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Phase field crystal simulation of dislocation configuration evolution in dynamic recovery in two dimensions

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ABSTRACT

Phase field crystal model is used for studying the grain boundary premelting system under an applied strain at high temperature. The evolution of the dislocation configuration and proliferation and annihilation process of the dislocation and also the characteristic of the morphology of the premelting regions are observed. The results show that the extension premelting domain of the dislocation induced by the applied strain can be regarded as a new phase region (the softening crystal phase domain, SCPD). Due to the lattice softening of the SCPD, two alternant slipping systems exist in it. The cycle processes of the dislocation proliferation by blocking and annihilation by gliding in the SCPD can be regarded as two processes of dynamic recoveries. The evolution of the dislocation configuration and the microscopic mechanism of the cycle dynamic recovery-controlled dislocation at high temperature under plastic deformation in SCPD can well be revealed by the improved KM model.

1. Introduction

The properties of modern materials, especially for those superplastic, nanocrystalline and composite materials, greatly depend on the structure of the interface and dislocations in materials. The structural transformation of grain boundary (GB) is an important embodiment of these processes [1]. At present, GB research is the most fundamental and active study field in interface science, in particular, in the GB motion coupling with the applied stress or strain [2]. Recent research has led to the recognition that many grain boundaries (GBs) in crystalline materials can couple to applied shear stresses and are moved by them in a manner similar to dislocation glide [3–10]. The coupling can be responsible for the stress-induced grain growth in nanocrystalline materials and can influence the nucleation of new grain during recrystallization. There are two main modes of nanograin growth [11–13], *i.e.*, tha shear-coupled migration (SCM) of the grain boundary, and nanograin rotation (NGR). The dominant mode of the operation depends on grain size, and that these two modes are usually coupled [14]. Now researchers not only still pay more attention to structural transitions of the GBs coupling with stress or strain, but also to the GB character at high temperature [15,16] and GB premelting (GBPM) [17–23]. GBPM was firstly observed in aluminum grain boundary [24] at $0.96T_m$, and then the premelting [25–27] occurred at GBs of Cu and Ag and Cu–Bi alloy at $0.96T_m$ were also reported. GBPM is induced not only as a consequence of the local inner stress around defects, but also by the external stress. The experiment observation of the GBPM induced by the external applied stress on bicrystal of Cu thin-film at temperatures of approximately 0.5 T_m was firstly reported by Inoko et al. [28,29], who refer this type of the GBPM as strain induced GB premeling (SIGBPM).

Due to the fact that the width of the GB usually has a few atom thicknesses, it is difficult to observe the GBPM directly in experiment [17], thus the development of computational simulation experiment can make up for the shortcomings [30]. Molecular-dynamic (MD) [31–33] has been used for simulating the

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evolution of the GBPM at different temperatures close to the bulk melting point. Although much success is obtained by MD simulations of the GBPM, a weakness [34] of the MD approach is that the applied strain rate in simulations is likely to diverge several orders from the actual results. Traditional phase field (PF) approach [35] is also used to simulate the GBPM [36,37], while it is difficult to describe the details of the GBPM on the atomic scale. Elder et al. [38,39] proposed a phase field crystal (PFC) model based on density functional theory in recent years, which can model the evolution of the microscopic structure of the polycrystalline materials on diffusive time and atomic scales, and the applied strain rate in the PFC simulations is good agreement with the actual results. Therefore, PFC has a great advantage in simulating the evolution of microstructure. In the past few years, PFC has been successfully used in many fields of research [40–49]. At present, there have been several studies [50–52] focused on the GBPM phenomenon by PFC approach, in which the GBPM phenomenon is induced by local inner stress surrounding dislocations of GB. For example, these studies include that the transformation of the GB structure due to the premelting individual dislocations merge in the GBPM at symmetric tilt grain boundaries (STGB) takes place to form double dislocation pairs under internal stress [50]. Since the atomic lattice in premelting domain is softening at 0.96T$_m$ high temperature [53], the stick-slip character of the dislocation movement becomes more significant [53]. Because the structure transformation [54,55] of the dislocation of the GBPM can be induced by internal stress, in this condition, if the external stress is applied to exert on the GBPM [52,56,57], what will happen to the GBPM ? This aroused our great interest! That is the motivation for us to study evolution of the GBPM under the external applied strain at high temperature.

In this paper we observe that the initial GBPM regions grow up bigger areas of the softening crystal phase domain (SCPD) under the applied strain at the temperature, and also observe the dislocation interactions including the multiplication of dislocation pairs, the rotation of dislocation pairs and their annihilation. The shape of the SCPD changing with the applied strain increasing is presented. The dislocation configuration evolution which process is very similar to the dynamic process of strain hardening-softening recovery at high temperature under plastic deformation is shown in the SCPD. The microscopic mechanism can well be revealed for the process of the dynamic recovery–controlled dislocation.

