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Grain boundary migration and grain rotation studied by molecular dynamics

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Abstract

We report on molecular dynamics simulations of an isolated cylindrical grain in copper shrinking under capillary forces. At low temperatures, the coupling between grain boundary (GB) migration and grain translation induces rotation of the grain towards higher or lower misorientation angles, depending on the initial misorientation. The dynamics of the GB motion and grain rotation are studied as functions of the initial misorientation angle and temperature. The effects of imposed constraints blocking the grain rotation or exerting a cyclic torque are examined. The simulation results verify several predictions of the model proposed by Cahn and Taylor [Acta Mater 52, 4887 (2004)]. They also indicate that the GB motion is never perfectly coupled but instead involves at least some amount of sliding. This, in turn, requires continual changes (annihilation or nucleation) in the GB dislocation content. Dislocation mechanisms that can be responsible for the motion of curved GBs and dislocation annihilation in them are proposed.

Keywords: Molecular dynamics; Grain boundary; Dislocation; Grain rotation

1. Introduction

Grain rotation in polycrystalline materials is part of microstructure evolution, along with other processes such as phase transformations, grain coarsening and dislocation motion. Grain rotation was observed experimentally during plastic deformation [1,2], recrystallization [3] and grain growth [4,5]. It was also found to accompany stress-driven grain boundary (GB) motion in bicrystals subject to a tensile load [6]. Several theories have been proposed to explain the driving forces and mechanisms of grain rotation. In particular, it was suggested that grains rotate to decrease the GB free energy γ [4]. This process was indeed observed in atomistic computer simulations [7,8]. It was also shown [9,10] that grain rotation can be induced by GB motion due to the coupling effect, which will be discussed below. In the latter case, grain rotation can lead to an increase in γ, provided that the GB area shrinks sufficiently fast to produce a net decrease in the total GB free energy [9]. As a mechanism of grain rotation, diffusion-controlled viscous flow along GBs was adopted in several models [3,11,12]. For low-angle GBs, models combining dislocation glide with climb were developed to explain subgrain rotation and coalescence during recovery and early stages of recrystallization [3,5,11,13,14].

Cahn and Taylor [10] proposed a unified approach to GB motion, grain translation and grain rotation. The underlying idea of their approach is the existence of coupling between GB migration and rigid translations of the grains parallel to the boundary. A coupled GB produces plastic shear deformation of the lattice regions swept by its motion, which in turn causes grain translation. Conversely, a shear stress applied parallel to a coupled GB induces its normal motion. Stress-induced GB motion was observed experimentally [6,15–25] and by atomistic simulations [9,26–30], and is considered to be responsible for stress-induced grain growth in nanocrystalline materials [19,31–34]. The reader is referred to [35] for a recent review of the coupling effect.

An interesting consequence of the coupling effect, pointed out in [9,10], is that coupled motion of a curved

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GB must induce grain rotation. Cahn and Taylor [10] proposed a model of grain rotation based on a linear dissipation approximation. They applied this model to describe evolution of an isolated cylindrical grain with a circular cross-section shrinking by capillary forces. A number of possible scenarios were discussed, depending on the presence or absence of coupling, GB sliding, applied shear stresses and other factors [10]. In particular, the model predicts that a low-angle GB induces grain rotation towards higher angles and thus larger γ. Such a rotation was indeed observed in molecular dynamics (MD) simulations of a cylindrical grain in a Lennard–Jones system [9]. More recently, Wu and Voorhees [36] applied the phase field crystal (PFC) method to model the shrinkage of an isolated circular grain in a two-dimension hexagonal system. At misorientation angles below 10°, the grain shrinkage produced grain rotation towards increasing angles.

Since the publication of [9], significant progress has been achieved in understanding the geometric rules and atomic mechanisms of coupled GB motion through a series of experimental studies [6,15–25] and MD simulations [26–30]. It seems timely to revisit the grain rotation problem, building on the new knowledge combined with recent improvements in computational methodologies and power. The goals of this work are to conduct a systematic MD study of a cylindrical grain similar to [9], compare the results with the Cahn–Taylor model [10], and gain insights into microscopic mechanisms of GB motion and grain rotation. Our simulations are based on a realistic interatomic potential for copper, which was employed in previous work on coupled GBs [26–29]. We study a wide range of temperatures and examine the effects of imposed constraints and applied torque on GB dynamics.

