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Effects of a disconnection dipole on the shear-coupled grain boundary migration

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ABSTRACT

Effects of a preexisting disconnection dipole on the migration of a $\Sigma 5(\bar{3}10)/[001]$ grain boundary (GB) at low shear rates have been investigated by using the minimized bulk dissipation phase field crystal model. Simulation results show that the two disconnections play different roles during the process of shear-coupled GB migration *via* different behaviors regarding heterogeneous nucleation and propagation of disconnections. Specifically, the different roles can be attributed to their structural deviation from the equilibrated crystallographic structure caused by shear loading: one disconnection contributes to the onset of GB migration by heterogeneous nucleation of disconnections, while the other one slows down the corresponding GB migration dynamics through the impediment of homogeneous nucleation in the flat GB plane.

1. Introduction

In nanocrystalline materials, stress-induced grain boundary (GB) migration is an important deformation mechanism, especially under shear stress. It is believed that GB migration under shear is operated by different "coupling modes" [1–4] depending on GB structures. A GB can migrate at a velocity v_n coupled with the tangential motion $v_{//}$ of abutting grains along the GB plane by a coupling factor β, i.e., $v_n = \beta v_{//}$, which is usually used to characterize the coupling mode. To determine the mechanism of shear-coupled GB migration, it is important to predict the coupling modes (or coupling factors β) with different kinds of GBs. Hypnotizing that a GB is simply composed of lattice dislocations, Cahn and Taylor [1] proposed a geometrical model (usually called as the Cahn model) for symmetrical tilt GBs, which has been conspicuously evidenced by experiments and simulations [5–9]. As a phenomenological model, however, the Cahn model predicts the coupling modes macroscopically only based on the orientation relationship of GBs but without taking their atomic structural details into account, leading to the limitation of its application in general GB migrations [10]. For instance, it is still debated that lattice dislocations are significant or not if the misorientation is larger than 15° [10]. To overcome this obstacle, Cahn et al. [2] have suggested that the coupling motion can be alternatively interpreted by the motion of step dislocations in GB planes, as explained in the displacement shift complete dislocation model [10]. In fact, step dislocations, i.e., disconnections, were first used by Hirth [11] to characterize the interfacial defects which have a close relationship with GBs, in accordance with the discussion by Kröner [12] in the crystallographic theory of connectivity at interfaces. In fact, disconnections are very suitable to describe the GB motion [13] and other related phenomena, such as deforming twinning [14]. By means of the disconnection description, later, Calliard et al. [3,4] developed a new geometrical model to predict a spectrum of coupling modes in general GBs [15], which has also been verified by experiments [10]. Although it is unlikely to consider details of interatomic interactions in GB migrations [16] in this new geometrical model, the introduction of disconnections sheds some lights on further study of this phenomenon.

Based on the disconnection description, the GB migration under shear stress σ is illustrated as nucleation and propagation of disconnections. For an ideally planar GB, accordingly, when σ reaches a critical value σ_c^{hom}, a number of disconnections will nucleate homogeneously in the normal direction and propagate rapidly along the GB plane, resulting in the coalescence of adjacent disconnections and thus the stick–slip behavior of GB migration [17]. In this case, the homogenous nucleation (HON) of disconnections is the limiting process. However, if there are some preexisting disconnections in curved GBs, which are commonly introduced in real materials by lattice dislocation decomposition or emission from triple junctions [18], heterogeneous nucleation (HEN) near the

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preexisting disconnections can easily occur under a critical stress σ_c^{het} expected to be much smaller than σ_c^{hom}. Numerically, Khater et al. [19] observed that the preexisting disconnections in high angle GBs start to move under a stress σ_c^{het} as small as $\sigma_c^{hom}/100$, while in experiments, the measured σ_c^{het} could also be smaller than $\sigma_c^{hom}/6$ [20]. Therefore, even under a very low shear strain, e.g. far below σ_c^{hom}, the preexisting disconnections in the curved GB are possible to evolve to a large extent and thus affect the whole GB migration behaviors. Recently, Rajabzadeh et al. [18] experimentally found that disconnections will propagate in different behaviors depending on their crystallographic structures. When disconnections are sessile, the whole GB dynamics will be hampered. In fact, the evolution of disconnections, including nucleation and propagation, can be very sensitive to the precise details of their structures. Under a shear strain, disconnections will be strained and thus deviate from the relaxed crystallographic structures. Despite that this deviation is not large, it is still likely to affect the evolution of disconnections as well as the whole GB. Consequently, the preexisting disconnections can impose significant effects on the intrinsic behaviors of shear-coupled GB migration *via* heterogeneous nucleation and propagation.

Unfortunately, these effects are still not fully understood at the atomic scale. The reason for this failure is that, the evolution of disconnections involves not only the atomic length scale but also the diffusive time scale because their burgers vectors often have climb components [18], which makes the molecular dynamic method, a widely used approach to describe atomic scale structure evolution, not suitable any more in this case. The recent proposed phase field crystal (PFC) model [21,22], is a good candidate for studying the atomic GB motion at the diffusive scale and behaviors of GB migration at low rates of shear. To illustrate the effects of preexisting disconnections on GB migration, we choose a curved $\Sigma5(\bar{3}10)/[001]$ GB in body-centered-cubic (BCC) crystals as the study object. An ideally flat GB of $\Sigma5(\bar{3}10)/[001]$ has the lowest Σ value among those with rotation axis [001] in a BCC lattice, which results in some advantages with respect to the structural stability over other GBs, and the stress-induced motion of this GB has also attracted a lot of attentions [20,23–25]. Thus, this kind of GB is typical in studying the shear-coupled migration of GBs with preexisting disconnections. In this study, we employ the PFC model to investigate the effects of a preexisting disconnection dipole on the migration of $\Sigma5(\bar{3}10)/[001]$ GB under low shear strain rates, with emphasis on the HEN and propagation of disconnections.

