Journal of the Mechanics and Physics of Solids 117 (2018) 157–178

Contents lists available at ScienceDirect

Journal of the Mechanics and Physics of Solids

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

Motion of grain boundaries incorporating dislocation structure

Luchan Zhang, Yang Xiang*

Department of Mathematics, The Hong Kong University of Science and Technology, Clear Water Bay, Kowloon, Hong Kong

ARTICLE INFO

Article history:
Received 6 October 2017
Revised 23 April 2018
Accepted 4 May 2018
Available online 5 May 2018

Keywords:
Grain boundary dynamics
Dislocation dynamics
Long-range elastic interaction
Grain rotation
Coupling and sliding

ABSTRACT

In this paper, we present a continuum model for the dynamics of low angle grain boundaries in two dimensions based on the motion of constituent dislocations of the grain boundaries. The continuum model consists of an equation for the motion of grain boundaries (i.e., motion of the constituent dislocations in the grain boundary normal direction) and equations for the dislocation structure evolution on the grain boundaries. This model is derived from the discrete dislocation dynamics model. The long-range elastic interaction between dislocations is included in the continuum model, which ensures that the dislocation structure on a grain boundary is consistent with the Frank's formula. These evolutions of the grain boundary and its dislocation structure are able to describe both normal motion and tangential translation of the grain boundary and grain rotation due to both coupling and sliding. Since the continuum model is based upon dislocation structure, it naturally accounts for the grain boundary shape change during the motion and rotation of the grain boundary by motion and reaction of the constituent dislocations. Using the derived continuum grain boundary dynamics model, simulations are performed for the dynamics of circular and non-circular two dimensional grain boundaries, and the results are validated by discrete dislocation dynamics simulations.

1. Introduction

Grain boundaries are the interfaces of grains with different orientations and they play essential roles in the polycrystalline materials (Sutton and Balluffi, 1995). Grain boundaries migrate under various driving forces such as the capillarity force, the bulk energy difference, the concentration gradients across the boundary, and the applied stress field. The motion of grain boundaries crucially determines the mechanical and plastic behaviors of the materials. The classical grain boundary dynamics models are based upon the motion by mean curvature to reduce the total interfacial energy (Herring, 1951; Mullins, 1956; Sutton and Balluffi, 1995) using the misorientation-dependent grain boundary energy (Read and Shockley, 1950). There are extensive studies in the literature on such motion of grain boundaries by using molecular dynamics or continuum simulations, e.g. (Chen and Yang, 1994; Elsey et al., 2009; Esedoglu, 2016; Kazaryan et al., 2000; Kirch et al., 2006; Kobayashi et al., 2000; Lazar et al., 2010; Upmanyu et al., 2002; 1998; 2006; Zhang et al., 2005).

It has been shown that the grain boundary normal motion can induce a coupled tangential motion which is proportional to the normal motion, as a result of the geometric constraint that the lattice planes must be continuous across the grain boundary (Cahn and Taylor, 2004; Li et al., 1953; Srinivasan and Cahn, 2002). Besides the tangential motion coupled with normal motion, there is another type of tangential motion that is the relative rigid-body translation of the grains along

---

* Corresponding author.
E-mail address: maxiang@ust.hk (Y. Xiang).

https://doi.org/10.1016/j.jmps.2018.05.001

the boundary by sliding to reduce the grain boundary energy (Esedoglu, 2016; Harris et al., 1998; Kobayashi et al., 2000; Li, 1962; Shewmon, 1966; Upmanyu et al., 2006). This sliding motion is independent of all other grain boundary motions. When a grain is embedded in another one, the tangential motions along a grain boundary give rise to a relative rotation between the two grains, leading to change of the misorientation of the grain boundary. In the grain rotation due to sliding, the misorientation angle goes to the nearby local energy minimum state (decreases for a low angle grain boundary), whereas in the grain rotation due to coupling, the misorientation angle increases. The coupling and sliding motions depend on the grain boundary structure and mechanisms of the dynamics. Rath et al. (2007) showed by a simple dislocation model and experimental observations that grain boundary motion does not have to couple with tangential motion. In fact, the coupling and sliding effects cancel out in their case.

Cahn and Taylor (2004) and Taylor and Cahn (2007) proposed a unified approach to the phenomena of the coupling and sliding associated with the grain boundary motion. They formulated the total tangential velocity $v_{\parallel}$ as the superposition of the coupling and sliding effects: $v_{\parallel} = \beta v_{\perp} + v_s$, where the tangential velocity induced by coupling effect is proportional to the normal velocity $v_{\perp}$ with the coupling parameter β, and v_s is the tangential velocity produced by sliding effect. They discussed different cases for the rotation of a circular cylindrical grain embedded in another one (Cahn and Taylor, 2004). When the grain does not have such symmetry, they proposed a generalized theory based on mass transfer by diffusion confined on the grain boundary (Taylor and Cahn, 2007).