To make the paper self-contained, we start with a brief overview of the Cahn–Taylor model (Section 2) and point to several predictions that can be directly compared with atomistic simulations. Our simulation methodology is introduced in Section 3. In Sections 4–7 we present our simulation results for the dynamics of GB motion and grain rotation, including simulations with prohibited grain rotation and applied torque. In Section 8 we compare our simulation results with the Cahn–Taylor model and discuss possible dislocation mechanisms that could be responsible for the coupled GB migration, GB sliding and grain rotation. Our conclusions are summarized in Section 9.

2. The Cahn–Taylor model of grain shrinkage and rotation

Fig. 1 illustrates the geometry and conventions adopted in the Cahn–Taylor model [10]. We consider an isolated cylindrical grain with a circular cross-section and an instantaneous radius R. The grain is embedded in an outer grain and its lattice is rotated around the cylinder axis by an angle θ relative to the outer grain. The unit normal of the GB, **n**, is pointing towards the center of the embedded grain. The GB velocity is denoted v_n and is considered positive if parallel to **n** and negative if anti-parallel. The

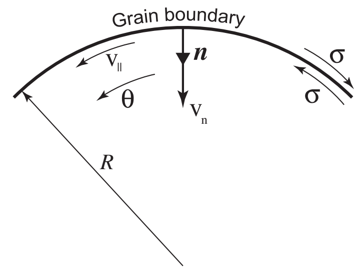

Fig. 1. Geometry and sign conventions in the Cahn–Taylor model [10] of an isolated cylindrical grain.

misorientation angle θ and the grain rotation velocity $v_{\parallel}$ next to the GB are positive in the counter-clockwise direction and negative otherwise. The shear stress σ is considered positive if it tries to rotate the grain in the counter-clockwise direction. The following kinematic relations are obvious:

$$v_n = -\dot{R} \tag{1}$$

$$v_{\parallel} = R\dot{\theta} \tag{2}$$

where the dot denotes the time derivative. Let the initial grain radius and angle be R_0 and θ_0, respectively.

It is postulated that the tangential velocity $v_{\parallel}$ is composed of the GB sliding velocity $\tilde{v}_{\parallel}$ and the coupling velocity βv_n,

$$v_{\parallel} = \tilde{v}_{\parallel} + \beta v_n \tag{3}$$

where β is the coupling factor introduced in Refs. [10,28]. Generally, β can depend not only on θ but also on the GB plane inclination, which varies along the GB. Eq. (3) assumes that the coupling factor has been averaged over all inclinations spanned by the GB and became a function θ only: $\beta = \beta(\theta)$.

To obtain the equations of GB motion, we first calculate the rate of total free energy change per unit height of the cylinder. The latter equals the rate of free energy change of the bicrystal, $\dot{f}$, minus the rate of work, $\dot{w}$, done against the applied shear stress $\sigma : \dot{f}_{tot} = \dot{f} - \dot{w}$. The two components of f are the GB free energy $2\pi R\gamma$ and the excess volume free energy density, p, inside the grain relative to its environment:

$$f = 2\pi R\gamma + \pi R^2 p \tag{4}$$

The excess p can be due to a defect concentration, magnetic energy or other factors. This excess is assumed to be homogeneous and independent of time. The GB free energy γ is assumed to be uniform over the boundary and depend on θ only: $\gamma = \gamma(\theta)$. Thus,

$$\dot{f} = 2\pi\dot{R}\gamma + 2\pi R\gamma'\dot{\theta} + 2\pi Rp\dot{R} \tag{5}$$

where $\gamma' := d\gamma/d\theta$. Also,

$$\dot{w} = 2\pi R\sigma v_{\parallel} \tag{6}$$

Combining the above equations,

$$\dot{f}_{tot} = -2\pi R(P_n v_n + P_{\parallel}\tilde{v}_{\parallel}) \tag{7}$$