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Simultaneous grain boundary motion, grain rotation, and sliding in a tricrystal

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ABSTRACT

Grain rotation and grain boundary (GB) sliding are two important mechanisms for grain coarsening and plastic deformation in nanocrystalline materials. They are in general coupled with GB migration and the resulting dynamics, driven by capillary and external stress, is significantly affected by the presence of junctions. Our aim is to develop and apply a novel continuum theory of incoherent interfaces with junctions to derive the kinetic relations for the coupled motion in a tricrystalline arrangement. The considered tricrystal consists of a columnar grain embedded at the center of a non-planar GB of a much larger bicrystal made of two rectangular grains. We examine the shape evolution of the embedded grain numerically using a finite difference scheme while emphasizing the role of coupled motion as well as junction mobility and external stress. The shape accommodation at the GB, necessary to maintain coherency, is achieved by allowing for GB diffusion along the boundary.

1. Introduction

Grain boundaries (GBs) and junctions play an important role in various deformation processes within nanocrystalline (NC) materials which have an average grain size of few tens of nanometers and hence contain a large volume fraction of boundaries and junctions. The microstructural evolution in NC materials, especially during grain coarsening and plastic deformation, is dominated by grain rotation and relative grain translation coupled with GB migration (Meyers et al., 2006; Wang et al., 2014; Koch et al., 2007; Harris et al., 1998). The resulting motion is called coupled GB motion (Cahn and Taylor, 2004; Taylor and Cahn, 2007). The presence of triple junctions, which can occupy up to 3% volume fraction in NC materials when the average grain size is around 10 nm (Chapter 5 of Koch et al. (2007)), induces drag on GB migration and affects the coupled motion in a significant way (Czubayko et al., 1998; Wu and Voorhees, 2012). For an illustration of the coupled motion consider an isolated tricrystal arrangement, as shown in Fig. 1(a), where a grain is embedded at the center of the planar GB of a large bicrystal. In the absence of external stress, the embedded grain spontaneously rotates due to GB capillarity, thus changing its orientation, while shrinking to a size shown in Fig. 1(b). The embedded grain can disappear either by shrinking to a vanishing volume or by reorienting itself to one of the neighboring grains. Grain rotation can be accomplished through either a pure viscous sliding, or a tangential motion geometrically coupled with GB migration, or a combination of both (Cahn and Taylor, 2004; Taylor and Cahn, 2007). If the tricrystal is subjected to external stress, the grains can accomplish relative translational motion as well (Trautt and Mishin, 2014); the center of rotation of the embedded grain then need not remain fixed in space.

Our aim is to develop a thermodynamically consistent framework to study the coupled GB motion in the presence

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of triple junctions as driven by GB capillarity and external stress. More precisely, the main results of the present contribution are:

(i) Developing a novel continuum framework, restricted to two dimensions, to study the dynamics of incoherent interfaces with junctions. An irreversible thermodynamical theory of incoherent interfaces, excluding junctions, has been previously developed by Cermelli and Gurtin (1994). On the other hand, junctions have been studied only with respect to coherent interfaces (Simha and Bhattacharya, 1998). Furthermore, these previous studies were based on the configurational mechanics framework which requires *a priori* postulation of configurational forces and their balances. In the present formulation the configurational forces appear as mechanisms of internal power generation so as to ensure that the excess entropy production remains restricted to only interfaces and junctions.

(ii) Extending the existing theory of coupled GB motion to include triple junctions and relative tangential translation. The earlier work on coupled motion was restricted to bicrystals with a grain embedded within a larger grain such that the center of rotation of the embedded grain remains fixed (Cahn and Taylor, 2004; Taylor and Cahn, 2007; Basak and Gupta, 2014). The possibility of including junctions and relative translation of the grains was ignored in these models. These extensions were nevertheless mentioned by Taylor and Cahn (2007) in their list of open problems related to coupled GB motion.

(iii) Performing numerical simulations for shape evolution of grains and GBs during coupled motion. Towards this end, we consider a tricrystalline arrangement (as shown in Fig. 3) and solve the coupled kinetic relations for GB motion, rotational and translational movements of the grains, and junction dynamics. The dynamical equations are solved using a finite difference scheme adapted from a recent work on triple junctions of purely migrating GBs (Fischer et al., 2012). Our results are qualitatively in agreement with a recent paper (Trautt and Mishin, 2014) concerned with molecular dynamics (MD) simulations of the coupled motion in a tricrystal.

We assume that the grains are rigid, free of defects, and do not posses any stored energy. The defect content as well as the energy density are confined to grain boundaries. Isothermal condition is maintained throughout. The assumption of grain rigidity is justified since we consider the magnitude of the external stress to be much lower than the yield stress. Also, in the present scenario the GBs do not exert any far-field stress and GB capillary exerts very low pressure on the neighboring grains. The shape accommodation process, required to avoid nucleation of void or interpenetration of the grains at the GBs during relative rotation of the embedded grain, is controlled by allowing for diffusion along the GBs. Bulk diffusion in the grains, as well as across the GBs, is taken to be negligible compared to GB diffusion (Koch et al., 2007). Furthermore, since both GBs and grains move at much smaller velocities than the velocity of sound in that material, the inertial effects are ignored. The above assumptions provide the simplest setting to pursue a rigorous study of coupled GB dynamics.

The paper has been organized as follows. After developing the pertinent thermodynamic formalism in Section 2, the kinetic relations for the tricrystalline configuration are derived in Section 3. The numerical results are presented in Section 4. Finally, Section 5 concludes our communication.

2. Thermodynamic formalism

The dissipation inequalities at GBs and junctions are now derived within the framework of Gibbs thermodynamics, where various thermodynamic quantities (such as energy, entropy, etc.) defined over interfaces and junctions are understood as excess quantities of the system. We begin by fixing the notation before deriving the consequences of the second law of thermodynamics in terms of various dissipation inequalities.

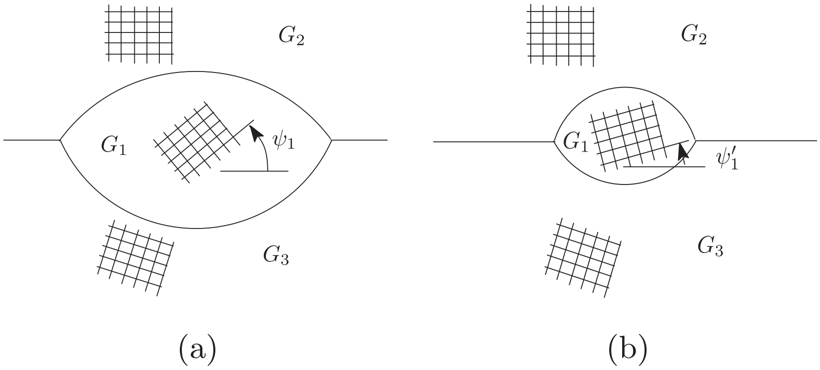

Fig. 1. A schematic to depict the coupling between GB motion and rotation of grain G_1 under GB capillary force in a tricrystal. Diagram (a) shows the initial configuration which evolves to (b) at a later time. The outer grains G_2 and G_3, being much larger than G_1, are taken to be stationary (after Trautt and Mishin (2014)).