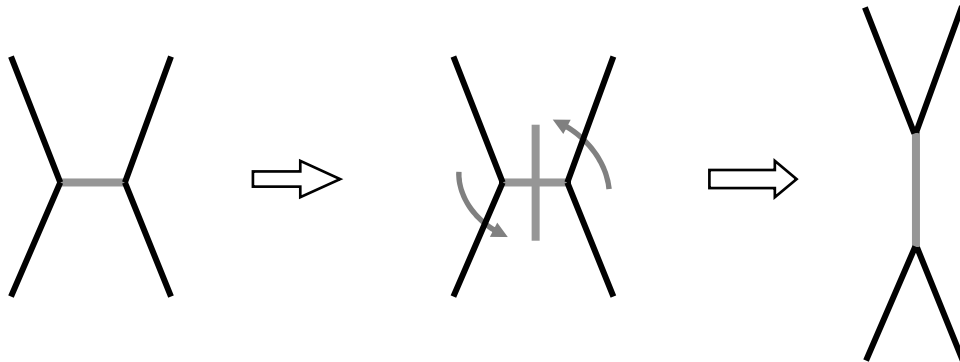


Figure 2. Topological change of the first kind (T1) in front tracking methods

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 are each decreased. 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.

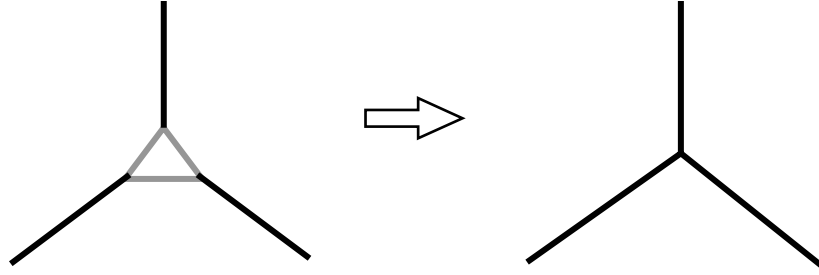


Figure 3. Topological change of the second kind (T2) in front tracking methods

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 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

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

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

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

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.

Ideally,

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

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

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

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 derivatives $\phi(\mathbf{x}, t)$. 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:

$$\mathbf{n} = \frac{\nabla \phi}{|\nabla \phi|} \quad (9)$$

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

In this study we consider the curvature 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:

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

In this work, a second-order ENO scheme is used for spatial derivative approximation of level set equation [43]. 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^* [36]:

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

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

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

From Eq. (12), we can see that ϕ^* remains unchanged at the interface, and the zero level set of ϕ_0 and ϕ^* are the same. Away from the interface ϕ^* will converge to $|\nabla \phi| = 1$ which is the distance function. This algorithm is efficient for numerical implementation and it avoids finding the interface using time consuming geometric procedures.

4. Multiple Level Set Method for Multiphase Problem

The level set method has been used to track the interfaces between materials with two phases. In a typical polycrystalline material, each grain has a different grain orientation and thus we have a multiphase problem where the grain boundaries cannot be described with a single level set function. Moreover, an implicit geometric representation of triple junctions requires special treatment. In this work, the coupled level set method proposed in [26] is employed.

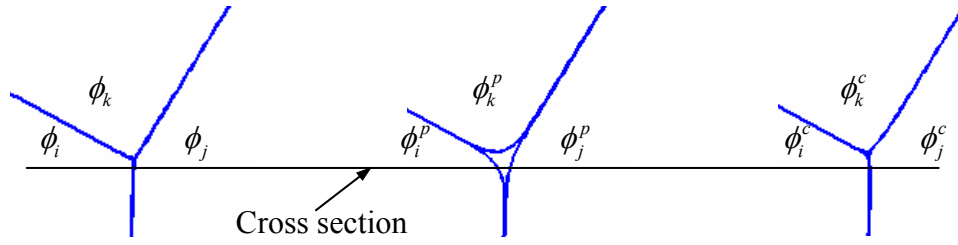
4.1 Coupling of multiple level set functions

As in [26], we assign each grain an independent level set function ϕ_i and first evolve each level set function ϕ_i with Eq. (11) as a predictor ϕ_i^p . Then the coupled level set functions are corrected as

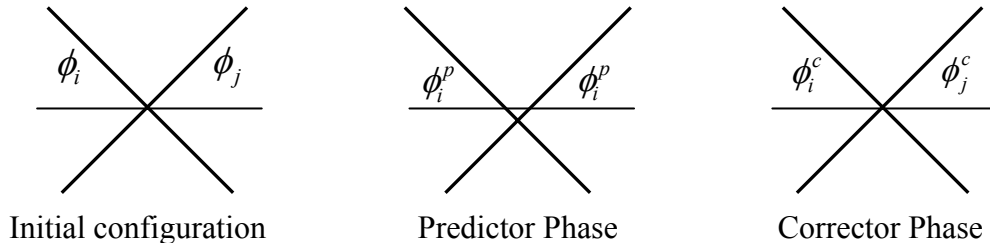
$$\phi_i^c = \frac{1}{2}(\phi_i^p - \max_{i \neq j} \phi_j^p) \quad (14)$$

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 (b). In the corrector phase, each of the level set

functions is corrected according to Eq. (14) as shown in Fig. 4 (c). The predictor-corrector procedures for a multiple grain structure evolution are shown in Fig. 5.



(a) Top view of level set function evolution



(b) Cross sectional view of level set functions evolution

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

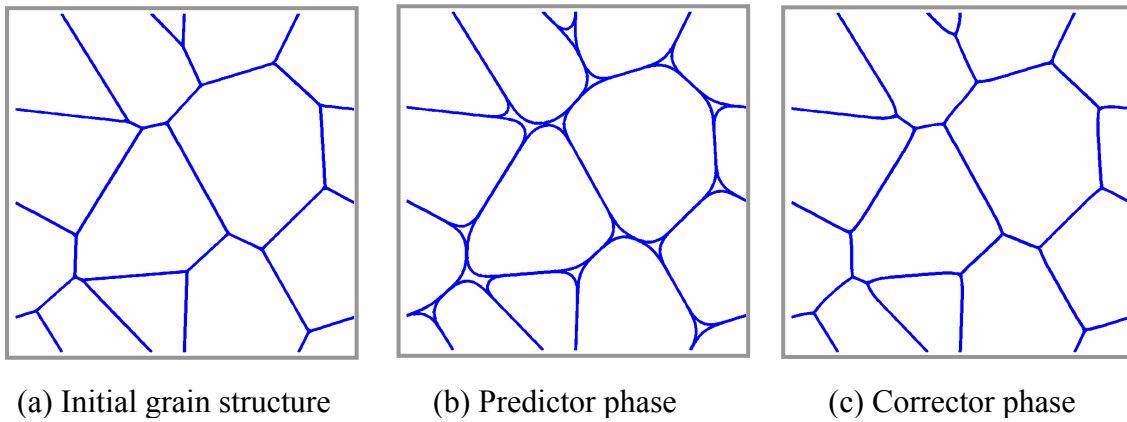


Figure 5. Coupling of multiple level set functions in multiple grain structure

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 [31]. 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

