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INFLUENCE OF TEMPERATURE AND GRAIN-SIZE ON PHASE FIELD CRYSTAL DEFORMATION SIMULATION

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Summary. We performed deformation simulations of nanopolycrystalline metal under different temperature and grain-size conditions using the phase-field crystal (PFC) method with our proposed scheme, and demonstrated that the PFC deformation simulation could have a potential of solving deformation problems depending on temperature and grain size.

1 INTRODUCTION

It is well known that defects, such as dislocation and grain boundary (GB), have a great effect on mechanical property of metallic materials. Although behaviors of defects have been studied by experiments and computer simulations by molecular dynamics (MD)[1], it is difficult to observe detailed dynamics at atomic level in experiments and MD simulations are limited inherently in small time scales. Therefore, the investigation of atomic behaviors in more realistic time scale is of great importance.

Recently, Elder et al. has developed the phase-field crystal (PFC) method[2], which enables one to simulate atomic behaviors in diffusive time scale. In our previous study[3], to express isovolmetic state during plastic deformation of metallic material employing this method, we proposed a new numerical scheme where computational grid size was changed and confirmed that the PFC deformation simulation with our scheme could reproduce appropriate behaviors of dislocations and GBs. However, these simulations were conducted under the limited temperature and grain-size condition.

In this study, to reveal that the PFC deformation simulation with our scheme can reproduce the behaviors of defects under various conditions, we performed deformation simulations of

nanopolycrystalline materials under different temperature and grain-size conditions.

2 PHASE-FIELD CRYSTAL METHOD

Unlike the conventional phase-field method, the PFC method introduces a periodic order parameter or the phase field ϕ, which represents a local-time-averaged atomic number density and is a conserved value. To express atomic states in solid and liquid phases of metallic materials, ϕ becomes periodic and constant, respectively. The free energy functional is minimized when ϕ has periodic profile and can be expressed as

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

where α is proportional to the deviation of temperature from a melting temperature. Also, following the Chan-Hilliard equation, the dynamics are described in dimensionless form by

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

In PFC deformation simulations, we employ the proposed numerical scheme in two dimensions[3]. To reproduce tensile deformation under isovolumetic condition, the grid size in x-direction increases by the displacement increment $d = \dot{\varepsilon}\Delta x\Delta t$ 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 during deformation, and Δt and $\dot{\varepsilon}$ are the time increment and the 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.

3 DEFORMATION SIMULATION

In this section, we study behaviors of defects in nanopolycrystalline structure under different temperature and grain-size conditions using the PFC method with our scheme.

3.1 Computational model and condition

Fig. 1(a) shows the schematic illustration of nanopolycrystalline structure with predefined crystal orientations. Crystal orientation θ is defined as shown in Fig. 1(b), and Fig. 1(c) shows a sample of phase field profile with $\theta = 15°$. Fig. 1(d) shows the definition of deviation angle ψ of the actual GB plane from the symmetrical GB plane. In Fig. 1(a), θ is represented in the center of hexagonal grains, and misorientaion $\Delta\theta$ and deviation angle ψ, which is described in parentheses, are on the GBs, respectively. GB within $\Delta\theta = 20°$ is treated as low-angle GB in this study. To investigate the influence of grain size on deformation behavior, we prepare two types of polycrystalline structure and call them Model A and B. The computational domain sizes of Model A and B are set to be $50a \times 44a$(500 × 440 lattices) and $150a \times 132a$(1500 × 1320 lattices) respectively, where a is the distance between atoms as shown in Fig. 1(c). Grain size of Model B is three times as large as that of Model A. Additionally, to perform the deformation simulation under two different temperatures, $\alpha = -0.25$ and -0.50 are employed. The temperature state corresponding to $\alpha = -0.25$ is the state near a melting temperature and higher than that of

