Computational Materials Science 132 (2017) 125–131

Contents lists available at ScienceDirect

Computational Materials Science

journal homepage: www.elsevier.com/locate/commatsci

Coupled motion of grain boundaries and the influence of microcracks: A phase-field-crystal study

Shi Hu *, Wen Xi, Zheng Chen, Song Wang, Ting-Hui Zhang

State Key Laboratory of Solidification Processing, School of Materials Science and Engineering, Northwestern Polytechnical University, Xi'an 710072, China

ARTICLE INFO

Article history:
Received 10 November 2016
Received in revised form 14 February 2017
Accepted 16 February 2017

Keywords:
Phase-field-crystal
Grain boundary
Coupled motion
Microcrack
Grain growth

ABSTRACT

With phase-field-crystal, the two-dimensional coupled motion of grain boundary (GB) in triangular lattice crystal is studied. The migration mechanism of symmetric and asymmetric GBs in bicrystals is explored. Considering microcracks can hardly be avoided in materials, it is necessary to study the influence of microcracks on coupled GB motion. As shown in our simulation results, the influence of microcracks can be classified into three categories: (I) GB passes microcracks and is not impeded, cracks maintain unchanged; (II) Microcracks hinder GB motion, cracks migrate along GB and shrink; (III) GB motion is blocked by microcracks, cracks extend along GB and enlarge. The three kinds of results have great dependence on the misorientation and inclination angles of GB. Moreover, coupled GB motion can also lead to grain growth. The shear-induced grain growth process is simulated. As cracks can impede coupled GB motion, the shear-induced grain growth can also be hindered by cracks.

1. Introduction

The vast majority of natural and man-made metals and alloys are polycrystals. The existence of grain boundaries (GBs) is the main characteristic that distinguishes polycrystals from monocrystals. GBs can have great influence on the physicochemical properties of materials. Many phenomena, such as corrosion, strengthening and premelting, are closely related to GBs. One interesting feature of GB is that it can migrate under applied stress. Cahn and Taylor [1] have proposed a model to explain coupled GB motion. Recently, many experimental and simulation results [2–7] have indicated that GBs can be moved by the coupled effect [8] of applied shear stress. Usually, we can use the coupled factor $\beta = v_\tau / v_n$ to characterize the coupled effect, where v_τ is the velocity of the shear stress parallel to the GB and v_n is the normal GB velocity. The applied shear stress parallel to the GB plane can generate normal GB motion, which is responsible for many grain growth behaviors [9,10].

Although traditional experimental methods, like transmission electron microscope (TEM), can be used to observe microstructural evolution in materials, they are not convenient and effective for directly observing GB motion. In recent years, Elder et al. [11–13] put forward the phase-field-crystal (PFC) method, which is derived from dynamical density functional theory and thermodynamic concepts. As the PFC method operates on atomic length and diffusive time scales, it develops into an efficient alternative to molecular simulation methods, e.g. molecular dynamics (MD), traditional phase-field method, etc. Many microscopic research results [14–17] have been published by using the original PFC model [11–13]. Inspired by these new exciting findings which cannot be effectively achieved by experimental or other simulation methods, the PFC method has been widely utilized and greatly improved. Many modified PFC methods [18–20] have been proposed, promoting the continuous development of PFC method. Some previous works conducted by the PFC simulation have already reproduced the coupled effect for symmetric tilt boundaries in two-dimension (2-D) [21] and 3-D [22]. Specifically, Trautt et al. [23] have investigated the influence of misorientation and inclination angles on the coupled factor of symmetric tilt GBs between 2-D square lattices, using the two-mode PFC model [24].

In the processing and manufacturing processes, microcracks can be inevitably generated on the surface or in the interior of materials. And more microcracks can be initiated during using and depositing. Under external influential factors, these microcracks can expand and lead to fracture failure. However, almost all materials are working with microcracks, provided that the microcracks can maintain stability under certain working conditions. Therefore, it is necessary to study the influence of stable microcracks on material properties. The interaction between microcracks and cou-

* Corresponding author.
E-mail address: hshi@mail.ustc.edu.cn (S. Hu).

http://dx.doi.org/10.1016/j.commatsci.2017.02.021
0927-0256/

pled GB motion is an interesting topic, which has been seldom touched by PFC method. Furthermore, as coupled GB motion can lead to grain growth, the influence of microcracks on the stress-assisted grain growth is also worth studying.

The goals of this work are to explore the coupled GB motion and the influence of microcracks in triangular lattice crystals in 2-D space. The rest of this paper is organized as follows. In Section 2, the PFC equations, system geometry, applied shear stress, and dynamics equation are outlined. In Section 3, the mechanisms of coupled GB motion are studied from microstructural perspective. In Section 4, the influence of microcracks on coupled GB motion in systems with different misorientation and inclination angles is studied. Lastly, the shear-induced grain growth, related to coupled GB motion, and the influence of microcracks are investigated in Section 5.

2. PFC simulation methods

In this work, we select the one-mode PFC model [11], which is much more convenient and efficient to be modeled and analyzed, to simulate 2-D GBs between triangular lattices. The free energy of the PFC model has been derived from the perturbative density functional theory proposed by Ramakrishnan and Yussouff [25] in the late 1970s. The dynamics of the number density field ρ is assumed to be dissipative and driven to minimize the free energy functional F, which is given by [11]:

$$F = \int d\boldsymbol{r}\left\{\frac{\omega}{2}\left[-\zeta + (1+\nabla^2)^2\right]\omega + \frac{1}{4}\omega^4 + \omega V_{ext}\right\} \tag{1}$$

$\omega(r, t)$, the crystal density field, is defined as $\omega(r, t) = (\rho(r, t) - \rho_0)/\rho_0$, where ρ_0 is the reference value of liquid phase. ∇^2 stands for Laplace operator and ζ is the super-cooling degree related to temperature. The quantities involved in Eq. (1) are all dimensionless. V_{ext}, specified below, represents an external potential applied to shear the simulated system.