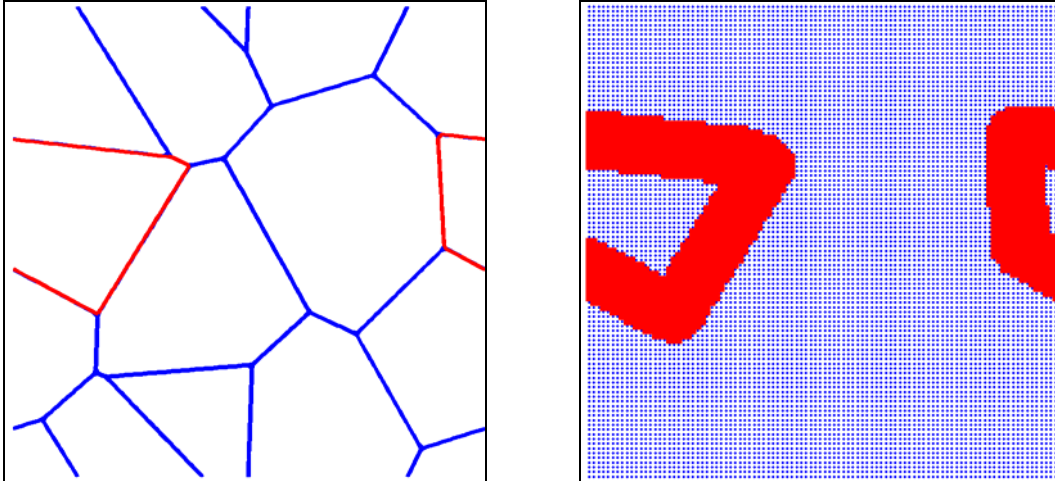
$$\phi|_{\Gamma^+} = \phi|_{\Gamma^-} \quad (15)$$

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

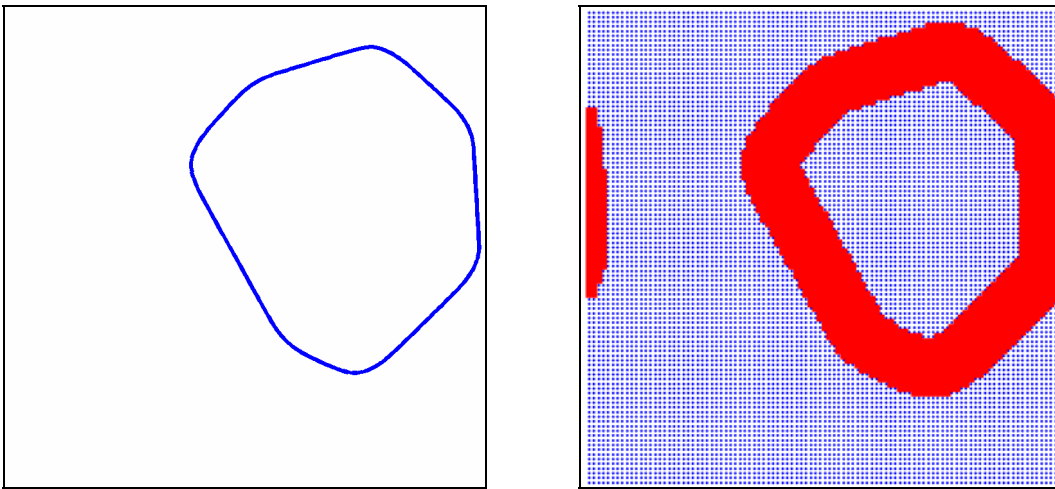
To avoid imposing periodicity as a constraint condition, we consider a layer of ghost cells along the periodic boundaries created by copying the geometry and the signed distance function of the grains on the opposite sides of the unit cell, as shown in Fig. 6. With this ghost cell approach, periodicity can also be imposed in the local calculation. Figure 7 shows the local level set of the grains near the unit cell boundaries using this ghost cell approach.

<i>16</i>	<i>13</i>	<i>14</i>	<i>15</i>	<i>16</i>	<i>13</i>
<i>4</i>	<i>1</i>	<i>2</i>	<i>3</i>	<i>4</i>	<i>1</i>
<i>8</i>	<i>5</i>	<i>6</i>	<i>7</i>	<i>8</i>	<i>5</i>
<i>12</i>	<i>9</i>	<i>10</i>	<i>11</i>	<i>12</i>	<i>9</i>
<i>16</i>	<i>13</i>	<i>14</i>	<i>15</i>	<i>16</i>	<i>13</i>
<i>4</i>	<i>1</i>	<i>2</i>	<i>3</i>	<i>4</i>	<i>1</i>

Figure 6. Ghost cells for the calculation of grain boundary curvature along the unit cell boundaries



(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

Figure 7. Periodic boundary conditions for construction of local level set

5. Numerical examples

5.1 Fundamental topological changes by the multiple level set method

The grain boundary migration of two unstable grain structures using the multiple level set method is examined. 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. 8 is modeled by four level set functions, and each function is only computed and updated by the local level set approach near the grain boundaries associated with the designated grain. In the initial grain configuration, the resultant driving forces at the two triple junctions act toward the centers of grains 1 and 2, forcing the two triple junctions to move toward each other horizontally. As the two triple junctions coincide, the driving force acting on each grain boundary further moves the grain boundaries toward the

centers of grains 1 and 2, forcing triple junctions to separate and move vertically as shown in Fig. 8. The grain boundaries migrate until they reach a stable configuration, where the 3 vertices at each triple junction are in a balanced 120° angle. These topology changes of 4 grains and the resulting triple junction evolution is represented entirely by the interactions of the zeros of evolving level set functions, without imposing any geometric rules. In the second grain structure shown in Fig. 9, 4 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° angle. The T1 and T2 topology changes in this example are again naturally represented by the interaction of level set functions.

