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MESOSCALE MODELING OF GRAIN BOUNDARY MIGRATION UNDER STRESS USING COUPLED FINITE ELEMENT AND MESHFREE METHODS

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ABSTRACT

The process of grain boundary migration involves moving interfaces and topological changes of grain boundary geometry. This can not be effectively modeled by Lagrangian, Eulerian, or arbitrary Lagrangian Eulerian finite element formulation when stress effect is considered. A coupled finite element and meshfree approach is proposed for modeling of grain boundary migration under stress. In this formulation, the material grid carries material kinematic and kinetic variables, whereas the grain boundary grid carries grain boundary kinematic variables. The material domain is discretized by a reproducing kernel partition of unity with built-in strain discontinuity across the grain boundaries. The grain boundaries, on the other hand, are discretized by the standard finite elements. This approach allows an arbitrary evolution of grain boundaries without continuous remeshing.

Keywords: grain boundary migration, meshfree method, reproducing kernel approximation, double-gird method

INTRODUCTION

Grain growth is the process by which the average grain size in a polycrystalline material increases in time. The evolution of the microstructure during the grain growth takes place via the migration of the grain boundaries towards their centers of curvature, the driving force being provided by the decrease in energy associated with the decrease of the length of the grain boundaries. There have been many experimental and theoretical investigations of grain growth process starting from 1950s. In recent years, various types of computer simulation models have been developed with the aim of simulating the detailed evolution of microstructure during grain growth. These simulation models fall mainly into two classes: probabilistic (Anderson *et al*., 1984) and deterministic (Soares *et al.*, 1985, Frost *et al.*, 1988, Kawasaki *et al.*,1989, Cocks *et al.*, 1996, Moldovan *et al*., 2002).

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Probabilistic models are generally of Monte-Carlo type and have their basis in the classical spin models of statistical physics; the most investigated is Potts model (Anderson *et al*., 1984). In the Potts model approach grains are subdivided into small-area elements and growth dynamics are simulated by exchange of area elements between grains. Growth takes place as a consequence of the minimization of the internal energy of the system. The exchange step of area elements from one grain to the neighboring grain is carried out using a Monte Carlo algorithm. The advantage of this method is its simplicity and the ease of its 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 the deterministic models, the motion of grain boundaries is followed by time integration of their position assuming the normal velocity of the grain boundary to be proportional to the boundary curvature. A purely deterministic approach was proposed first by Fullman (1952) and is referred to as "vertex model". Later, this was improved by Soares *et al*. (1985) and Kawasaki *et al.* (1989) assuming straight grain boundaries, and by Frost *et al*. (1988), Cocks and Gill (1996), Weygand *et al*. (1998) by extending it to curved grain boundaries. Using the theoretical approach of Needleman and Rice (1980) based on a variational principle for dissipative systems, Cocks and Gill (1996) have proposed a new method to simulate curvature-driven grain growth. Their modification describes the rate of power dissipation due to the competition between the reduction in the grain boundary energy and the viscous drag during grain boundary migration. Moreover, the grain boundaries are discretized using finite elements.

In general in a polycrystalline microstructure subject to an externally applied stress an additional driving force to that given by the grain boundary curvature has to be considered. This is due to the elastic anisotropy of the grains comprising the microstructure, which in general store different amounts of elastic energies. Our focus in this study is to investigate the grain growth in the presence of both curvature driven and stress induced grain boundary migration. This requires the coupling of elastic deformation of grains with grain boundary migration and thus necessitates the discretization of grain boundaries and grain domains. Using finite element method, the migration of grain boundary leads to a severe mesh distortion in each grain, and the topological changes of grain structures further demand a complete remeshing. In this work, a double-grid method is proposed. The elastic deformation of grains is modeled by reproducing kernel discretization with built-in strain discontinuities along the grain boundaries (Chen *et al.* 1996, 2002), whereas the migration kinematics of discretized grain boundaries is modeled using the standard finite element formulation.

The numerical examples we provide in this study demonstrate that the evolution of grain growth can be effectively simulated without any remeshing. Moreover, the study also shows the proper time evolution of the grain structures in an idealized grain network with an imperfection using the proposed methods.

GRAIN GROWTH KINEMATICS

In general, the grain boundaries migrate at a wide range of velocities, which depend on the magnitude of both the driving force and the grain boundary mobility (which dependent on temperature, and impurities concentration). Using a simplified model, Burke and Turnbull (1952)

proposed a parabolic relationship for the grain growth kinetic.