As triangular lattice is simulated, the approximation for ω can be written as [11]

$$\omega = \omega_0 + A_t\left[\cos(q_t x)\cos\left(\frac{\sqrt{3}}{3}q_t y\right) - \frac{1}{2}\cos\left(\frac{2\sqrt{3}}{3}q_t y\right)\right] \tag{2}$$

where q_t is wave number. By means of free energy minimization, A_t and q_t can be acquired as shown below [11]

$$A_t = -\frac{4}{15}\left(-3\phi_0 - \sqrt{15r - 36\phi_0^2}\right), \quad q_t = \frac{\sqrt{3}}{2} \tag{3}$$

To determine the values of ω, we need to compute the phase diagram. By taking a derivative of the free energy with respect to the density fields of the triangular and liquid phases, and then using the common tangent rule, the 2-D phase diagram [15,26] can be derived as shown in Fig. 1.

The schematic arrangement of the constructed simulation system is given in Fig. 2. To create a stable GB, we construct two separate crystals and join them along a plane normal to the y-direction. Periodic boundary condition is imposed in the x-direction, and apparently fails in the y-direction. The orientation angle of grain, θ_1 and θ_2, is defined as the angle rotated clockwise relative to the y-direction. The misorientation angle θ is defined as the angle between the $[\bar{1}\,2\,\bar{1}]_1$ axis in grain 1 and the $[\bar{1}\,2\,\bar{1}]_2$ axis in grain 2. Then we can get $\theta = \theta_1 - \theta_2$, with $\theta > 0$ corresponding to the $[\bar{1}\,2\,\bar{1}]_1$ axis rotated clockwise relative to the $[\bar{1}\,2\,\bar{1}]_2$ axis. The inclination angle φ is defined as the angle between the y-direction and the internal bisector between the $[1\,\bar{2}\,1]_1$ and $[\bar{1}\,2\,\bar{1}]_2$ axes. Therefore, $\varphi = (\theta_1 + \theta_2)/2$. We take $\varphi \geq 0$ if the bisector is rotated clockwise relative to the y-direction. Similarly, we can obtain two GBs by adding a third grain. Considering the sixfold symmetry of triangular lattice, all possible combinations of θ and φ can be found in the domain $\{-\pi/6 \leq \theta < \pi/6, -\pi/6 \leq \varphi < \pi/6\}$.

Since the PFC method is not able to model solid-vacuum interfaces [17,23,27], we cannot use free surfaces to simulate shearing deformation process. However, we can simulate free surfaces by making the atomic density ω vary spatially over narrow strips near the solid-liquid interfaces, as illustrated in Fig. 2. ω varies from ω_s to ω_l along the y-direction, normal to the solid0liquid interface. ω_s and ω_l are the atomic densities of the solid and liquid phases, respectively.

Applied shear stress is imposed by choosing

$$V_{ext}(x,y) = \omega_0 + A\left\{\cos[q_t(x \pm n\varepsilon\Delta t)]\cos\left(\frac{\sqrt{3}}{3}q_t y\right) - \frac{1}{2}\cos\left(\frac{2\sqrt{3}}{3}q_t y\right)\right\} \tag{4}$$

where ε is the constant shear rate. n is time steps the solid-liquid interface needed to move a grid distance. Δt is the time-step size. A, adopted as $A = A_t$ here, stands for the amplitude of shear stress. V_{ext} is applied on the two solid-liquid interfaces (the gray zones shown in Fig. 2). Eq. (4) is consistent with Eq. (2) in form, which can produce coupled effect and simulate shearing effects more efficiently.

According to the modified PFC equation proposed by Stefanovic et al. [18], the dimensionless time evolution equation for ω can be expressed as following:

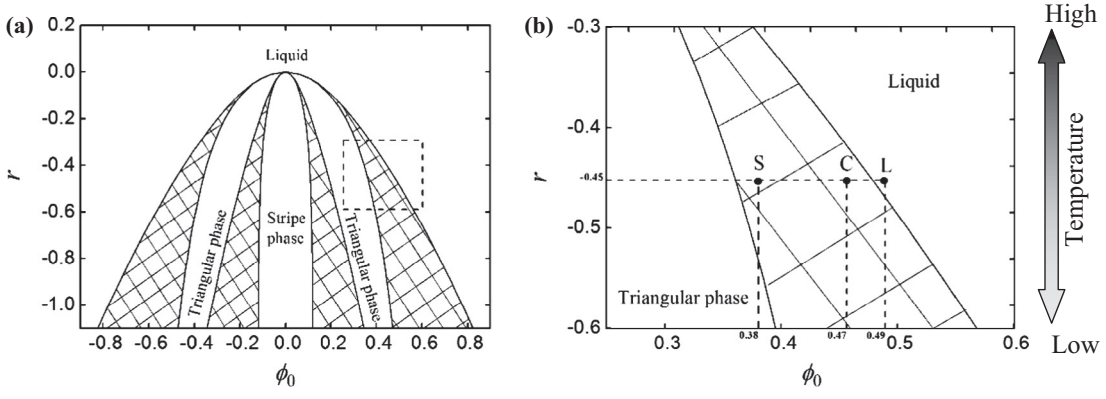

Fig. 1. (a) 2-D phase diagram as calculated by one-mode approximation (the meshed areas correspond to two-phase coexistence regions). (b) Enlarged image of the region enclosed by dashed box in (a).