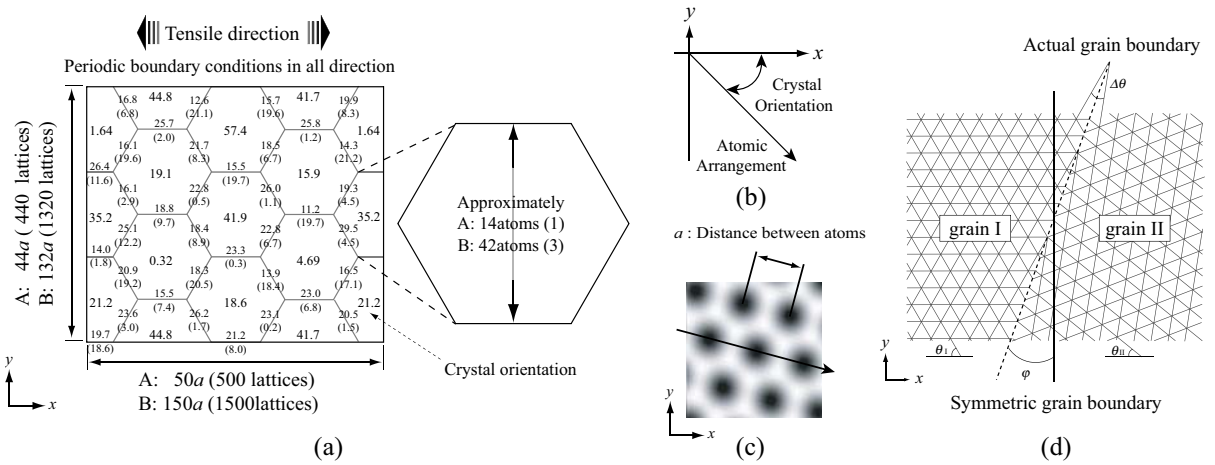

Figure 1: (a) Nanopolycrystalline model with predefined crystal orientations. (b) Definition of crystal orientation. (c) A sample of phase field profile with $\theta = 15°$. (d) Definition of deviation angle ψ.

$\alpha = -0.50$. To use the same initial structure for $\alpha = -0.25$ and -0.50 in the deformation simulation, the structure is formed by solidification simulation with $\alpha = -0.25$ and following the solidification simulation, a relaxation simulation with $\alpha = -0.50$ is performed to create the initial structure for $\alpha = -0.50$. The obtained initial structures for Model A and B are shown in Fig. 2(a). Tensile deformation simulations are performed under the following condition, $d = 4.0 \times 10^{-9}$ and $\Delta t = 3.00 \times 10^{-3} (\alpha = -0.25), 2.55 \times 10^{-3} (\alpha = -0.50)$, which corresponds to deformation condition under realistic strain rates of approximately $10^0 s^{-1}$ to $10^1 s^{-1}$. Periodic boundary conditions are also adopted in all direction.

3.2 Numerical results and discussions

Fig. 2 shows deformation behaviors of nanopolycrystalline structure. In Model A ($\alpha = -0.25$), as the strain increases, grain coalescence by grain rotation occur and grain growth results from curvature-driven GB motions. On the other hand, in Model A ($\alpha = -0.50$), although grain rotation and GB migration are also observed, they aren't remarkable comparing to the case of $\alpha = -0.25$ due to lower temperature. Alternatively, the migrations of dislocations comprising of low-angle GB contribute to the plastic deformation (Circle A in Fig. 2(b)). In Model B ($\alpha = -0.25$), due to larger grain size, grain rotation becomes harder to occur. By contrast, GB migration becomes dominant deformation mechanism. These GB migrations are mainly observed at GBs that aren't parallel to the tensile direction. Interestingly, symmetric low-angle GBs ($\psi < 5°$) displace greatly (GB B in Fig. 2(c)), whereas high-angle GBs migrate hardly. In Ref.[4], under high temperature, these low-angle GB motions are induced by the shear stress and high-angle GB motions are interrupted by GB sliding occurred during deformation. We can't, however, reveal clearly the detailed mechanism. In Model B ($\alpha = -0.50$), more dislocations move into grains from low-angle GBs and the above GB migrations are also observed. Comparing the results of Model A with B, we can consider that grain boundary property affects strongly on deformation behaviors of the nanopolycrystalline structure with larger grain size. Thus, we can confirm that the PFC deformation simulation with our scheme can reproduce deformation behaviors of nanopolycrystalline structure as shown in experiments and MD simulations.

