



# Modified Young's equation for equilibrium dihedral angles of grain boundary grooves in thin films at the nanoscale



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## ARTICLE INFO

### Article history:

Received 11 August 2015

Received in revised form

15 September 2015

Accepted 20 September 2015

Available online 8 October 2015

### Keywords:

Grain boundary groove

Atomistic modelling

Young's equation

Surface energy

Dislocations

## ABSTRACT

We derive the modified Young's equation for the equilibrium dihedral angle at the triple junction of the grain boundary groove by taking into account the discrete structure of the low angle grain boundary. For low angle grain boundaries, the geometric relation that the misorientation of the bicrystal is inversely proportional to the dislocation spacing naturally gives rise to the variation in the misorientation when the grain boundary length changes (holding the number of dislocations constant). The fact that the grain boundary energy increases as the grain boundary length decreases due to a smaller dislocation spacing leads to a larger dihedral angle compared to that of the classical theory. Two atomistic continuum modelling tools, namely the phase field crystal model and the amplitude equations, are used to simulate the equilibrium dihedral angle. The numerical results are in quantitatively good agreement with the derived modified Young's equation. Furthermore, the amplitude equations are employed to investigate the kinetics of the grain boundary grooving. The time-independent groove shape as predicted by Mullins is observed for bicrystal with high misorientation, and the groove width scales with time approximately as a power law  $t^{1/4}$ . For bicrystals with small misorientations, the groove root exhibits a stick-slip motion due to volatile dislocation motion toward the liquid phase as it is close to the triple junction.

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## 1. Introduction

Solid–solid and solid–liquid interfaces play crucial role in many metallurgical and materials processes such as the microstructural evolution during solidification from melts [1–8], grain growth in polycrystalline materials [9–13], and grain boundary grooving – be it thermal [14–22], liquid [23–25] or electrochemical [26,27].

The evolution of microstructures is closely related to the energetic and kinetic properties of interfaces; in the case of grain boundary grooving, it is also influenced by the junctions where multiple interfaces meet. The dihedral angle at the triple junction is one of the important physical quantities that influences the morphology of microstructures.

The equilibrium dihedral angle at the triple junction is a result of a balance between grain boundary energy and solid–vapour interfacial energy in the case of thermal grooving and grain boundary energy and solid–liquid interfacial energy in the case of liquid grooving; in the classical description, it is given by the Young's

equation. The classical Young's equation for the grain boundary grooving rests on the assumptions that the solid–vapour/solid–liquid interfacial energy is isotropic and the grain boundary energy is fixed for the bicrystal. Then the dihedral angle is related to the ratio of the grain boundary energy and the solid–vapour/solid–liquid interfacial energy.

At this point, it should be noted that coherency strain energies, electrochemical processes and impressed fields such as electric field can also influence grooving (liquid and electrochemical) [26–28]. However, in this paper, we restrict our attention to only those cases in which only the grain boundary and interfacial energies play the crucial role. In addition, as in the case of liquid grooving, the diffusion kinetics can also play a crucial role. Again, in this paper, we restrict ourselves to systems where there are no such fast diffusion paths influencing the groove structure.

In thermal grooving, the local equilibrium dihedral angle is shown to dictate the time-independent groove shape under the assumption that the local equilibrium dihedral angle remains constant at the groove root by Mullins [14]. However, the fixed grain boundary energy assumption requires revision as one considers the atomistic details of the grain boundary.

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For bicrystals with small misorientations, the structure of the grain boundary is composed of an array of dislocations whose spacing is inversely proportional to the misorientation. Read and Shockley derived a relation between the grain boundary energy and the misorientation based on the above-mentioned grain boundary structure and elastic properties of edge dislocations [29]. For small misorientation, the Read–Shockley relation predicts that the grain boundary energy increases with the misorientation. By considering the discreteness of the grain boundary for bicrystals with small misorientations, as the length of the grain boundary varies the dislocation spacing varies accordingly which gives rise to the variation in the misorientation (i.e., variation in the grain boundary energy). Therefore, the grain boundary energy can no longer be treated as a constant in finding the dihedral angle at the triple junction using the variational principle.

In this paper, we derive a modified Young's equation that takes into account the discrete structure of the grain boundary for small misorientations, and the prediction of the modified Young's equation is examined using the phase field crystal (PFC) model and its amplitude equations.