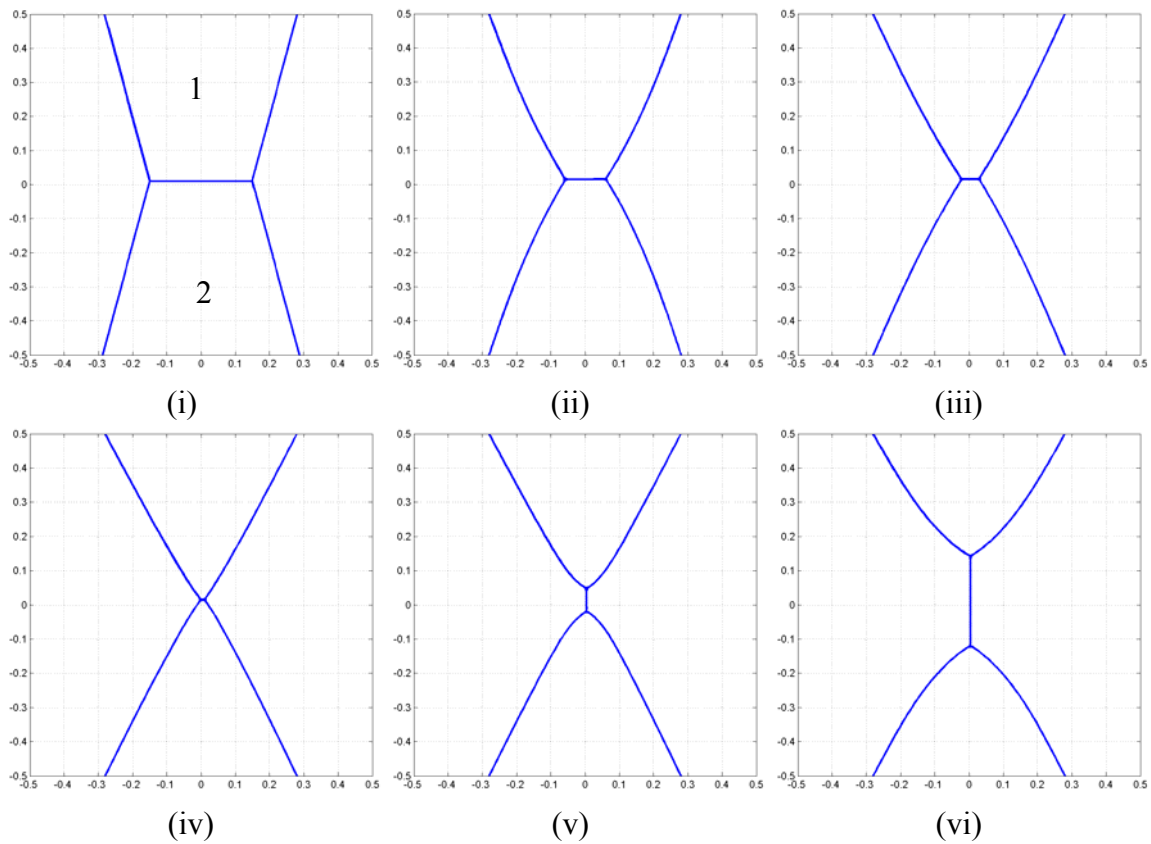


Figure. 8. Topological change of the first kind (T1) by multiple level set method

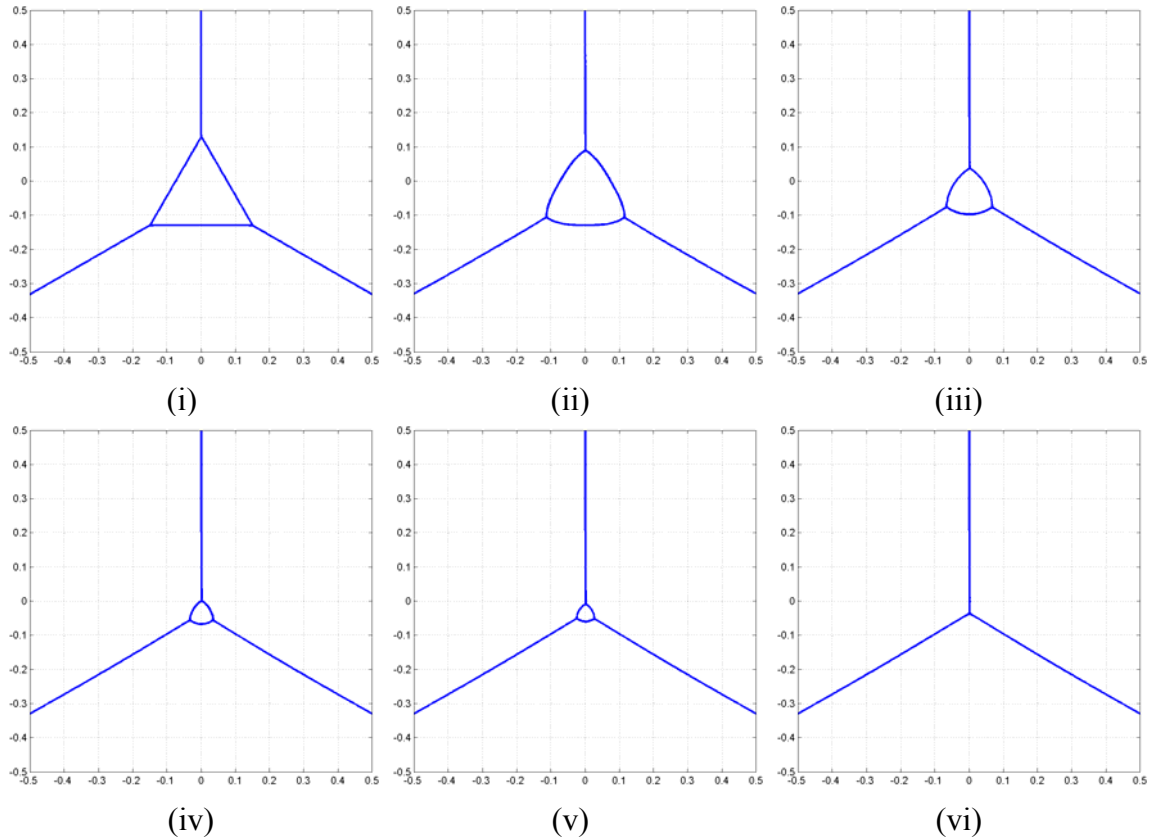


Figure. 9. Topological change of the second kind (T2) by multiple level set method

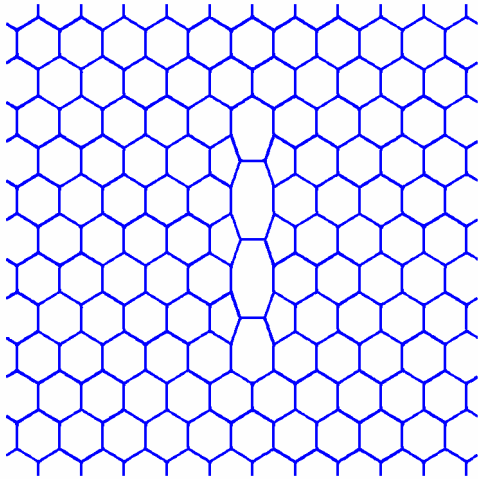
5.2 Uniform grain growth with geometric imperfection

In this example, abnormal grain growth is studied by introducing a geometric imperfection in an otherwise perfect grain structure of uniform hexagonal grains, as shown in Fig. 10(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.

