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Capillary-driven grain boundary motion and grain rotation in a tricrystal: A molecular dynamics study

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Abstract

We report on molecular dynamics (MD) simulations of a tricrystal composed of a cylindrical grain embedded at the center of a plane grain boundary (GB). The embedded grain shrinks by capillary forces and eventually vanishes. This process is often accompanied by rotation of the embedded grain in either a clockwise or counter-clockwise direction. Using the geometric theory of coupling between GB motion and grain translations, we propose a model capable of predicting the direction of the grain rotation depending on the crystallographic parameters of the three grains. Full agreement has been found between the model predictions and the MD simulation results for both spontaneous grain shrinkage and in the presence of applied shear stresses. The consequences of these results for grain rotation in polycrystalline materials and possible extensions of the model to multiple grains are discussed.

Keywords: Modeling; Grain boundary; Rotation; Capillary

1. Introduction

Grain rotation is part of microstructure evolution in polycrystalline materials and has been observed experimentally during plastic deformation [1,2], recrystallization [3] and grain growth [4,5]. Rotation of an isolated cylindrical grain was predicted theoretically [6–8] and observed in computer simulations by molecular dynamics (MD) [6,9–12] and the phase-field crystal (PFC) method [13]. In most cases the grain rotation could be explained by the existence of coupling between grain boundary (GB) motion and shear deformation of the lattice [6–8,14,15].

In real materials, isolated grains are extremely rare. Most grains are surrounded by several other grains and are separated from those by multiple GBs and triple junctions. One could expect that this complexity would suppress the grain rotation, or at least make it a rare occurrence, for at least two reasons. First, the triple lines can be expected to act as pinning sites since the grain rotation requires accommodation of incompatibilities along the triple lines [16–18]. Second, assuming that the magnitude and sign of the grain rotation depend on geometric parameters of the GB, different GBs would try to rotate the grain in different directions, reducing or even blocking the net rotation. Nevertheless, in certain cases the individual GBs can exert forces acting in the same direction and collectively causing the grain to rotate. The ability to predict such cases requires a better understanding of the geometric conditions for grain rotation by individual GBs and the role of triple junctions in this process.

Because of the complexity of the general polycrystalline problem, it is strategically meaningful to start with a relatively simple configuration amenable to quantitative analysis and then continue to build up the complexity by adding more grains. As such, a perfect starting point is offered by a tricrystal consisting of a cylindrical grain sitting on a plane GB. This configuration involves two different GBs surrounding the embedded grain and two different triple lines. The embedded grain spontaneously shrinks by capillary forces and may or may not rotate in the process.

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This tricrystalline structure was studied by MD simulations in a two-dimensional Lennard–Jones system with a triangular lattice [11]. No rotation was found when the two curved GBs were symmetrically equivalent, leading to cancellation of the rotational forces. When the symmetry was broken, rotation was observed in some cases but not in others, and was apparently influenced by the presence of open surfaces in the simulated models. The important observation was, however, that the presence of two different GBs and two triple lines did not prevent the grain rotation. More recently, Wu and Voorhees [13] reported on two-dimensional PFC simulations of a similar tricrystalline system with hexagonal lattices. The geometry was symmetrical with the curved GBs having opposing misorientations of $\pm 5.2^\circ$. As expected from this symmetry, no grain rotation was observed, in agreement with the MD simulations [11]. Although interesting insights into the dislocation mechanisms of GB migration were obtained, grain rotation under asymmetric conditions was not tested.

In this work we address the same tricrystalline configuration but in a more systematic manner. Based on the analysis of geometric coupling factors, we propose a simple analytical model that permits predictions of the direction of grain rotation, depending on the misorientation angles of the GBs. We then conduct a series of MD simulations designed to test this model. All three GBs are chosen to be [0 0 1] tilt type. The atomic interactions are modeled with an accurate atomistic potential to ensure realistic character of the results. As a further test of the model, we conduct simulations under a shear stress applied parallel to the plane GB and driving the collective motion of all three boundaries.

