

New Computational Technique for Evaluating Deformation of Nanocrystalline Metal using Phase Field Crystal Method

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ABSTRACT

The phase field crystal (PFC) method is anticipated as a new multiscale method, because this method can reproduce physical phenomena depending on atomic structures in metallic materials on the diffusion time scale. Although the PFC method has been applied to some phenomena, there are few studies related to evaluations of mechanical behaviors of materials by appropriate PFC simulation. In a previous work using the PFC method, tensile deformation simulations have been performed under conditions where the volume change was unavoidable during plastic deformation. In this study, to reproduce deformation under isovolumetric conditions, we proposed a novel numerical technique for PFC deformation simulation. Moreover, to evaluate the contribution of the driving force α (temperature) on deformation behaviors, we performed the tensile deformation simulations of nanopolycrystalline structures with different temperatures. The results confirmed that the resistance to dislocation motions increased by lowering temperature. As a results, grain rotation and grain boundary migration were restrained.

1. Introduction

It is of great importance to predict macroscopic properties of industrial metallic materials depending on defects in microstructures to improve material properties and/or create novel functions of such materials. Therefore, the development of a multiscale model bridging a molecular description and a continuum field theory is an urgent need. Recently, the phase field crystal (PFC) method [1] has been developed as a new multiscale numerical method that operates for atomic length scale with diffusive time scale. The PFC model introduces a periodic order parameter, which represents a local-time-averaged atomic density field to express regular arrangements of atoms in a solid phase. Therefore, this model inherently includes features of crystal systems, elasticity, plasticity and multiple orientations. Although, the PFC method has been applied to some phenomena, there are few studies on appropriate deformation simulation using this method. In previous PFC simulations of tensile deformation [1, 2], the volume of polycrystalline structure increases during plastic deformation simulation due to the difficulty in setting the boundary conditions appropriately. In this study, we propose a novel numerical technique for deformation simulation by the PFC method. By employing this technique, the deformation behaviours of nanopolycrystalline structures are studied at different temperatures.

2. Phase Field Crystal Method

The free energy functional in the PFC method is minimized by a periodic order parameter or the phase field ϕ , which is defined as the local-time-averaged atomic density and is a conserved value [1]. Therefore, this model can reproduce the dynamics based on individual atoms on the diffusion time scale that is much larger than the atomic vibrational time scale. In the steady solid phase of metallic materials, atomic locations are independent of time and become regular arrangements. Therefore, to express these periodic states, the phase field ϕ must have periodic profiles. Here, the local maxima of the phase field ϕ correspond to atomic positions. On the other hand, since atomic positions in the liquid phase become random depending on time, the phase field ϕ is averaged and becomes a constant value ϕ_0 . From the phase field ϕ defined above, the dimensionless free energy functional F is given by [1]

$$F = \int \left[\frac{\alpha}{2} \phi^2 + \frac{\phi^4}{4} + \frac{\phi}{2} (1 + \nabla^2)^2 \phi \right] dV, \quad (1)$$

where α is the driving force, which is proportional to a distance in temperature from a melting point, $T - T_m$. Here, T is a temperature and T_m is a melting point. Since ϕ is the time-averaged density and a conserved value, the Chan-Hilliard equation provides the evolution of ϕ as

$$\frac{\partial \phi}{\partial t} = \nabla^2 \frac{\delta F}{\delta \phi} = \nabla^2 \left[\alpha \phi + \phi^3 + (1 + \nabla^2)^2 \phi \right]. \quad (2)$$

Fig. 1(a) schematically shows the proposed numerical scheme for PFC deformation simulation in two dimensions. To reproduce tensile deformation under isovolumetric condition, the grid size in x-direction increases by the displacement increment $d = \dot{\epsilon} \Delta x \Delta t$ at every time step, and the grid size in y-direction decreases so as to maintain $\Delta x \Delta y = \Delta x' \Delta y'$. Here, Δx and Δy are initial grid sizes, and $\Delta x'$ and $\Delta y'$ are grid sizes changed during deformation, and Δt and $\dot{\epsilon}$ are the time increment and dimensionless strain rate, respectively. In this methodology, since a constant strain rate is applied to all atoms, the deformation state becomes the affine deformation state, and periodic conditions can be used as boundary conditions.