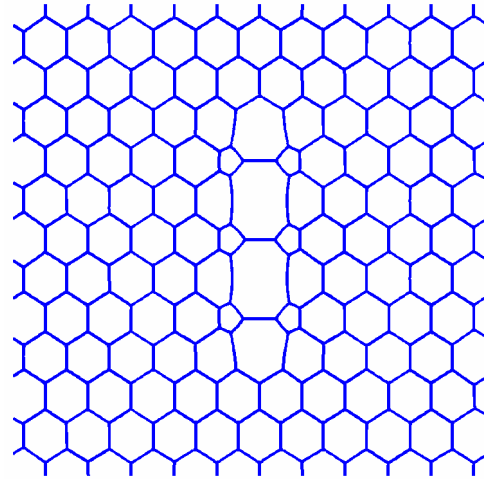
The grains with less than six edges generate larger driving forces towards the center of the grains, compared to that of the adjacent grains with more than six edges. Thus the grains with less than six edges continue to shrink while the ones with more than six edges continue to grow. A grid size of 200×200 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. The

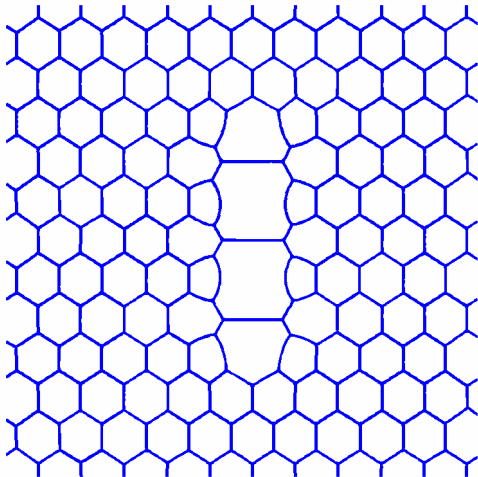
progressive evolution of grain boundaries is shown in Fig. 10. Since the local level set method is employed for each grain, the coupling of multiple level set functions is indeed localized.



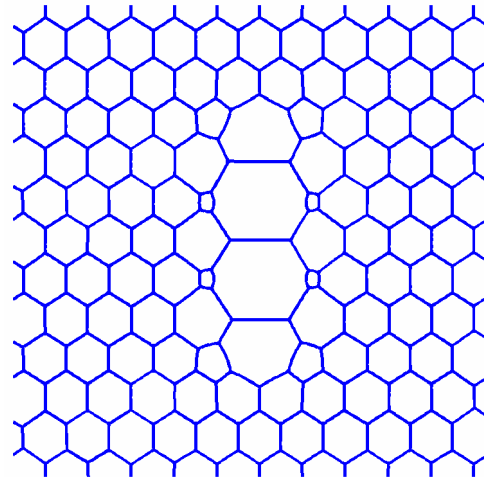
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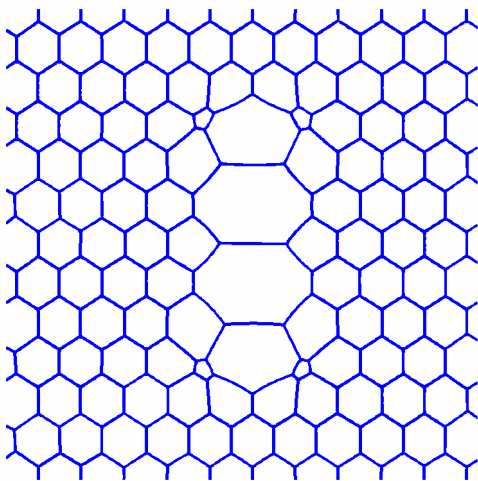
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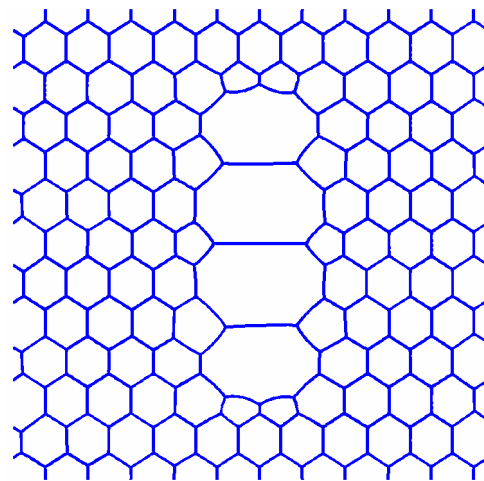
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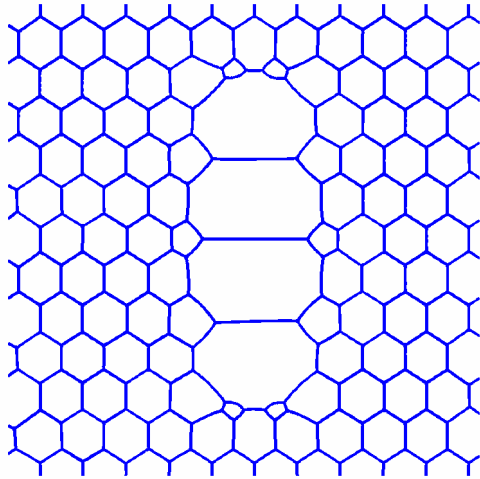
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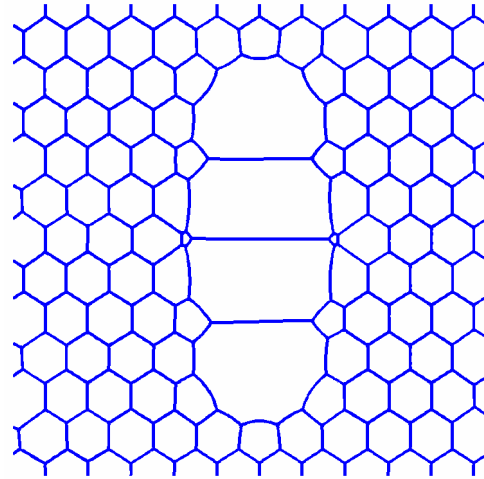
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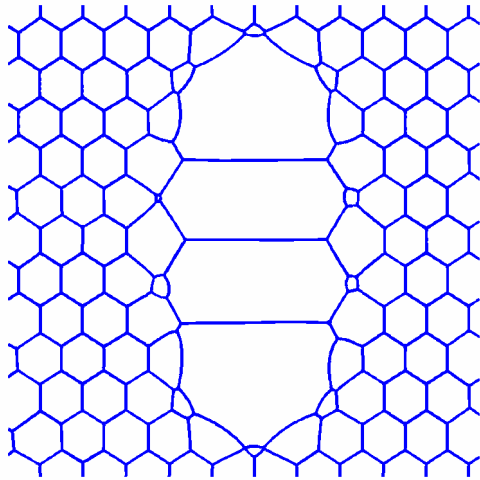
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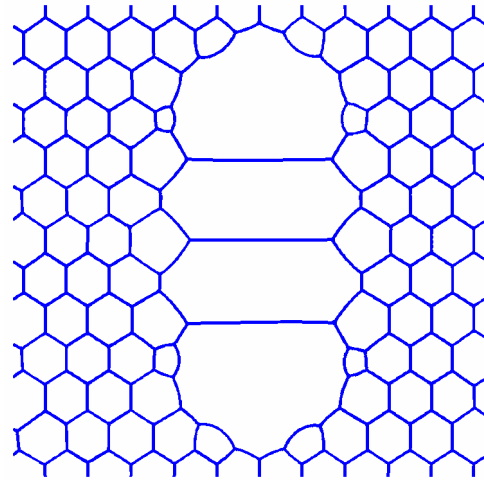
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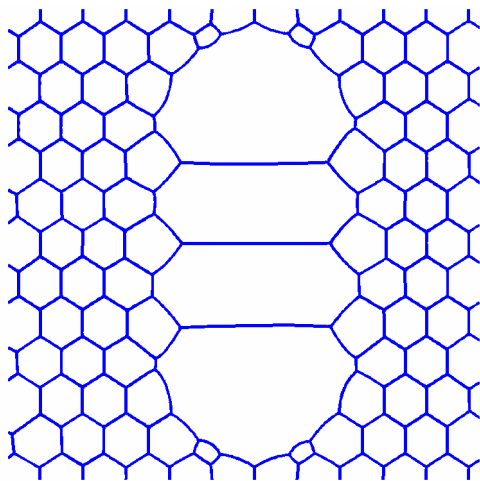
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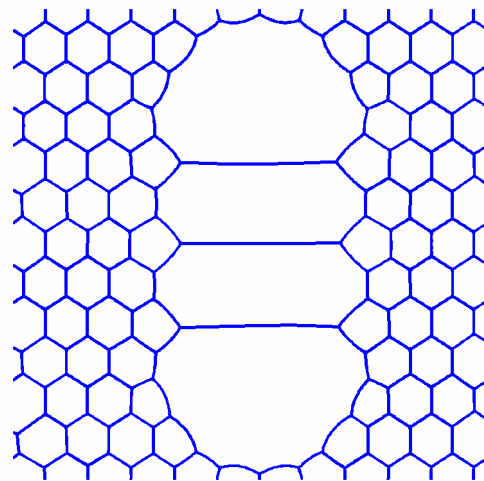
(ix)