The PFC method has been developed as an efficient computational approach to model elastic and plastic deformations in crystals on atomistic length scales, and on a time scale that is much larger than molecular dynamics (MD) simulations [30–32]. The free-energy functional used in the PFC is closely related to classical density functional theory (DFT) [32–35], and many interface properties are realistic and comparable to those found in MD simulations [34,36,37]. The elastic properties of crystals, the structure of grain boundaries, and the behaviour of edge dislocations in the PFC model have been investigated previously [31,38–44]. The density field in the PFC model represents the average density over time, thus it averages out fluctuations at short time scales, therefore, the atomistic details of the evolution of grain boundaries and dislocations can be easily identified. However, the PFC model is computational intensive in resolving atoms spatially while it evolves at the diffusive time scale. Therefore, the amplitude equations of the PFC model [35,45–47] which reduce the computational costs by separating the length scales of the envelope of the density waves and the lattice periodicity are introduced to simulate grain boundary grooves for large domains. In this paper, both the PFC model and amplitude equations are employed to determine the solid–liquid interfacial energy, the grain boundary energy, and the dihedral angle of the triple junction. The results are compared to the classical Young's equation and the modified Young's equation for various misorientations.

This article is organized as follows. In section 2 we derive an analytical expression for the equilibrium dihedral angle of the grain boundary groove using the variational principle. We introduce the PFC model, the amplitude equations, and the coexistent properties in section 3. In section 4 simulation details and results of the equilibrium dihedral angle are given along with the comparison between simulations and theory. Moreover, the dynamics of grain boundary grooving are investigated numerically for small and large misorientations, and the results are compared with Mullins theory of thermal grooving. The conclusions are presented in section 5.

## 2. Equilibrium dihedral angles of grain boundary grooves

### 2.1. Young's equation

In classical theory, the equilibrium dihedral angle is a result of the minimization of total surface energies or equivalently the balance of surface tensions at the triple junction. Assume that the misorientation of the bicrystal remains constant and isotropic solid–liquid interfaces. The dihedral angle at the grain boundary

groove is related to the solid–liquid interfacial energy,  $\gamma_{sl}$ , and the grain boundary energy,  $\gamma_{gb}$ , by Young's relation,

$$\cos \frac{\Psi}{2} = \frac{\gamma_{gb}}{2\gamma_{sl}}. \quad (1)$$

The dihedral angle decreases while the grain boundary energy increases, and the dihedral angle ceases to exist as the grain boundary energy is greater than twice the solid–liquid interfacial energy,  $\gamma_{gb} > 2\gamma_{sl}$ .

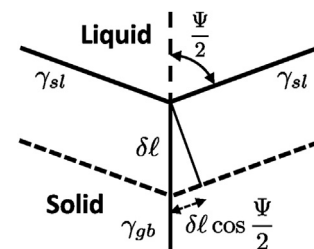
### 2.2. Modified Young's equation

However, the Young's relation is derived based on the continuum picture where the spatial structure of the solid–liquid interface and the grain boundary is homogeneous, and the grain boundary and solid–liquid interfacial energies remain constant during grooving. Nevertheless, for low angle grain boundaries, the structure of the grain boundary is composed of discrete dislocations. For low angle grain boundaries, we assume that the number of dislocations is conserved. As shown by Bachurin et al. [48], if the misorientation is small enough, the dislocations attain metastable equilibrium points and do not egress. Thus when the length of the grain boundary decreases, the dislocations have to re-arrange themselves spatially to remain evenly spaced to avoid excess strain energy accumulated in the crystal. The resulting dislocation spacing becomes smaller which leads to larger misorientation due to the geometric constraint for a symmetric tilt grain boundary  $\theta = b/d$ , where  $b$  is the magnitude of Burgers vector and  $d$  is the spacing between dislocations. The grain boundary energy changes with the misorientation according to the Read–Shockley relation. Thus it is crucial to incorporate the variation of the grain boundary energy in predicting the dihedral angle of grain boundary grooves.

In order to give a quantitative argument, we consider the grain boundary groove consists of two isotropic solid–liquid interfaces and a grain boundary of length  $\ell$ . As depicted in Fig. 1, the variation of the total surface energy due to a small variation of the length of the grain boundary,  $\delta\ell$ , is

$$\delta F = \gamma_{gb}\delta\ell + \delta\gamma_{gb}\ell - 2\gamma_{sl}\delta\ell\cos\frac{\Psi}{2}, \quad (2)$$

where the physical origin of the second term is the rearrangement of dislocations which leads to variation of the grain boundary energy. Assume that the number of dislocations,  $n_0$ , remains the same as we vary the grain boundary length, then the variation of the misorientation of the bicrystal increases (decreases) while the length of the grain boundary decreases (increases),  $\delta\theta = -b\delta d/d^2$ . If the grain boundary consists large amount of dislocations, the dislocation spacing is approximately the length of the grain boundary divided by the number of dislocations,  $d \approx \ell/n_0$ . The



**Fig. 1.** Schematic plot of solid–liquid interfaces and the grain boundary at the groove root. The variation of the length of the grain boundary gives rise to not only the variation of the length of the solid–liquid interfaces but also the variation of the misorientation of the bicrystal.

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