Equilibrium Morphology of Crystal-Melt Grain Boundary Grooves

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Abstract:

A general solution is presented for coupled grain boundary groove morphology at a crystal-melt interface in a thermal gradient. The analysis employs a variational solution for the solid-liquid grain boundary groove and incorporates a general Fourier-series description of anisotropic interfacial energy in two dimensions. Numerically computed groove morphologies illustrate the dramatic effect of anisotropy on the coupled groove depth and overall shape. In the case where the included grains are oriented symmetrically about the grain boundary, the junction condition was rigorously shown to be equivalent to that given by Herring's equation. For asymmetric groove configurations, however, Herring's equation does not adequately address the constraints of local equilibrium. Because of the mismatch in the normal interface energies, asymmetric grain orientations give rise to an effective remote migration force, not accounted for by local force-balance at the junction. Moreover, calculations of asymmetric groove energy reveal that the equilibrium structure must exhibit a tilted grain boundary, where the angle is sufficient to balance the migration force.

Recent Results

We consider the morphology of a crystal-melt interface in the vicinity of a grain boundary which is normal to the solid-liquid interface and normal to the 2-D analysis frame. The orientation of each grain is specified by the inward in-plane rotation angle, ϕ, between the macroscopic normal, $\boldsymbol{N}$, and a common crystallographic reference direction. It is further assumed that the two included grains are symmetrically orientated with respect to the grain boundary plane and that the grain misorientation is far from any "special" low-energy condition such that the grain boundary energy can be assumed to be isotropic. The solid-liquid interfacial energy is considered generally anisotropic but small in magnitude so that no orientations are missing from the equilibrium shape. Given this construction, the task at hand is to specifically describe a self-consistent shape, $y(x)$ or $y(\theta)$, which everywhere satisfies the conditions for local equilibrium.

The variational solution yields the locus of possible groove junctions $h(a)$,

$$h^2\lambda - 2\gamma_N + 2\gamma_a \sec\theta_a - \gamma_{gb}\tan\theta_a = 0 \qquad (1)$$

where γ is an arbitrary, low amplitude function of θ. Integration of the undercooling along the boundary yields

$$h^2 = 2\int_0^{\theta_a} \xi \sin\theta d\theta \qquad (2)$$

where ξ is the normalized interfacial stiffness, $(\gamma+\gamma_{\theta\theta})/\gamma_0$. Here, all spatial coordinates have been scaled by a characteristic gradient length, $l_g=(\gamma_0/G\Delta S)^{1/2}$, and all interfacial energies have been normalized by γ_0.

Defining the interfacial energy, generally, on this plane as

$$\gamma(\theta) = \sum_{k=-n}^{n} A_k e^{ik\beta} \qquad (3)$$

and combining (1) and (2), the coupled groove solution is obtained as

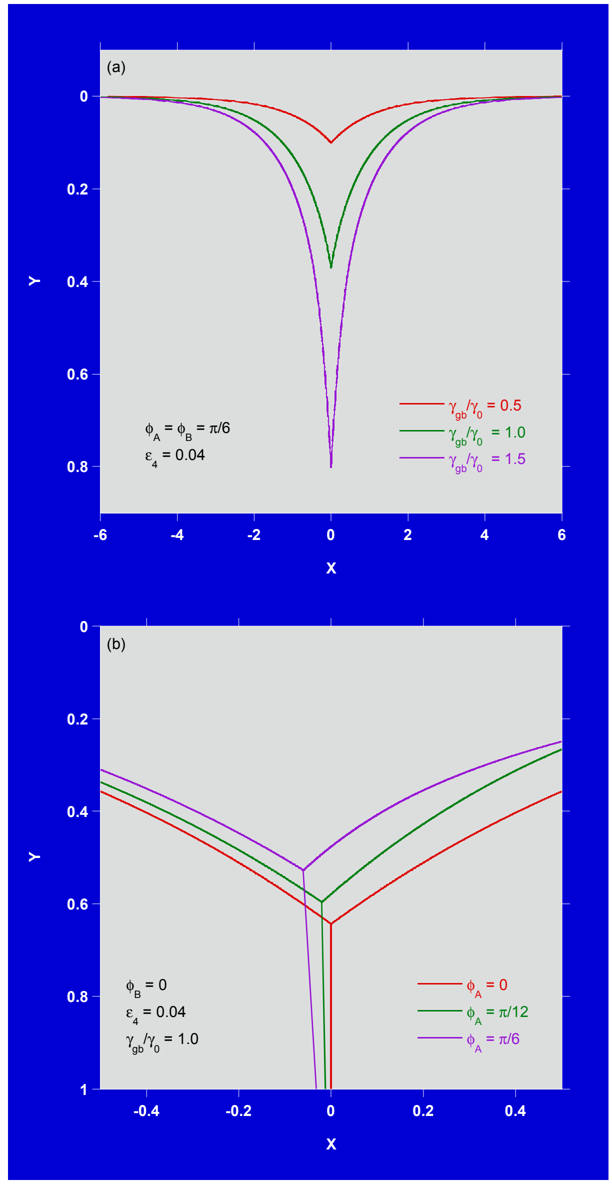
$$\frac{1}{2}\bar{\gamma}_{gb}\tan\theta - \bar{\gamma}\sec\theta + \cos\theta = \sum_{k=1}^{n}\varepsilon_k f_k(\theta,\phi) \qquad (4)$$

where

$$f_k(\theta,\phi) = \begin{bmatrix}\cos(k\phi)\\ -\sin(k\phi)\end{bmatrix} \bullet \begin{bmatrix}\cos(k\theta) & \sin(k\theta)\\ -\sin(k\theta) & \cos(k\theta)\end{bmatrix}\begin{bmatrix}\cos\theta\\ k\sin\theta\end{bmatrix}$$

and the subscript, a, has been dropped for convenience. Eq. (4) represents a general solution for the fully coupled groove morphology, where interfacial energy is generally anisotropic with arbitrary periodicity. Corresponding computed groove shapes are shown in Fig.(a), illustrating the effects of anisotropy, grain boundary energy, and grain orientation.

For the asymmetric case, the groove will tend to migrate laterally (from the reference state) in the direction of the grain with highest γ^N. Examples of asymmetric groove shapes (for $\Delta\phi$=3.5x10^{-4}=0.02°), are given in Fig.(b) for several grain configurations.



Significance

Grain boundary (and phase boundary) grooves at solid-liquid interfaces play a critical role in pattern formation during solidification. Such grooves serve as initiation sites for morphological instability in single-phase solidification. In addition, the conditions at triple junctions are important in the selection of eutectic and other coupled growth morphologies. Beyond their importance as microstructural features, grain boundary grooves offer a means for the measurement of interfacial properties. Indeed the periodicity of the constrained equilibrium shape of a grain boundary groove may be used to experimentally probe the anisotropy of interfacial energy, which is a critical parameter in morphological selection in metallic systems.

Future Work

The theory of grain boundary groove morphology will be extended to include more detailed descriptions of anisotropy. Experimental measurement of grain boundary grooves is also in progress for the determination of interface energy anisotropy in metallic systems.

Interactions

The work described here is related to the general investigation of interfacial properties and their effects on solidification dynamics. Accordingly, there are various interactions with Ames Laboratory researchers in other focus areas as well as outside of Ames Laboratory. For example, the determination of interfacial properties is an integral part of the efforts of the DOE-CMSN.