The driving force f_c due to the surface curvature (the capillarity effect) is

$$f_c = \gamma(\theta)(\frac{1}{R_1} + \frac{1}{R_2}) \tag{1}$$

where $\gamma(\theta)$ is the surface tension (the boundary energy per unit area) which in general dependents on the grain-boundary misorientation θ, and R_1 and R_2 are the principal radii of the surface curvature.

Assuming the only forces acting on a grain boundary are those given by Eq.(1) $\gamma(\theta)$ is constant for all boundaries, the parabolic equation is deduced as:

$$\overline{R}^n(t) - \overline{R}^n(0) = kt \tag{2}$$

where, n takes the value of 2 and is known as the grain growth exponent $\overline{R}(t)$ is the mean grain radius at time *t* and *k* is a constant. The grain growth exponent is one of the most important characteristics of the growth and the experimental value ranges from n=2 to n=4.

In general at small grain sizes the most significant driving force for grain boundary migration is the surface tension. However at larger grain sizes, and in the presence of strain energy, additional driving forces due to difference in elastic strain energies in the volumes of neighboring grains, may also play a key role in grain boundary migration. For instance, this driving force f_e can be expressed as:

$$f_e = \frac{|\Delta U|}{\Delta V} \tag{3}$$

where ΔU is the difference in strain energy between adjacent grains in volume ΔV, ΔV is the volume through which the grain boundary segment has swept during a migration step.

The following creep law is used for the elastic deformation of the grain

$$\sigma_{ij} = C_{ijkl}\dot{\varepsilon}_{kl} \tag{4}$$

$$\dot{\varepsilon}_{ij} = \frac{1}{2}(\frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i}) \tag{5}$$

where v_i is material velocity, and C_{ijkl} for each grain is assumed to be orthotropic following the crystallographic orientation of grain.

Due to the grain boundary migration with velocities components $\overline{v}_n$ and $\overline{v}_s$ as shown in Fig. 1, the rate of elongation per unit length of grain boundaries can be calculated as

$$\dot{\overline{\varepsilon}}_s = \frac{\overline{v}_n}{R} + \frac{\partial \overline{v}_s}{\partial s} \tag{6}$$

where R is grain boundary radius of curvature.

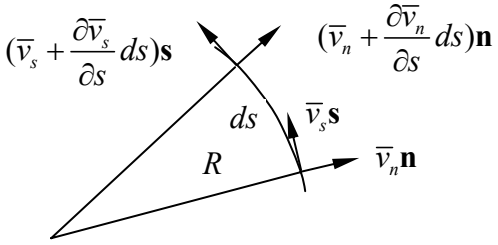

Fig. 1. A segment of grain boundary

GEOMETRY OF POLYCRYSTALLINE MATERIALS

The geometry of a 2D polycrystalline material is determined by the arrangement of the fundamental elements such as vertices, edges and faces as shown in Fig. 2. These elements obey the following Euler relation:

$$F - E + V = 1 \tag{7}$$

where F, E, and V are the numbers of faces, edges and vertices respectively.

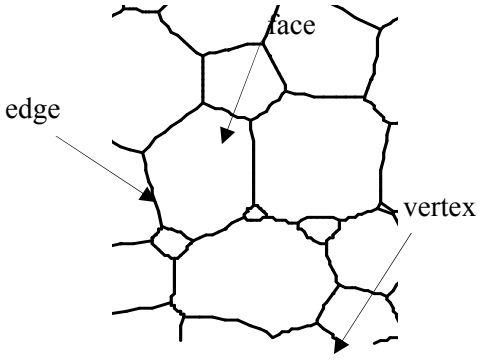

Fig. 2. 2-D grain structure

Although any number of edges can join in a vertex, the threefold vertices are the one favored energetically in 2D polycrystalline materials, and it follows

$$3V = 2E = \overline{n}F \tag{8}$$

where $\overline{n}$ is the mean number of vertices per face (grain). For a system with a large number of grains $N \gg 1$, this implies $\overline{n} = 6$.

In 2D, unless the microstructure consists of a regular array of hexagons, grain growth is inevitable. According to Eq. (8), each grain disappearance is accompanied by vanishing of two vertices and three edges. In addition to this the von Neumann (1952) relation predicts that any grain with more than 6 edges will grow, while those having less 6 edges will shrink. The topology of the system evolves continuously during growth. In order to provide solutions for the necessary topological transformations during growth typical topological transformations have been proposed. These are T1, T2 and T3 topological changes as shown in Fig. 3.