3. Deformation Simulation

The deformation behaviors of a nanopolycrystalline structure are simulated by the PFC method with our technique. Before deformation simulation, a regular hexagonal grain structure with predetermined orientations is prepared by solidification simulation.

3.1 Computational model and conditions

Fig. 1(b) is a schematic illustration of the desired nanopolycrystalline structure with regular hexagonal grains of which a distance between two sides is approximately 14 atoms. The predefined crystal orientations of each grain are shown at the center of each grain. The computa-

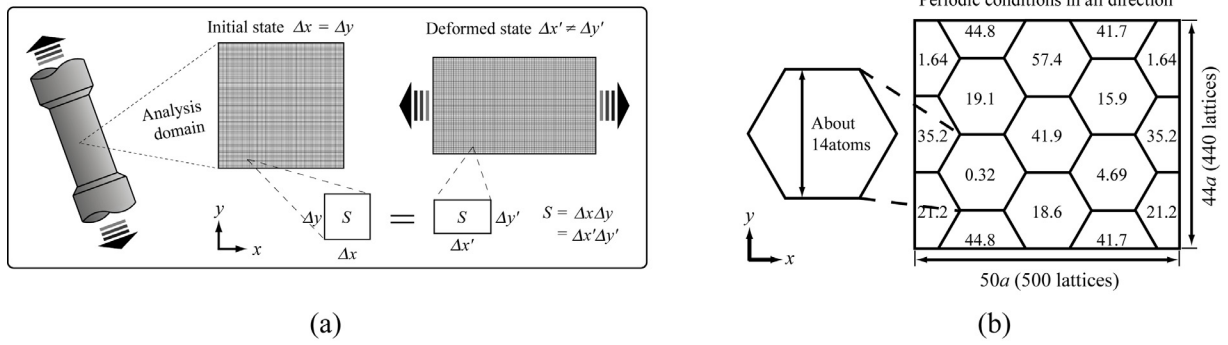


Figure 1. (a) Numerical scheme of tensile deformation simulation in two dimensions and (b) desired nanopolycrystalline structure with regular hexagonal grains and crystal orientations.

tional domain size is set to be $50a \times 44a$ (500×440 lattices) and $\phi_0 = -0.285$ is selected. Here, a is a distance between nearest atoms. To perform the deformation simulations under two different temperatures, $\alpha = -0.25$ and -0.50 are employed. The temperature corresponding to $\alpha = -0.25$ is higher than that of $\alpha = -0.50$. The initial structure is formed by solidification simulation that starts from nuclei with predefined crystal orientations. As a result of solidification simulation with $\alpha = -0.25$, the initial structure shown in Fig. 2(a) is obtained. To prepare same atomic structure for $\alpha = -0.50$, after obtaining the structure shown in Fig. 2(a), further relaxation simulation is performed by changing to $\alpha = -0.50$. The computed structure is shown in Fig. 3(a). Tensile deformation simulations are performed under a constant dimensionless strain rate $\dot{\epsilon}$ of 1.84×10^{-6} , which corresponds to realistic strain rates of approximately 10^0s^{-1} to 10^1s^{-1} , and use the dimensionless time step $\Delta t = 3.0 \times 10^{-3}$. Periodic conditions are used in all directions.

3.2 Numerical results and discussion

Fig. 2 indicates the deformation states of the nanopolycrystalline structure for the case of $\alpha = -0.25$. As the strain increases, grain rotations occur and cause the motions of dislocation at grain boundaries, such as the dislocation shown in the circle of Fig. 2(a). It is also observed that grain rotation occurs between two neighboring grains with a relatively small misorientation (arrows in Figs. 2(a)(b)). As a result of coalescence due to grain rotation, the grain boundary between integrated grains disappears and the grain boundary migration driven by curvature is accelerated, such as the grain boundary in the circle of Fig. 2(c). With further deformation, grain rotations and grain boundary migrations occur continuously in other grains (Figs. 2(d)(e)).

