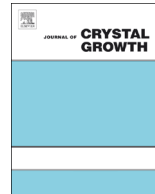




Contents lists available at ScienceDirect

Journal of Crystal Growth

journal homepage: www.elsevier.com/locate/jcrysgro

Surface rippling during solidification of binary polycrystalline alloy: Insights from 3-D phase-field simulations

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ARTICLE INFO

Keywords:

Phase-field modeling
Solidification
Morphological instabilities
Growth models
Diffusion-limited patterns

ABSTRACT

The mechanisms by which crystalline imperfections initiate breakdown of a planar front during directional solidification remain a topic of longstanding interest. Previous experimental findings show that the solid-liquid interface adjacent to a grain boundary provides a potential site where morphological instabilities initiate. However, interpretation of experimental data is difficult for complex 3-D diffusion fields that develop around grain multi-junctions and boundary ridges. We apply a phase-field approach to investigate factors that induce interfacial instabilities during directional solidification of a binary polycrystalline alloy. Using 2-D simulations, we establish the influence of solid-liquid interfacial energies on the spatial localization of initial interfacial perturbations. Based on parametric studies, we predict that grain misorientation and supersaturation in the melt provide major crystal growth factors determining solute segregation responsible for surface rippling. Subsequent breakdown of boundary ridges into periodic rows of hills, as simulated in 3-D, conform well with experiments. Finally, the significance of crystal misorientation relationships is elucidated in inducing spatial alignment of surface ripples.

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1. Introduction

The mechanism by which interfacial free energy is minimized by grain boundary grooving at triple junctions is well known. By definition, thermal grooves pertain to solid-vapor, whereas liquid grooves correspond to solid-melt interfaces. In the present article, we focus on the influence of liquid grooves in instigating surface instability during solidification.

The dihedral angle, θ_d , at the triple point of a grain boundary groove develops at equilibrium as a result of solute diffusion. The equilibrated groove exhibits a pair of convex ridges that are symmetrically disposed about the line of intersection of the solid-liquid interface and the grain boundary, provided that the interfacial energy of the adjacent grains does not depend on the local grain orientation to the melt. When constitutional supercooling overcomes the interface-stabilizing thermal gradient, instability arises and protruding ridges progressively amplify from the groove. Mullins [1,2] established the kinetic law for grain boundary grooving with corresponding power-law exponents of $\frac{1}{4}$ and $\frac{1}{3}$ for surface and volume diffusion-controlled kinetic regimes,

respectively. Several works discussing theoretical aspects of boundary grooving have been reported since the 1960s [3–6]. Bolling and Tiller [3] described stationary groove profiles of pure materials analytically with solid-liquid interfacial energy, thermal gradient, and dihedral angle. It is reported that the preferred growth directions depend upon the anisotropy in surface energy.

Coriell and Sekerka [4,5] elucidated grain boundary-mediated morphological instabilities by applying linear stability theory for unidirectional solidification of pure materials and binary alloys. The spreading of instabilities from initial perturbations can be described by a Green's function [7]. Bokstein et al. [6] propose a model of liquid grooving to investigate the kinetic (dissolution) and diffusion regimes at grain boundaries with zero (or nearly zero) dihedral angles.

Grain boundary grooving has been observed and reported in numerous experiments on alloy solidification. By experimentally analyzing the isothermal grain boundary grooving in the Sn–Pb alloy, Hardy et al. [8] establish synergies with Mullins' power-law. Independent experimental investigations on solidification of dilute Pb–Sb [9] and Al–Cu [10] alloys also reveal that grain boundary grooves provide potent sites for initial perturbations; all these findings agree with theoretical predictions. Further, it is suggested that crystal orientation has a strong influence on morphological

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amplification of ridges and patterns evolving at later stages [9].

In order to expose and analyze the mechanisms by which interfacial morphological instability initiates adjacent to grain boundary grooves, optically transparent analogues, such as succinonitrile-based alloys (SCN) and $\text{CBr}_2\text{-C}_2\text{Cl}_6$, were frequently employed for such directional solidification experiments. The pioneering study on morphological instabilities adjacent to crystalline imperfections by Schaefer and Glicksman [11] shows that grain boundaries play a key role by initiating morphological instability of primary ridges. As the initial ridges amplify, parallel secondary ridges appear beside them. The primary ridges progressively break down into periodic rows of hillocks and knobs, some of which eventually evolve to ramified dendritic patterns. A detailed elaboration of these concomitant events is provided in Section 5.