(x)



(xi)

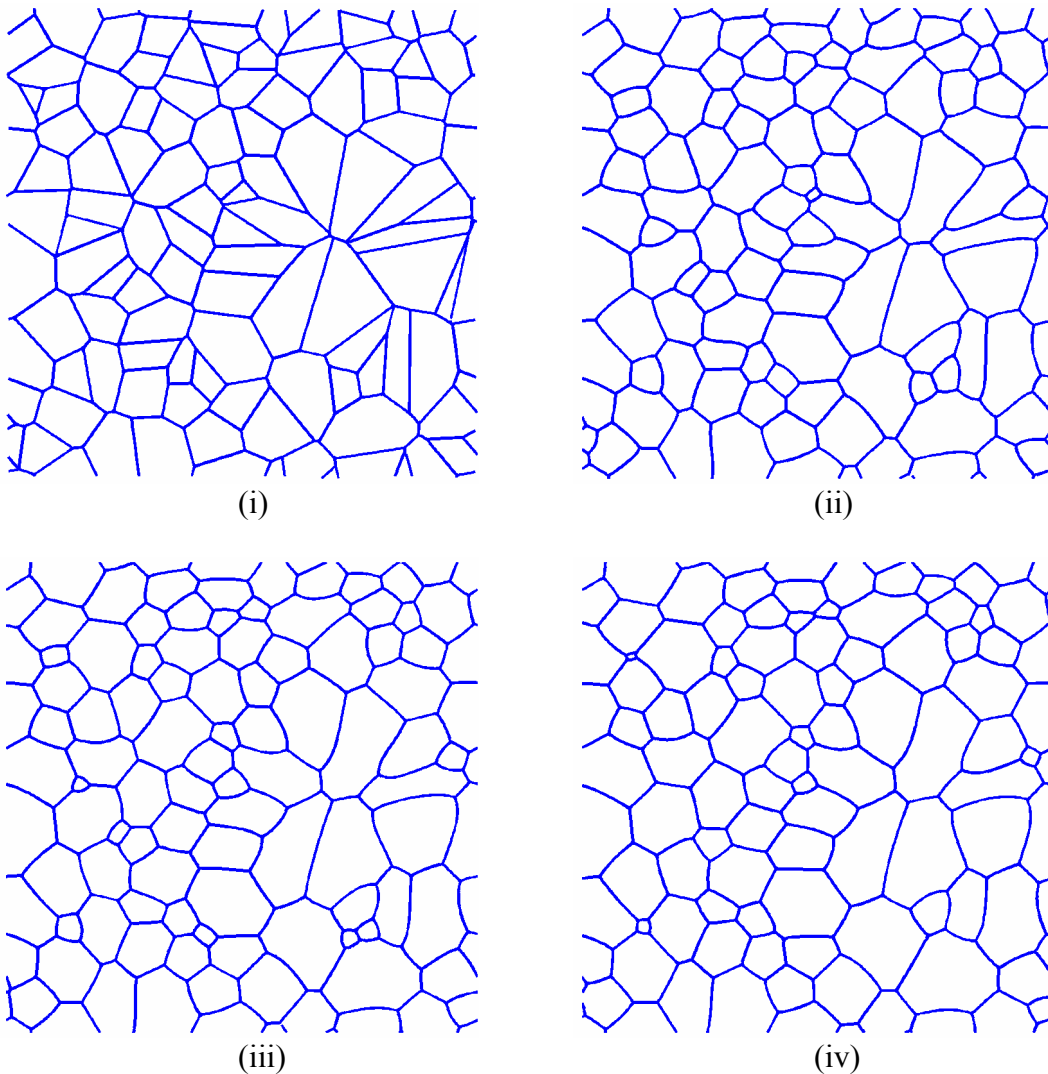


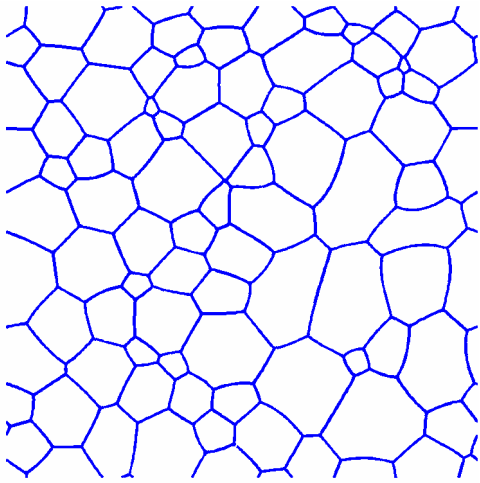
(xii)