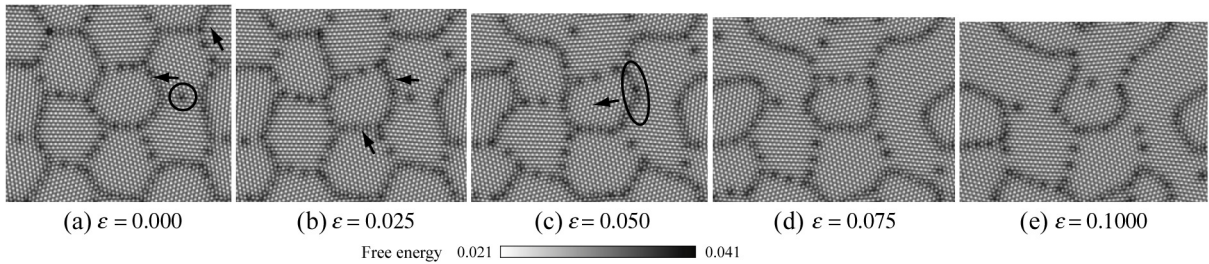


Figure 2. Deformation process of nanopolycrystalline structures in the case of $\alpha = -0.25$.

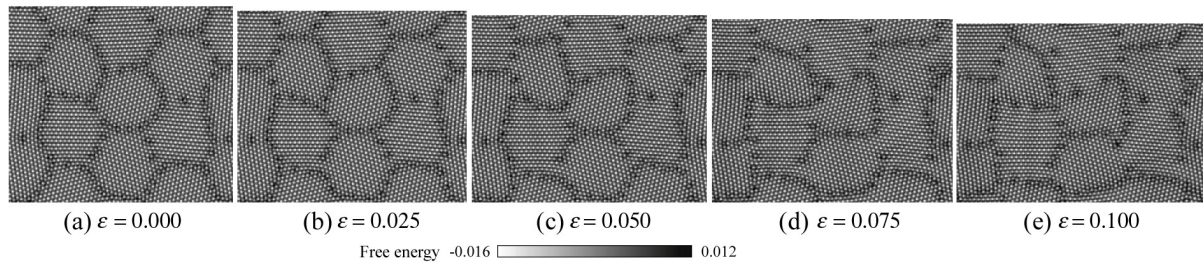


Figure 3. Deformation process of nanocrystalline structures in the case of $\alpha = -0.50$.

Fig.3 shows the deformation states in the case of $\alpha = -0.50$ that is a lower-temperature state than the former. The comparison between Figs. 2(a)-(c) and Figs. 3(a)-(c) suggests that the dislocation motion at grain boundary becomes slower than those at higher temperature. Moreover, grain rotation is harder to occur. As a result, grain coalescence observed in the former can't be confirmed. With further deformation as shown in Figs. 3(d)(e), unlike the former, it can be confirmed that grain boundary migration is restrained. These results clarify that the PFC deformation simulation with our technique can reproduce the increase of the resistance to dislocation motion by lowering temperature.

4. Conclusion

To express deformation under isovolumetric condition, we proposed the novel numerical scheme for PFC deformation simulation. Moreover, to evaluate the influence of the driving force α on deformation behaviours, we performed the tensile deformation simulation of nanopolycrystalline models at two different temperatures. At higher temperature ($\alpha = -0.25$), the intergranular deformation such as grain rotation, grain boundary migration and grain growth became the dominant deformation mechanism. On the other hand, at lower temperature ($\alpha = -0.50$), unlike the former, the resistance to dislocation motions at grain boundary increased by lowering temperature. As a result, grain rotation and grain boundary migration were restrained.

Acknowledgements

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