Molecular dynamics simulations have been performed to validate the theory of Cahn and Taylor on the coupling grain boundary motion to shear deformation for planar grain boundary (Cahn et al., 2006a; 2006b), and grain boundary migration and grain rotation for closed circle cylindrical grain boundaries (Srinivasan and Cahn, 2002; Trautt and Mishin, 2012). Experimental observations have also been reported on the migration of low angle planar tilt boundaries coupled to shear deformation in Al bicrystal with stress (Gorkaya et al., 2009; Molodov et al., 2007). The ratios of the normal to the lateral motion that they measured are complied with the coupling factors in the theory and atomistic simulations by Cahn and Taylor (2004) and Cahn et al. (2006a,b). Phase field crystal model (an atomistic-level model) was employed to simulate the dynamics of a two-dimensional circular grain, and grain rotation and translation by motion and reaction of the constituent dislocations were observed (Wu and Voorhees, 2012). Phase field crystal simulations also showed that the coupling of grain boundary motion in polycrystalline systems can give rise to a rigid body translation of the lattice as a grain shrinks and that this process is mediated by dislocation climb and dislocation reactions (McReynolds et al., 2016). Three-dimensional phase field crystal simulations were further performed to investigate the motion, rotation and dislocation reactions on a spherical grain in a BCC bicrystal (Yamanaka et al., 2017). Numerical simulations based upon the generalization of the Cahn–Taylor theory to noncircular grains (Taylor and Cahn, 2007) were performed using the level set method (Basak and Gupta, 2014).

In this paper, we present a continuum model for the dynamics of low angle grain boundaries in two dimensions based on the motion of constituent dislocations of the grain boundaries. The continuum model consists of an equation for the motion of grain boundaries (i.e., motion of the constituent dislocations in the grain boundary normal direction) and equations for the dislocation structure evolution on the grain boundaries (Eqs. (12) and (13), or Eqs. (14) and (15) in Section 3). The long-range elastic interaction between dislocations is included in the continuum model, which ensures that the dislocation structures on the grain boundaries are consistent with the Frank's formula for grain boundaries (the condition of cancellation of the far-field elastic fields). These evolutions of the grain boundary and its dislocation structure are able to describe both normal motion and tangential translation of grain boundaries and grain rotation due to both coupling and sliding effects. Since the continuum model is based upon dislocation structure, it naturally accounts for the grain boundary shape change during the motion and rotation of the grain boundary by motion and reaction of the constituent dislocations without explicit mass transfer. Unlike the Cahn–Taylor theory (Cahn and Taylor, 2004) in which the coupling effect is an assumption, our model is based on the motion of the grain boundary dislocations and the coupling effect is a result. Our model also generalizes the Cahn–Taylor theory by incorporating detailed formulas of the driving forces for the normal and tangential grain boundary velocities that depend on the constituent dislocations, their Burgers vectors, and the grain boundary shape, as well as the shape change of the grain boundaries. Our model is different from their earlier generalization based on the assumption of the coupling effect and mass transfer via surface diffusion (Taylor and Cahn, 2007). Note that in some existing continuum models for the motion of grain boundaries and grain rotation (Esedoglu, 2016; Kobayashi et al., 2000; Li, 1962; Shewmon, 1966; Upmanyu et al., 2006), evolution of misorientation angle was included to reduce the grain boundary energy density. These models able to capture the grain boundary sliding but not coupling. In our continuum model, we use dislocation densities on the grain boundary as variables instead of the misorientation angle, which enables the incorporation both the grain boundary coupling and sliding motions. Using the derived continuum grain boundary dynamics model, simulations are performed for the dynamics of circular and non-circular two dimensional grain boundaries.

We also perform discrete dislocation dynamics simulations for the dynamics of these grain boundaries and the simulation results using the two models agree excellently with each other. In particular, both our continuum and discrete dislocation dynamics simulations show that without dislocation reaction, a non-circular grain boundary shrinks in a shape-preserving way due to the coupling effect, which is consistent with the prediction of the continuum model in Taylor and Cahn (2007) based on the assumption of the coupling effect and mass transfer via surface diffusion.

Our continuum grain boundary dynamics model is based upon the continuum framework for grain boundaries in Zhu and Xiang (2014) derived rigorously from the discrete dislocation dynamics model. Previously, a continuum model for the energy and dislocation structures on static grain boundaries has been developed (Zhang et al., 2017a) using this framework. In fact, the energetic and dynamic properties of grain boundaries were understood based on the underlying dislocation mechanisms