Figure. 10. Evolution of a uniform grain structure with geometric imperfection

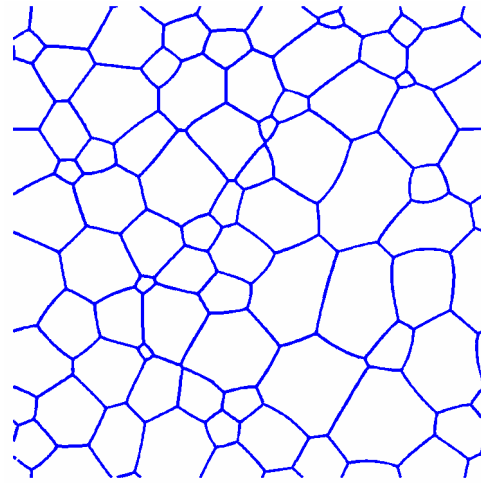
5.3 Random grain growth

The growth of a random grain structure with 100 grains shown in Fig. 11 is modeled. A total of 100 level set functions are assigned with one to each grain. The grid size and time step as of the previous numerical example are again used. As shown in Fig. 11 (ii), the grains with fewer than six edges in the initial configuration shrink quickly while the ones with more than six edges keep growing. As the grain boundaries migrate, the average grain size increases and is accompanied by a reduction of total grain boundary energy. The reduction of total grain number during the evolution process causes the corresponding number of level set functions and the amount of reinitiation processes to be reduced proportionately. 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 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.

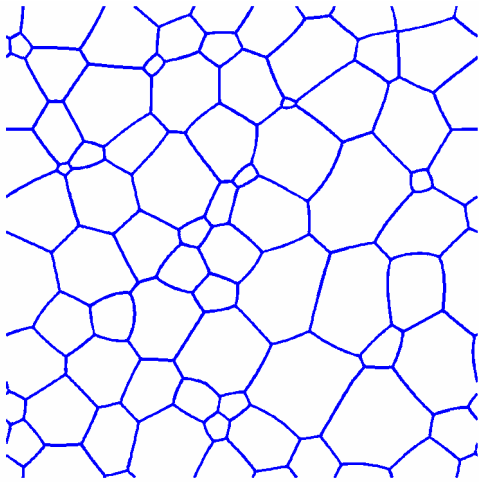




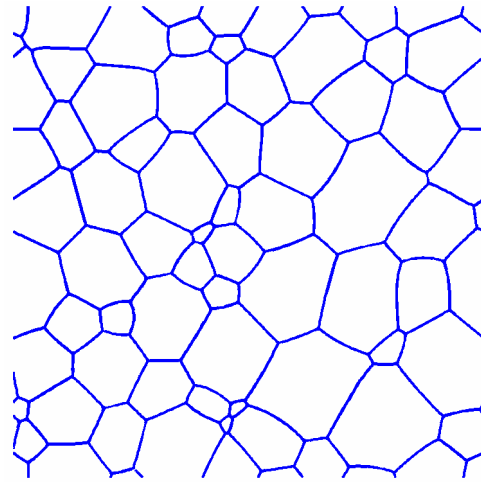
(v)



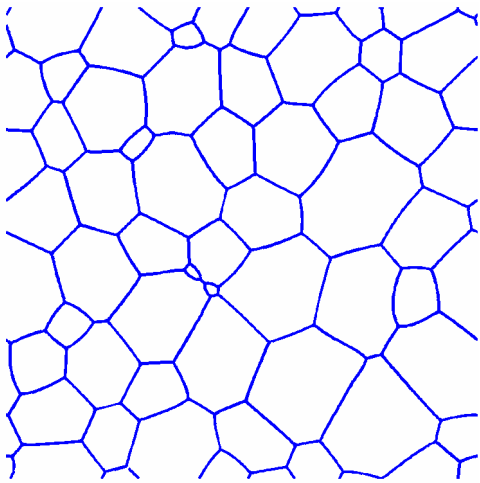
(vi)



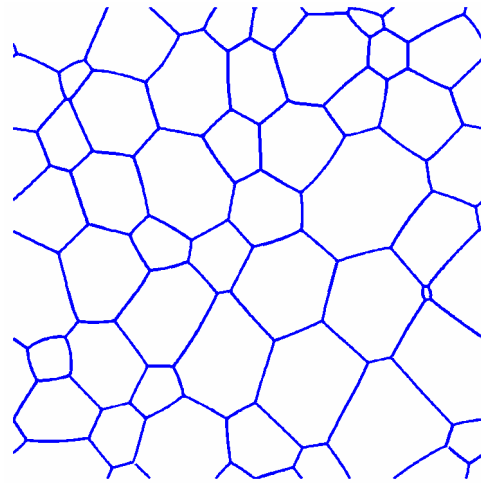
(vii)



(viii)



(ix)



(x)