2. The minimized bulk dissipation phase field crystal model

Here, we use the standard PFC free energy functional [21] with the conserved minimized bulk dissipation (MBD) dynamics proposed by Adland et al. [22,26]. This PFC model is able to relax elastic stress in bulk quickly enough and lets GBs evolve with diffusive dynamics. The standard PFC free energy functional is as follows:

$$\tilde{F} = \int d\vec{r}\left\{\frac{\psi}{2}[-\varepsilon + (\nabla^2+1)^2]\psi + \frac{\psi^4}{4}\right\}, \quad (1)$$

where ψ measures the dimensionless density field, and ε is related to temperature and crystal anisotropy [21]. The corresponding dynamical equation is

$$\frac{\partial^2\psi}{\partial t^2} + \eta h(\chi)\frac{\partial\psi}{\partial t} = \nabla^2\frac{\delta\tilde{F}}{\delta\psi}, \quad (2)$$

where $h(\chi) = (1-\xi)(\chi(\vec{r})-1)^4/(\chi_d-1)^4 + \xi$, is a weighted function to allow crystal and interface to evolve with different dynamics, here $\chi(\vec{r}) = C\int d\vec{r}'\exp(-|\vec{r}-\vec{r}'|^2/2w^2)|\nabla\psi(\vec{r}')|^2$, a function to distinguish between the bulk and GBs, $C = 1/\max\left\{\int d\vec{r}'\exp(-|\vec{r}-\vec{r}'|^2/2w^2)|\nabla\psi_0(\vec{r}')|^2\right\}$, $\psi_0(\vec{r})$ the equilibrated lattice density field that minimizes $\tilde{F}$, η controls the relative strength of elastic dynamics compared to the diffusive one, ξ the ratio of bulk dissipation to interface dissipation, and χ_d the preset value corresponding to $\chi(\vec{r})$ at a dislocation. The physical details of all the parameters and the solving procedure spectrally implemented in the Fourier space can be referenced to Ref. [27]. Here, parameters used in the simulation are $\varepsilon = 0.248, \psi_0 = -0.318$, $\Delta t = 0.05, a = 8.959, \xi = 0.0083$, $\eta = 0.001, \chi_d = 0.66, w = a/2$, where a is the lattice constant of BCC crystal and Δt is the time step. Periodic boundary conditions are used in the directions parallel to the GB plane, while free boundary conditions are employed in the normal directions to avoid another GB forming. It should be noted that there will always be liquids at the end of the simulation block in the normal direction since the system is evolving in the liquid–solid coexistence region. To observe the GB motion, a GB segmentation procedure [28] is conducted to extract the GB outline separating the two neighboring grains.

To implement the shear strain, two planes residing on the two sides of GB plane perpendicular to the y-axis are dragged at a constant velocity $v = a\times10^{-3}/\Delta t$ along the x-axis in opposite directions. Their intercepts with the y-axis are at $d_\mu = L_y/2 - 25a, d_\lambda = L_y/2 + 25a$, respectively, as shown in Fig. 1, where the subscripts λ and μ denote the abutting two grains. The dragging procedure is performed by adding an external function to the original free energy functional as $\tilde{F}_{ext} = \int d\vec{r}[G(y-d_\mu)\psi - \psi_0(x-vt,y,z)^2 + G(y-d_\lambda)\psi - \psi_0(x+vt,y,z)^2]$, where G is the standard Gaussian function.

3. Results and discussion

Fig. 1 shows a schematic representation of a curved $\Sigma5(\bar{3}10)/[001]$ GB containing a disconnection dipole under shear strain, projected onto the x–y plane. According to the Cahn model [2], the as-shown GB is expected to move downward along the negative y-axis by the evolution of disconnections, including the downward nucleation and the propagation along the GB plane. Initially, the equilibrated disconnection dipole in the $\Sigma5(\bar{3}10)/[001]$ GB contains two disconnections which can be represented by two narrow step planes in a mirror fashion, separating the main GB plane and a parallel terrace with a relative height h and a width l, as shown in Fig. 1. The terrace is crystallographically

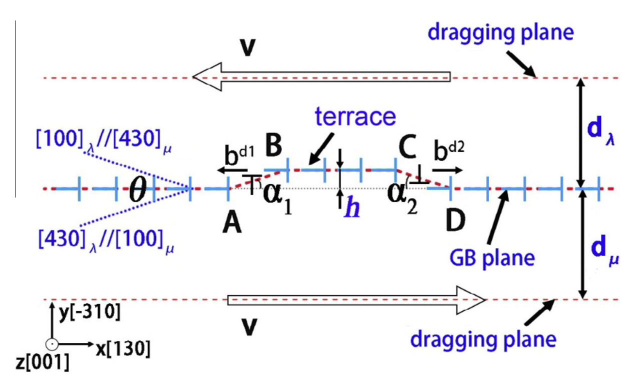

Fig. 1. Sketch of a disconnection dipole in a $\Sigma5(\bar{3}10)/[001]$ GB ($\theta = 36.87°$) separating two abutting grains λ (up) and μ (down), where the coordinate axis is shown at the bottom-left corner. A, B, C and D are four key points for the disconnection dipole. The length of the line segment BC denotes the terrace width l. Projection of GB plane and dragging planes into the x–y plane are displayed by dash lines.