DEFORMATION SIMULATION UNDER CONSTANT VOLUME CONDITION USING PHASE FIELD CRYSTAL METHOD

Tomoyuki Hirouchi*, Tomohiro Takaki** & Yoshihiro Tomita*
*_Graduate School of Engineering, Kobe University, Rokkodai, Nada, Kobe, 657-8501, Japan_
**_Graduate School of Science and Technology, Kyoto Institute of Technology, Kyoto, 606-8585, Japan_

Summary   We proposed a new technique for the deformation simulation using the phase field crystal (PFC) method, which keeps constant volume during deformation, and investigated the deformation behaviors of nano single crystal and bicrystal materials. We confirmed that the PFC model could reproduce the deformation simulation under the constant volume condition. Furthermore, we observed that grain boundary could be the source of dislocation emission and absorption.

INTRODUCTION

It is very important to predict macroscopic properties of industrial metallic materials depending on microstructures so as to improve the properties and/or create novel functions of such materials. Recently, the phase field crystal (PFC) method [1, 2] is developed as a new numerical approach in atomic level. In this method, a free energy is minimized by a periodic order parameter, which represents a local-averaged atomic density field. Therefore, this formulation can describe physical systems in diffusive time and interatomic length scales. In this sense, the PFC model is anticipated as a model that bridges between a molecular description and a continuum field theory, or a multi-scale model.

In general, it is well known that metallic materials actually keep the volume constant during plastic deformation. However, in the previous PFC simulations of tensile deformation [2, 3], the volume of the polycrystalline structure increased during the deformation simulation because it was difficult to set the boundary condition properly. Therefore, it is very important to develop an appropriate numerical condition for PFC deformation simulation.

In this study, we propose a new technique applying deformation by controlling computational grid sizes. By applying this technique, we study the deformation behaviors of nano single crystal and bicrystal structures to demonstrate basic properties of the proposed technique.

PHASE FILED CRYSTAL METHOD

Unlike conventional phase field models, a free energy in the PFC model is minimized by a periodic order parameter. This order parameter, or phase field ϕ, is defined as a local-time-averaged atomic density field. Therefore, the phase field is a conserved field. Figure 1(a) schematically shows the phase field profile for the PFC model. In the steady solid phase, ϕ has the periodic profile with a wavelength a to express atoms fixed in a periodic arrangement. Here, the local maxima of ϕ correspond to atomic positions. On the other hand, atomic positions in the liquid phase depend on time. Therefore, ϕ in the liquid phase becomes constant, $\phi = \phi_0$, as a local-time-averaged value.

Here, the dimensionless free energy functional F minimized by the phase field profile that generates a triangular lattice structure is given by [1, 2],

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

where α is the driving force related to temperature. This free energy gives rise to a phase diagram of solid (triangular), liquid (constant), striped phases and the coexistence of each phase as shown in Fig. 1(b). Since ϕ is a conserved value, the time evolution equation is derived from the functional derivative by the Chan-Hilliard equation,

$$\frac{\partial \phi}{\partial t} = \nabla^2 [\{\alpha + (1 + \nabla^2)^2\}\phi + \phi^3] \tag{2}$$

To perform deformation simulations using the PFC method, we propose a new technique enabling constant volume deformation by controlling computational grid sizes. Here, in the case of two-dimensional tensile deformation simulation, the grid size in x-direction, Δx, is increased and that in y-direction, Δy, is decreased by following a volume constant condition. Therefore, this technique enables constant volume deformation under periodic boundary condition.

RESULTS AND DISCCUSSION

First, to confirm the propriety of the proposed technique, we perform the uniaxial tensile deformation simulation of the single crystal at constant strain rate. Computation is performed on a domain of 880×20 lattices with $\Delta x = \Delta y = 4\pi/\sqrt{3}$ $(a/10)$. Model parameters are set to $(\alpha, \phi_0) = (-0.25, -0.285)$. Figure 2 shows atomic positions at the strained values. The data clearly shows that the response of the system satisfies linear elasticity. Thus, we could confirm the propriety of our technique. Second, to present the role of the grain boundary in plastic deformation, we perform the deformation simulation of the bicrystal. Figure 3(a) shows the free energy contribution at the initial condition. Crystal orientations of 20 and 40 degrees are selected to construct the high angle grain boundaries. Model parameters are set to $(\alpha, \phi_0) = (-0.25,$