(a) T1 change (b) T2 change (c) T3 change

Fig. 3. Topological change of grain boundaries

DOUBLE-GRID DISCRETIZATION

Grain boundary velocity and material velocity are the two primary variables describing the physic problem. As shown in Fig. 4, the material domain is discretized by material points carrying material velocity $\boldsymbol{v}$, whereas the grain boundary is discretized by grain boundary points carrying grain boundary velocity $\overline{\boldsymbol{v}}$. In this approach, the material velocity is approximated by a reproducing kernel approximation with strain discontinuity along material interface. The grain boundary velocity is approximated by the standard finite element shape function, i.e.,

$$v_i = \sum_{I=1}^{NPm} \Psi_I(\boldsymbol{x}) \upsilon_{iI} \tag{9}$$

$$\overline{v}_i = \sum_{I=1}^{NPgb} N_I(s) \overline{\upsilon}_{iI} \tag{10}$$

where *NPm* is the number of material points, *NPgb* is the number of grain boundary points, $N_I(s)$ is the 1-dimensional shape function defined along the grain boundary using grain boundary coordinate *s*, and $\Psi_I(\boldsymbol{x})$ is the reproducing kernel shape function defined in the 2-dimensional

material domain as follows

$$\Psi(\boldsymbol{x}) = \hat{\Psi}(\boldsymbol{x}) + \bar{\Psi}(\boldsymbol{x}) \tag{11}$$

In Eq.(11), $\hat{\Psi}(\boldsymbol{x})$ is primitive function employed to introduce derivative discontinuity along the brain boundary as shown in Fig. 5, and $\bar{\Psi}(\boldsymbol{x})$ is the enrichment function to impose completeness of the approximation. Following the procedures described in the work by Chen *et al.* (2002) and Wang *et al.* (2002), the enrichment function is expressed as

$$\bar{\Psi}_I(\boldsymbol{x}) = \boldsymbol{H}^T(\boldsymbol{x}-\boldsymbol{x}_I)\boldsymbol{M}^{-1}(\boldsymbol{x})[\boldsymbol{H}(\boldsymbol{0}) - \sum_{I=1}^{NPm} \hat{\Psi}(\boldsymbol{x})\boldsymbol{H}(\boldsymbol{x}-\boldsymbol{x}_I)]\Phi_a(\boldsymbol{x}-\boldsymbol{x}_I) \tag{12}$$

$$\boldsymbol{H}^T(\boldsymbol{x}-\boldsymbol{x}_I) = [1, x-x_I, y-y_I] \tag{13}$$

$$\boldsymbol{M}(\boldsymbol{x}) = \sum_{I=1}^{NPm} \boldsymbol{H}(\boldsymbol{x}-\boldsymbol{x}_I)\boldsymbol{H}^T(\boldsymbol{x}-\boldsymbol{x}_I)\Phi_a(\boldsymbol{x}-\boldsymbol{x}_I) \tag{14}$$

where $\Phi_a(\boldsymbol{x}-\boldsymbol{x}_I)$ is the kernel function with support size "*a*".

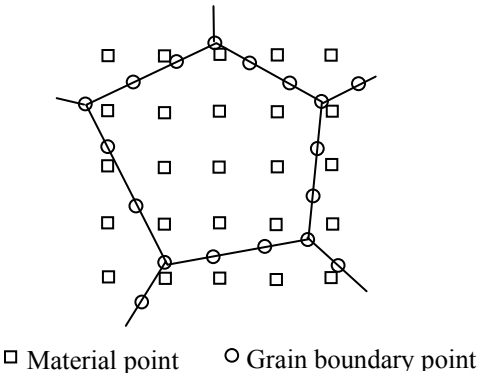

Fig. 4. Double grid discretization

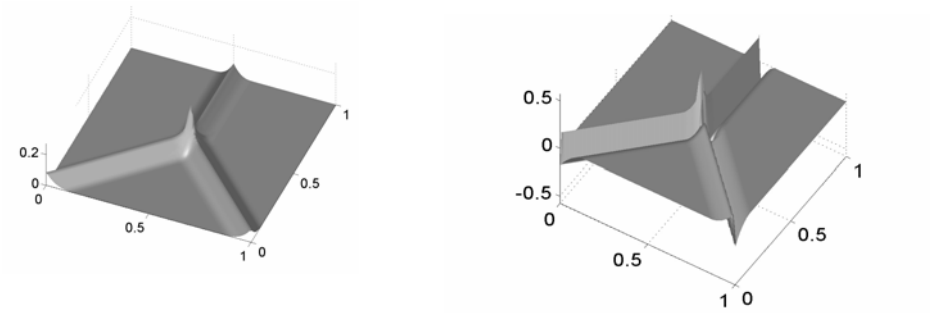

Fig. 5. Premitive function and its derivatives along the normal direction of the grain boundaries