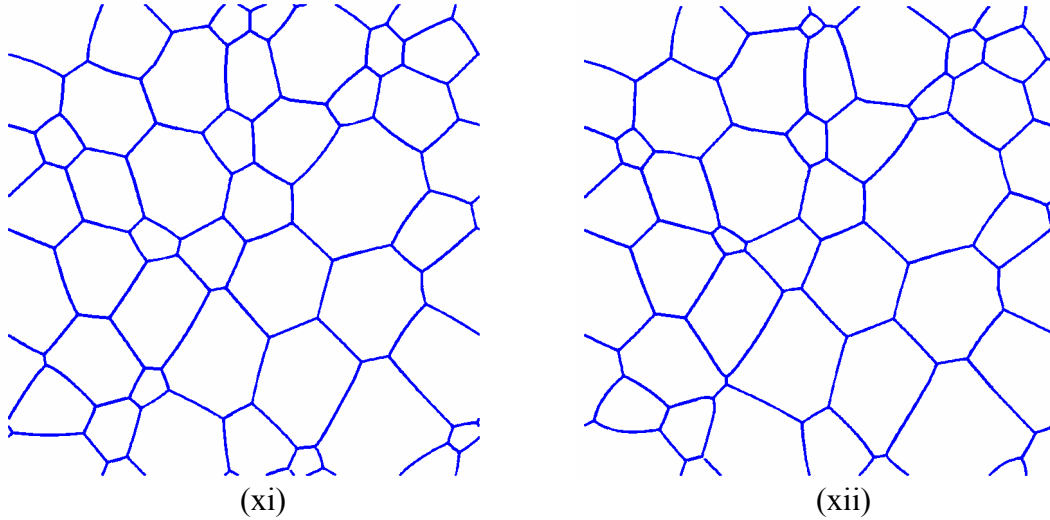


Figure. 11. Evolution of a random grain structure

5.4 Comparison with front tracking method

In this section, we compared our simulation results based on our multiple level set method with that of the front tracking method [7, 8]. Although similar results are obtained with the two methods in the uniform grain with imperfection, as shown in Fig. 12, some differences can be seen in the random grain structure evolution case as shown in Fig. 13. This is due to the errors associated with ad hoc rules of topological changes employed in the front tracking method. As marked with open circles in the initial grain structure of Fig. 13, the triple junctions within those circles are very close to each other in the initial grain structures. Thus, due to the pre-set minimum length of grain boundaries in front tracking method, the T1 changes are invoked prematurely, leading to some errors in the predicted grain structure evolution process. These kind of computational errors are avoided in the proposed multiple level set method.

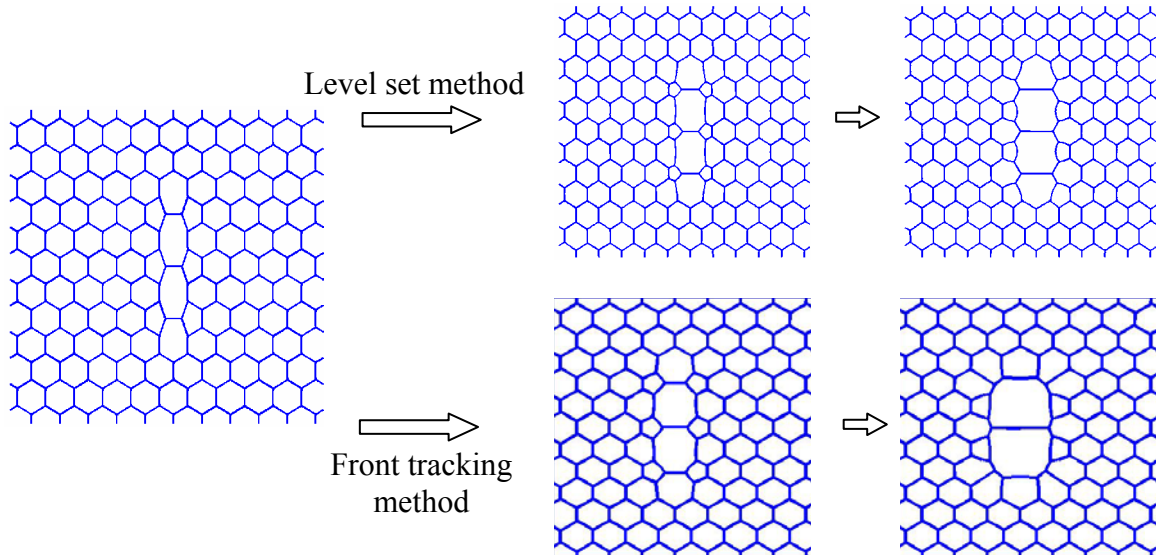


Figure. 12. Uniform grain growth modeled by multiple level set method and front tracking method [7, 8]

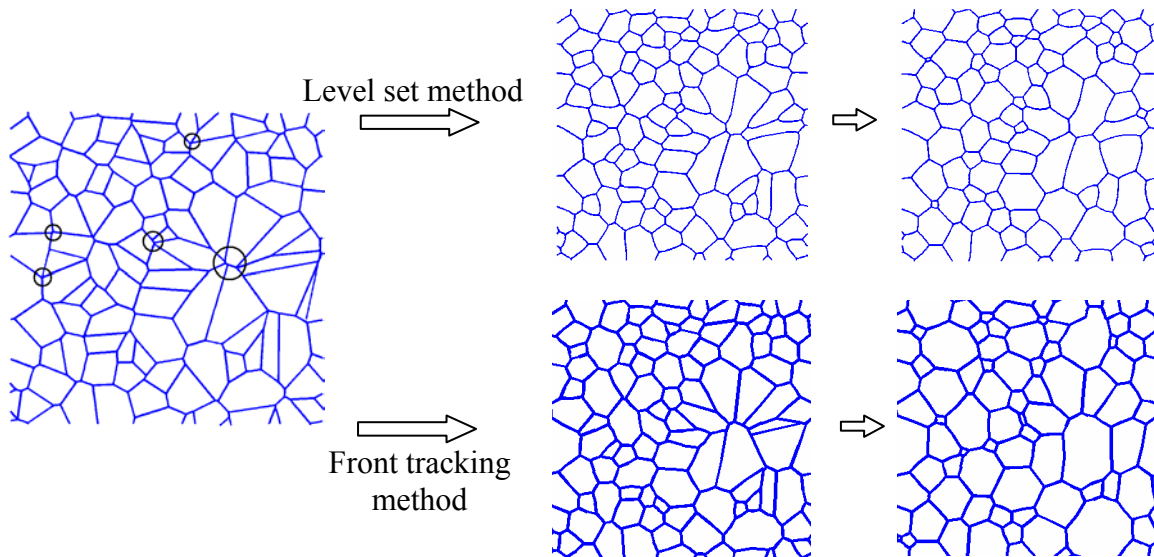


Figure. 13. Random grain growth modeled by multiple level set method and front tracking method [7, 8]

6. Conclusions

In this work, a multiple level set method for modeling grain boundary migration in polycrystalline materials has been presented. For grain boundary migration under curvature induced driving forces, the multiple level set method can naturally handle topological changes without 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, noting that the higher order 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. 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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References