2. Model and simulation technique

2.1. PFC model and equation

The simple PFC model proposed by Elder et al. which includes the direct correlation function can be deduced from the classical density functional theory (CDFT) of freezing. The free energy functional of pure materials can be derived from the CDFT [40],

$$\mathrm{F} = \int d\vec{x}\left\{\left[n\left(\vec{x}\right)^2/2 - wn\left(\vec{x}\right)^3/6 + vn\left(\vec{x}\right)^4/12\right] - \frac{1}{2}n\left(\vec{x}\right)K\left(\vec{x}\right)\right\}, \tag{1}$$

where $n(\vec{r})$ is the time-averaged atom number density measured with respect to a reference liquid state, w and v are fitting constants, and $\widehat{K}(\vec{k}) = \widehat{C}_2(\vec{k})\widehat{n}(\vec{k})$, more details of which can be seen in Appendix 1. The direct-correlation function Cˆ2(k) is related to the experimental structure factor $S(\vec{k})$. Defining the following parameters: $\vec{r} = \vec{x}q_0, \rho = n\sqrt{v/q_0^4}$, $e = (\alpha/\lambda q_0^4)$, and $\tilde{F} = (v/q_0^5)F$, the dimensionless free-energy functional can be written as

$$\widehat{F} = \int d\vec{r}\left\{\frac{\rho\left(\vec{r}\right)}{2}\left[e + \left(\nabla^2+1\right)^2\right]\rho\left(\vec{r}\right) + t^*\frac{\rho\left(\vec{r}\right)^3}{3} + \frac{\rho\left(\vec{r}\right)^4}{4}\right\}, \tag{2}$$

Where e and t^* are constants, and t^* relate to the anisotropy of interface; ρ is the rescaled time-averaged atom number density measured with respect to a reference liquid state.

Because our paper does not discuss solid-liquid interface anisotropy, we ignore it and set $t^* = 0$, then the original free energy of PFC model suggested by Elder can be gotten as:

$$\widehat{F} = \int d\vec{r}\left\{\frac{\rho\left(\vec{r}\right)}{2}\left[e + \left(\nabla^2+1\right)^2\right]\rho\left(\vec{r}\right) + \frac{\rho\left(\vec{r}\right)^4}{4}\right\} = \int f\left(\rho(x,y)\right)dV, \tag{2a}$$

Where e is a parameter relate to temperature, ∇^2 is the Laplace operator, and the $\rho(x,y)$ is the time-averaged atom number density measured with respect to a reference liquid state ρ_0 [40]. It can be obtained an analytical expression for equation (2a) in the one-mode approximation [39] under the minimum of the free energy. Then, the atomic density for two-dimensional triangular structure can be written as

$$\rho = A_T\left[\cos(qx)\cos\left(qy/\sqrt{3}\right) - \cos\left(2qy/\sqrt{3}\right)/2\right] + \rho_0, \tag{3}$$

Where ρ_0 is the average density value of liquid phase, the wave vector $q = \sqrt{3}/2$, $A_T = \frac{4}{15}(3\rho_0 - \sqrt{-36\rho_0^2 - 15r})$.

Here considering the external applied strain ε on the system with deviatoric deformation, we can write the energy of system under strain as

$$\widehat{F} = \int f(\rho(x(1-\varepsilon), y(1+\varepsilon)))dV = \int [f(\rho(x,y)) + E_{ext}(\varepsilon,x,y)]dV, \tag{4}$$

Where $E_{ext}(\varepsilon,x,y)$ is the energy change of the system due to the strain. According to reference [58–60], the form of the energy density change can be selected as $E_{ext} = V_{ext}\cdot\rho$, where V_{ext} is the external force field. The benefits of this approach is that the modified free energy in Eq. (3) has the same phase diagram as that in Eq. (2a). The more details for V_{ext} will be given in the next section.

The evolution of the atomic density of the conserved field variable under strain is described by the time-dependent Cahn-Hilliard dimensionless equation [39,56].

$$\frac{\partial\rho}{\partial t} = \nabla^2\left(\frac{\delta F}{\delta\rho}\right) = \nabla^2\left[e\rho + \rho^3 + \left(1+\nabla^2\right)^2\rho + V_{ext}\right]. \tag{5}$$

The evolution of the atomic density distribution in two-dimension is governed by Eq. (5), which is a six order nonlinear partial differential equation and can only be solved by numerical computation method. Here it is solved by using the semi-implicit Fourier spectral method [61,62]. Therefore Eq. (5) can be written in Fourier spaces as