NUMERICAL EXAMPLE

A network of uniform hexagonal grains with a central one whose elastic material property is different from the others (as shown in Figs. 6 and 7) is subject to a tensile stress in the vertical direction. In the first case, the Young's modulus of the center grain is larger than that of other grains. The time evolution of microstructure is shown in Fig. 6. Several T1 topological changes give rise to a grain with number of edges less than 6 which promotes its growth (see central grain in Fig. 6). Finally, after some time the central grain occupies most of the domain. In the second case, a central grain with lower Young's modulus is introduced. At the initial stage, this grain shrinks as shown in Fig. 7 in order to reduce the total strain energy of the system. After several T1 and T3 topological changes, the central grain disappears and leads to an unstable microstructure where several grains have less than 6 edges and one with more than 6 edges. The one grain with more than 6 edges continues to grow whereas the surrounding grains with less than 6 edges keep on reducing their sizes and eventually disappear.

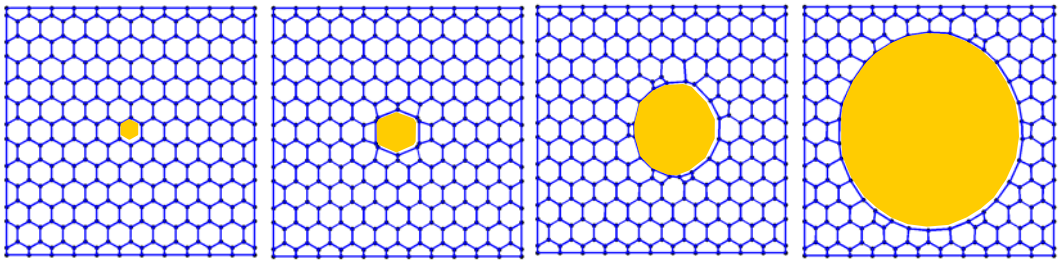

Fig. 6. Imperfection with stiffer grain

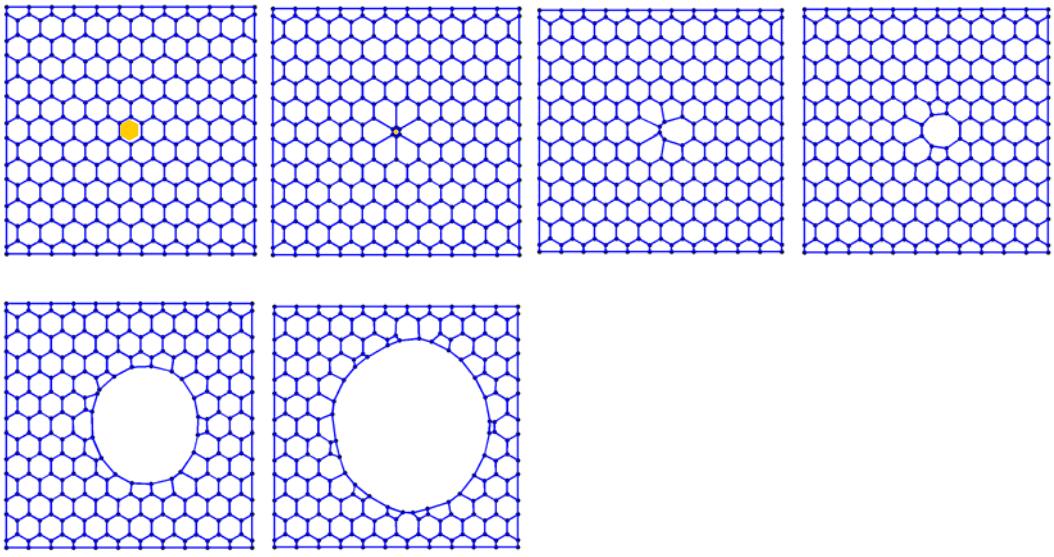

Fig. 7. Imperfection with softer grain

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