1. Anderson MP, Srolovitz DJ, Grest GS, Sahni PS. Computer simulation of grain growth—I: kinetics. *Acta Metall* 1984; 32:783–791.
2. Atkinson HV. Theories of normal grain growth in pure single phase systems. *Acta Metall* 1988; 36:469–491.
3. Bloomfield MO, Cale TS. Formation and evolution of grain structures in thin films. *Microelectronic Engineering* 2004; 76:195–204.
4. Bloomfield MO, Richards DF, Cale TS. A computational framework for modelling grain-structure evolution in three dimensions. *Philosophical Magazine* 2003; 83(31-34): 3549-3568.
5. Chadwick GA and Smith DA. *Grain Boundary Structure and Properties*. Academic Press, New York, 1976.
6. Chan TF and Vese LA. Active contours without edges. *IEEE Trans. Image Proc.* 2001; 10:266–277.
7. Chen JS, Lu H, Moldovan D and Wolf D. Mesoscale modeling of grain boundary migration under stress using coupled finite element and meshfree methods. *Proceeding, 5th ASCE Engineering Mechanics Conference, Columbia University, 2002; June 2-5.*
8. Chen JS, Lu H, Moldovan D and Wolf D. A double-grid method for modeling of microstructure evolution. *The 5th World Congress on Computational Mechanics, Proceeding, Vienna, Austria, 2002; July 7-12.*
9. Chen JS, Kotta V, Lu H, Wang D, Moldovan D, Wolf D. A variational formulation and a double-grid method for meso-scale modeling of stressed grain growth in polycrystalline materials. *Proceeding, Forum on Advanced Engineering Computation, Taiwan, National Taiwan University, 2004; February.*
10. Chen JS, Kotta V, Lu H, Wang D, Moldovan D, Wolf D. A variational formulation and a double-grid method for meso-scale modeling of stressed grain growth in polycrystalline materials. *Computer Methods in Applied Mechanics and Engineering* 2004; 193:1277-1303.

11. Chen JS, Kotta V, Lu H, Yoon S, Modolvan D, Wolf D. Modeling of grain boundary migration under stress. *6th US Congress on Computational Mechanics, Detroit, MI*, 2001; August 1-4.
12. Chiang CR. The grain size effect on the flow stress of polycrystals, *Scripta Metall* 1985; 19:1281–1283.
13. Coble L. A model for boundary diffusion controlled creep in polycrystalline materials. *J. Appl. Phys.* 1963; 34(6):1679-82.
14. Fan D, Chen LQ, Computer simulation of grain growth using a continuum field model. *Acta Mat.* 1997; 45:611–622.
15. Frost HJ, Thompson CV, Walton DT. Simulation of thin film grain structures: I. grain growth stagnation. *Acta Metallurgica et Materiala* 1990; 38:1455-1462.
16. Gottstein G, Shvindlerman LS. *Grain Boundary Migration in Metals: Thermodynamics, Kinetics, Applications*. CRC Press, Boca Raton, 1999.
17. Hall EO. The deformation and ageing of mild steel: III discussion of results. *Proc. Phys. Soc. Lond.* 1951; B64:747–753.
18. Herring C. Diffusional viscosity of a polycrystalline Solid. *J. Appl. Phys.* 1950; 21 (5):437-45.
19. Huang H, Gilmer GH and Diaz de la Rubia T. An Atomistic Simulator for Thin Film Deposition in Three Dimensions. *Journal of Applied Physics* 1998; 84:3636-3649.
20. Huang H, Gilmer GH, Texture competition during thin film deposition - effects of grain boundary migration. *Comp. Mater. Sci.* 2002; 23:190-196.
21. Humphreys FJ and Hatherly M. *Recrystallization and related annealing Phenomena*. Pergamon, Oxford, 1995.
22. Krill CE, Chen LQ. Computer simulation of 3-d grain growth using a phase-field model. *Acta Mat.* 2002; 50:3057–3073.
23. Kuprat A. Modeling Microstructure evolution using gradient-weighted moving finite elements. *SIAM J. Sci. Comput.* 2000; 22(2):535-560.
24. Lee TY and Chen JS. Modeling of Grain Growth Using Voronoi Discretization. *Proceeding, 6th World Congress on Computational Mechanics, Beijing, China, 2004*; September 5-10.
25. Lusk MT. A phase-field paradigm for grain growth and recrystallization, *Proc. Roy. Soc. Lond. A* 1999; 455:677–700.
26. Merriman B, Bence JK and Osher S. Motion of multiple junctions - a level set approach. *Journal of Computational Physics* 1994; 112:334–363.
27. Morral JE, Ashby MF. Dislocated cellular structures, *Acta Metall.* 1974; 22:567–575.
28. Novikov VYu, Computer simulation of normal grain growth. *Acta Metall.* 1978; 26: 1739–1744.
29. Osher S and Sethian JA. Fronts propagating with curvature dependent speed: Algorithms based on hamilton-jacobi formulations. *Journal of Computational Physics* 1998; 79:12–49.
30. Osher S and Fedkiw R. *Level set methods and dynamic implicit surfaces*. Springer-Verlag, 2002.
31. Peng D, Merriman B, Osher S, Zhao HK and Kang M. A PDE based fast local level set method. *Journal of Computational Physics* 1999; 155:410-438.
32. Petch NJ. The cleavage strength of polycrystals, *J. Iron and Steel Institute* 1953; 174:25–28.

33. Roosen AR and Carter WC. Simulations of microstructural evolution: anisotropic growth and coarsening. *Physica A* 1998; 261(1-2):232-247.
34. Sahni PS, Grest GS, Safran SA. Kinetics of the Q-state potts model in two dimensions., *Phys. Rev. Lett.* 1983; 50:263–266,.
35. Smith CS. *Grain shapes and other metallurgical applications of topology*, *Metal Interfaces*. American Society for Metals, Cleveland, Ohio 1952:65–108.
36. Sussman M, Smereka P and Osher S. A level set approach for computing solutions to incompressible two-phase flow. *Journal of Computational Physics* 1994; 114:146-159.
37. Thompson CV. Grain growth and evolution of other cellular structures. *Solid State Phys* 2000; 55:269–314.
38. Warren JA, Kobayashi R and Carter WC. Modeling grain boundaries using a phase-field technique. *Journal Crystal Growth* 2000; 211:18–20.
39. Zhao Hong-Kai, Chan T, Merriman B and Osher S. A variational level set approach to multiphase motion. *Journal of Computational Physics* 1996; 127:179-195.
40. Smereka P, Li XQ, Russo G, Srolovitz DJ. Simulation of faceted film growth in three dimensions: microstructure, morphology and texture. *Acta Materialia* 2005; 53(4): 1191-1204.
41. Osher S, Fedkiw RP. Level set methods: An overview and some recent results. *Journal of Computational Physics* 2001; 169(2):463-502.
42. Babuska I. The finite element method with Lagrangian multipliers. *Numer. Math* 1973; 20:179-182.
43. Engquist B, and Osher S. Stable and entropy satisfying approximations for transonic flow calculations, *Math.Comp.*, 1980; 34:45-75.