In Sections 2 and 3 we introduce our model and propose analytical expressions for the effective coupling factor governing the grain rotation. These two sections also serve to introduce a set of sign conventions for the angles and coupling factors; the nature of the problem makes it important to adopt and strictly follow such conventions in order to avoid confusion. In Section 4 we describe the simulation methodology and details of the GB geometries tested in this work. The results of the MD simulations for the spontaneous shrinkage of the embedded grain are presented in Section 5, followed by stress driven simulations in Section 6. We conclude the paper by discussing the comparison between the proposed model and the simulation results and outlining future work (Section 7).

2. Coupling model for curved grain boundaries

To set the stage for the discussion of curved GBs, we will first review the geometric theory of coupling for plane GBs. Fig. 1 illustrates the geometry of a plane asymmetrical [0 0 1] tilt GB between two face-centered cubic (fcc) crystals, defining the tilt angle θ and the inclination angle ϕ. Angle θ measures the misorientation between [1 0 0] directions in the grains, with $\theta = 0$ for a single crystal and $\theta > 0$ when the $[1\,0\,0]_U$ axis in the upper grain is rotated counter-clockwise

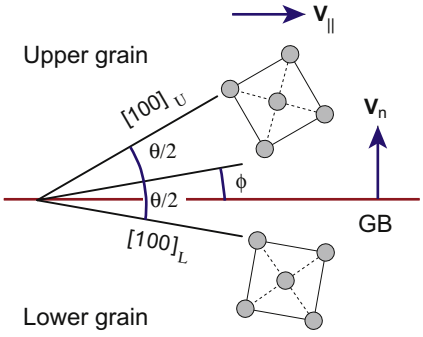

Fig. 1. Schematic geometry of [0 0 1] asymmetrical tilt GBs between fcc crystals defining the tilt angle θ, the inclination angle ϕ, the normal GB velocity v_n and the parallel grain translation velocity $v_{||}$ of the upper grain relative to the lower.

relative to $[1\,0\,0]_L$ in the lower grain. The inclination is characterized by the angle ϕ between the GB plane and the internal bisector between the [1 0 0] directions in the grains, with $\phi > 0$ if the bisector is rotated in the counter-clockwise direction relative to the GB plane. Due to the fourfold lattice symmetry around the [0 0 1] axis, all distinct GB structures can be found in the angular domain $\{0 \leqslant \theta < 90^\circ, -45^\circ \leqslant \phi < 45^\circ\}$. Symmetrical tilt GBs arise at $\phi = 0$ and again at $\phi = \pm 45^\circ$, all other boundaries being asymmetrical.

The coupling factor of the boundary is defined as the velocity ratio $\beta = v_{||}/v_n$ (Fig. 1). Following the sign convention of [8,14,15], $\beta > 0$ when the GB moves up while the upper grain translates to the right or when the GB moves down while the upper grain translates to the left. The coupling is called perfect, or pure, if β is a geometric constant depending only on the GB bicrystallography and not on the boundary velocity, driving force or any other physical parameter. An interesting feature of the coupling effect is that the coupling factor is a multi-valued function of the crystallographic angles. Owing to this multiplicity, physically the same GB can display different coupling factors and thus different mechanical responses to the same applied stress [8,14,15].

For symmetrical boundaries with $\phi = 0$, the fourfold symmetry generates four possible coupling modes with the coupling factors $\beta = 2\tan(\theta/2 - \pi k/4)$, $k = 0, 1, 2, 3$. Two of them, corresponding to the smallest magnitude of β, have been observed in simulations [8,14,15,19,20] and experiments [21–25], whereas the remaining two modes require exceedingly high stresses to activate and have never been reported. The two observed coupling modes are referred to as $\langle 1\,0\,0\rangle$ and $\langle 1\,1\,0\rangle$ type and have the coupling factors

$$\beta_{\langle 100\rangle} = 2\tan\left(\frac{\theta}{2}\right) > 0 \tag{1}$$

and

$$\beta_{\langle 110\rangle} = 2\tan\left(\frac{\theta}{2} - \frac{\pi}{4}\right) < 0 \tag{2}$$