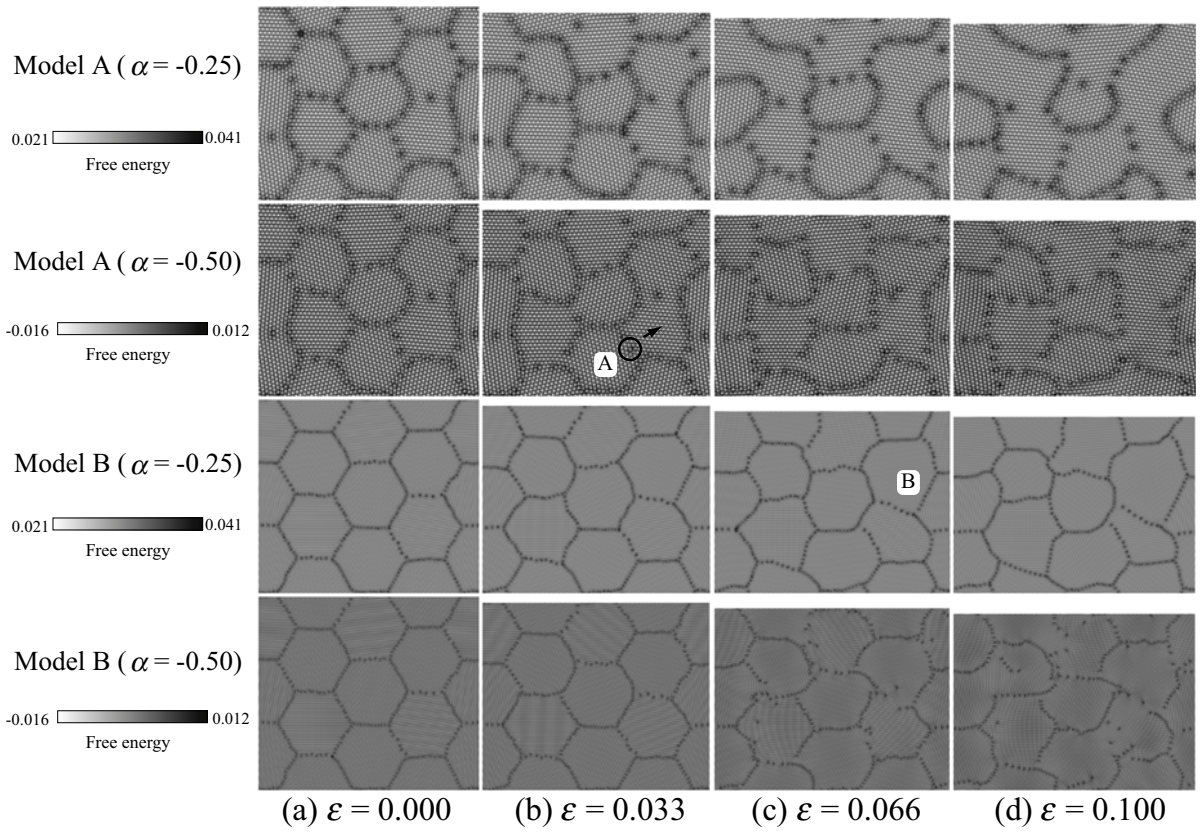

Figure 2: Deformation behaviors in nanopolycrystalline structure.

4 CONCLUSIONS

We conducted the PFC deformation simulations of nanopolycrystalline structure under different temperature and grain-size conditions. As a result, we could confirm that by lowering temperature and increasing grain size, grain rotation and GB migration became harder to occur and behaviors of dislocation and GB changed. Moreover, these deformation behaviors were in qualitative agreement with the results in experiments and MD simulations. Thus, we concluded that the PFC deformation simulation with our scheme could have a potential of solving deformation problems depending on temperature and grain size.

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