-0.285). The boundary conditions are periodic conditions in all direction. In Fig. 3(a), we can confirm two dislocations and grain boundaries as high energy. Figures. 3(b)-(d) show the deformation behavior of the bicrystal. As strain increases, the convex part of the grain boundary X in square region of Fig. 3(a) becomes sharp and the dislocation A is emitted from there in Fig. 3(b). We understand that this occur because of the stress concentration on there. Next, the dislocation A is absorbed into the grain boundary Y as shown in Figs. 3(c)-(d). On the other hand, the grain boundary Y starts to generate serration and to nucleate dislocations in Fig. 3(c). Thus, we observed that grain boundary could create and absorb dislocations. These behaviors of grain boundary are proved in molecular dynamics simulations [4, 5]. Therefore, we consider that the proposed technique can be used as the analysis tool simulating plastic deformation.
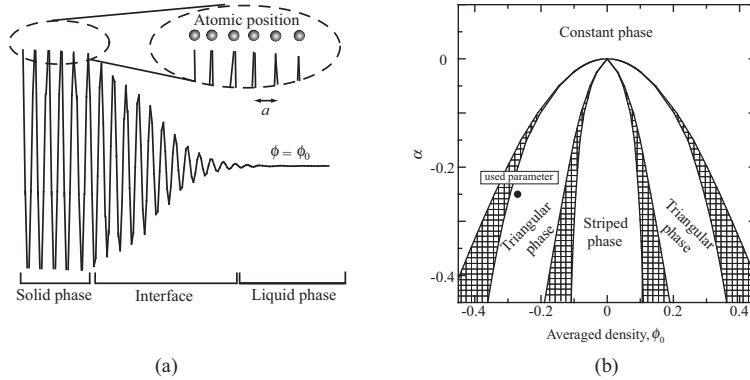

Figure 1. (a) Phase field profile for PFC model and (b) phase diagram in two dimensional problem.
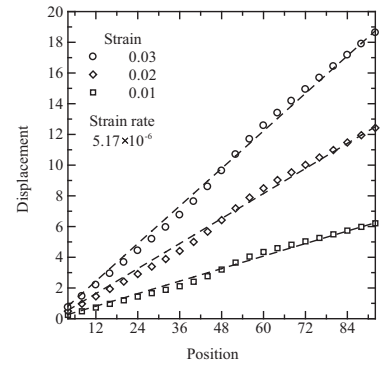
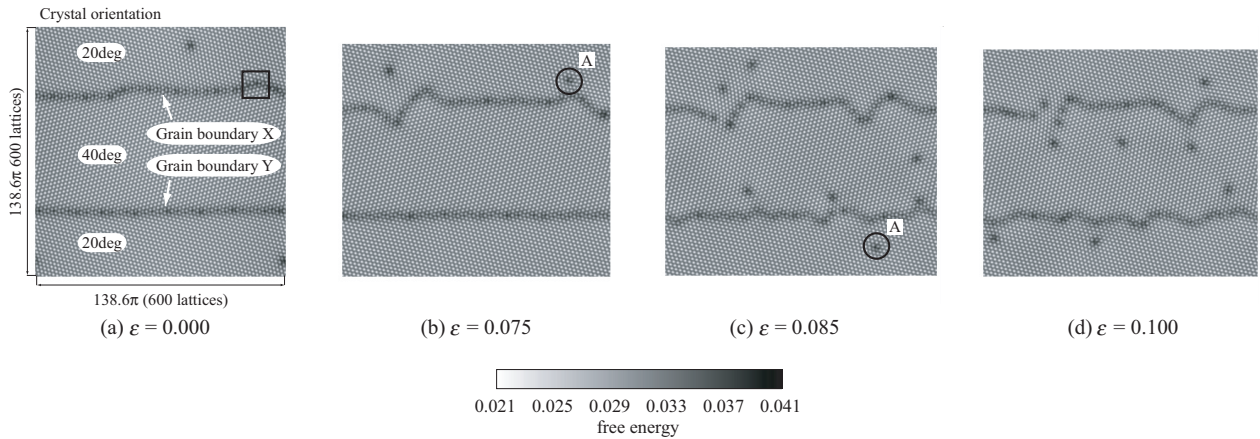**Figure 2.** Atomic displacement distribution under tension.

Figure 3. (a) Initial condition of the bicrystal, and deformation state with (b) $\varepsilon = 0.075$, (c) $\varepsilon = 0.085$ and (d) $\varepsilon = 0.100$.

CONCLUSIONS

In this work, we proposed a new technique enabling constant volume deformation simulation using the PFC model and studied the deformation behaviors of nanocrystalline materials to present the propriety of the proposed technique. In the case of the single crystal, we confirmed the propriety from the elastic response of the system. Moreover, in the case of the bicrystal, we observed the emission and absorption of the dislocations from grain boundary. Therefore, we conclude that this method enables us to simulate plastic deformation.

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