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Surface morphologies due to grooves at moving grain boundaries having stress-driven fluxes

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Abstract

We modify a previous steady-state description developed by Gènin [J. Appl. Phys. 77, 5130–5137 (1995)] for a grain boundary groove moving with a prescribed speed in a material subject to in-plane stress and a resultant grain boundary flux. The arbitrary assumption that the grain boundary flux is equally delivered to (or extracted from) the two adjacent free surfaces of the grains is replaced by a condition that requires continuity of surface chemical potentials at the grain boundary. Analytical results for the small-slope approximation as well as nonlinear results for large slopes are computed numerically for steady-state motion at a specified groove speed. We apply these results to a "partial loop" grain boundary geometry that moves by mean curvature induced by the groove conditions. In contrast to the ordinary effect that a grain boundary surface groove retards grain boundary motion, the presence of a compressive stress and resultant grain boundary flux toward the free surface can promote grain boundary motion.
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1. Introduction

Gènin [1,2] has developed a model for a moving grain boundary groove in a material under a compressive stress. The effect of a compressive normal stress on the grain boundary chemical potential causes a flux of material along the grain boundary toward the free surface. If the grain boundary is moving, this flux deposits preferentially on the trailing surface, causing the formation of a hillock. These results have been applied to understand the height profiles of hillock grains of Al measured by atomic force microscopy [3,4]. Gènin also noted that a flux from the interior onto the surface due to the existence of compressive in-plane stress could, under certain circumstances, augment the motion of the grain boundary, i.e. the groove could "push" the grain boundary. As pointed out by Gènin, increased motion of the grain boundary leads to a more efficient method to relieve the internal compressive stress by transferring material from the interior to the surface onto the trailing side of the moving grain boundary groove.

We generalize the Gènin model [1] to remove an unnecessary assumption regarding how the grain boundary flux is split onto the two adjacent sides of the moving grain boundary groove. Gènin employed the superposition of two solutions in the small-slope approximation: (i) the Mullins solution [5] for a grooved moving boundary but no grain boundary flux, and (ii) a new solution for a moving boundary with no groove but including a grain boundary flux produced by stress. Since the governing differential equation is linear within the small-slope approximation, superposition of solutions is certainly allowed. However, there is a problem with the superposition of the boundary conditions. The Mullins solution assumed equality of surface chemical potential on either side of the groove. For his new solution (ii), Gènin abandoned this condition and instead added the arbitrary condition that the grain boundary flux is split evenly, left

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and right, along the two surfaces. In this paper we solve the problem with a consistent set of boundary conditions that does not presume an equal split of the grain boundary flux, but instead assumes equality of surface chemical potential on either side of the groove.

The work of Gènin was based on research initiated by Mullins. Grain boundary grooving, wherein a groove forms at the perpendicular intersection of a stationary grain boundary with a free surface, was first modeled by Mullins [6]. Mullins showed in the small-slope approximation that the groove evolves with a self-similar shape whose dimensions enlarge with time as $t^{1/4}$ for surface diffusion or $t^{1/3}$ for volume diffusion. For volume diffusion in an adjacent liquid, this result was later extended to the large-slope nonlinear regime [7] and compared with experiment, resulting in agreement within 5% of measured surface tension. The small-slope theory was extended to include grain boundary motion [5], grain boundary fluxes produced by stress for a static grain boundary [8], and finally by Gènin to the case of both grain boundary motion and boundary fluxes produced by stress [1], as mentioned above. In all of these extensions, transport by bulk diffusion is ignored, since grain boundary and surface diffusion should dominate for groove sizes of experimental interest.

Under situations where there is no stress, a grain boundary groove normally exerts a drag on grain boundary motion. This drag is quantified by an angle, θ_c, introduced by Mullins for a moving groove. This angle is the deviation of the grain boundary from the perpendicular to the nominal surface. It is defined as positive if the grain boundary tilts toward the direction of motion as it goes into the interior. The Mullins paper showed, for steady-state grain boundary motion, that the angle was fixed at $M/6$ (M is the ratio of the grain boundary energy to the surface energy) independent of the speed of the groove if no barrier exists for atoms to cross the triple junction along the surface from the leading to the trailing side of the groove. (See details on this assumption under item iv of Section 3.1 below.) The work of Kanel et al. [9] confirmed the results of the critical angle of Mullins and quantified the drag effect of the grain boundary groove. They solved the coupled equations for the surface diffusion near the grain boundary groove and motion of the interior grain boundary due to curvature. They employed a quarter loop grain geometry that permits the existence of a steady-state motion [10]. The decreased speed of the grain boundary with a groove compared to the speed of a grain boundary without a groove was calculated.

When the substrate is stressed (and a grain boundary flux is present), Gènin showed that the critical angle was not constant at $M/6$. Indeed if the boundary is under compression and a flux of material on the grain boundary exits toward the surface, θ_c is decreased. For sufficiently high values of the flux, the angle becomes negative. Thus the drag of a grain boundary groove decreases as the flux increases and for sufficiently high values of flux the groove can push the grain boundary.

We first make the correction to the Gènin model mentioned above. The predicted shape of the moving groove is changed as is the expression for the tilt angle as a function of flux. Second, we extend this model by removing the small-slope approximation and determine the range of parameters where the small-slope approximation is valid. Third, we use a modification of the steady state quarter-loop model to develop an expression for the velocity of a grain boundary as a function of grain boundary flux toward the surface (biaxial compression) for a "partial loop," wherein the grain boundary is vertical at some distance below the surface. This model quantifies how a grain boundary flux toward the surface can push a grain boundary.

2. Fundamental equations

In this section we provide the fundamental nonlinear equations that underlie grain boundary grooving by surface diffusion under stress, including grain boundary fluxes. For a two-dimensional problem, we also develop the corresponding nonlinear boundary conditions. Then we discuss an approximate model, due to Gènin, Mullins and Wynblatt [8], that relates grain boundary flux to stress. Finally, we simplify these equations and boundary conditions by means of a small-slope approximation for steady-state problems.

2.1. Surface diffusion/accretion

The theory of Mullins [6] for a single-component system is based on Herring's formula [11] for the chemical potential on a curved surface, namely:

$$\mu_s = \mu_0 + \gamma_s \Omega K, \tag{1}$$

where μ_s is the chemical potential of an atom on the surface, μ_0 is the chemical potential of an atom on a flat surface, γ_s is the surface free energy (assumed to be isotropic), Ω is the atomic volume and K is the mean curvature. The surface flux (in units of atoms per unit length and time) due to surface diffusion and relative to bulk crystal is given by:

$$\mathbf{J} = -v_s \frac{D_s}{kT} \nabla_s \mu_s = -\frac{D_s v_s \gamma_s \Omega}{kT} \nabla_s K = -\frac{B}{\Omega} \nabla_s K, \tag{2}$$

where $B = D_s v_s \gamma_s \Omega^2 / kT$; here, D_s is the surface diffusion coefficient (in units of length squared divided by time), v_s is the number of atoms per unit area of the interface (usually taken as $v_s = \Omega^{-2/3}$), T is the absolute temperature, k is Boltzmann's constant, and ∇_s is the surface gradient operator. The negative of the surface divergence of $\mathbf{J}$, namely $-\nabla_s \cdot \mathbf{J}$, represents a local accumulation (atoms per unit area per unit time) of atoms which causes the surface to move normal to itself according to:

$$-\nabla_s \cdot \mathbf{J} = \frac{v_n}{\Omega}, \tag{3}$$