Noël et al. [12,13] investigated the influence of grain boundaries and natural convection on microstructure formation in cellular directional solidification of dilute SCN alloys. Their findings confirmed that the dynamic grooving of grains occurs by the propagation of ridges and depressions along grain boundaries. Experimental results by Xing et al. [35] accentuate the potency of grain boundaries in initiating morphological instabilities. The initial perturbations observed adjacent to the grain boundary are reported to be larger than others. Further, it is suggested that preferred grain orientations dominate during growth competition as the complex patterns evolve. Fig. 1(a–h) shows an exemplary evolution of the solid-liquid interface near the grain boundary of succinonitrile-0.9 wt% p-dichlorobenzene (SCN-DCB) alloy for an applied thermal gradient of 6.2 K/mm and a pulling velocity of 2.80 m/s.

The phase-field simulation method, long established in the material science community, provides a superlative numerical approach to describe microstructural evolution during solidification, solid-state and electrochemical transformations [14–18]. Two-dimensional phase-field simulations of morphological instability adjacent to liquid grooves were reported earlier by Yeh et al. [19] and by Miller et al. [20]. Both of these works capture the critical onset of morphological instability near the intersecting grain boundary that typically is characterized by “hump amplification.” However, the influence of lateral flux-assisted solute segregation results in a progressive breakdown of the solid-liquid interface—a process termed “rippling.” For further aspects of this process, which, heretofore, have not been addressed in detail, see Fig. 19 in Morris and Winegard [9]. Indeed, further investigation is warranted to achieve a more precise understanding of defect-induced interfacial breakdown during directional solidification.

The remainder of this study is organized as follows: we first describe the methodology, by using constructed free energy densities, to approximate the variation of the grand-potentials of the solid and liquid phases as functions of their chemical potentials. In Section 3, a validation is presented of phase-field grain boundary groove simulations checked against classical analytic solutions.

The importance of surface energy and grain misorientation in initiating morphological instability is elaborated using 2-D simulations in Section 4. Section 5 is devoted to 3-D analysis of the mechanisms by which primary ridges amplify, along with a discussion of the significance of crystal misorientation relationships inducing spatial alignment of surface ripples. Section 6 contains conclusions and the outlook from this study.

2. Thermodynamics

The grand-chemical potential phase-field model used for our numerical investigation is outlined in Appendix A. The free energy of a phase α , in a 2-phase model binary alloy (A-B), are described by the following form,

$$f_{\alpha}(c_A, c_B, T) = A^{\alpha}(T)c_A^2 + B^{\alpha}(T)c_B^2 + D^{\alpha}(T)c_A + E^{\alpha}(T)c_B + K^{\alpha}(T), \quad (1)$$

where c_A and c_B are the concentrations of components A and B, respectively, and A^{α} , B^{α} , D^{α} , E^{α} and K^{α} are the temperature-dependent coefficients for phase α . On imposing the binary alloy constraint $c_A + c_B = 1$, one may rewrite the Equation (1) as follows:

$$f_{\alpha}(c_A, T) = O^{\alpha}(T)c_A^2 + P^{\alpha}(T)c_A + Q^{\alpha}(T), \quad (2)$$

where $O^{\alpha} = A^{\alpha} + B^{\alpha}$, $P^{\alpha} = D^{\alpha} - 2A^{\alpha} - E^{\alpha}$ and $Q^{\alpha} = B^{\alpha} + E^{\alpha} + K^{\alpha}$. The corresponding grand-potential densities are calculated algorithmically as outlined by Choudhury et al. [21]. We point out that the present generalization of free energy density by a polynomial facilitates straightforward coupling with CALPHAD databases, as exemplified by previous numerical studies on binary alloys [22–27] and ternary alloys [28,29,21]. As the present investigation is not limited to a specific alloy, we construct the parabolic free energy densities such that the equilibrium mole fractions of B in the solid grains and liquid phase are conveniently calculated to be 0.8 ($c_B^{s,eq}$) and 0.2 ($c_B^{l,eq}$), respectively. The relevant simulation parameters are listed in their dimensional form in Table 1. Since we are primarily interested in generic features of ripple formation, the reported times are normalized by l_0^2/D^l , where $l_0 = \sigma/(RT/V_m)$ is the capillary length, T denotes the isothermal transformation

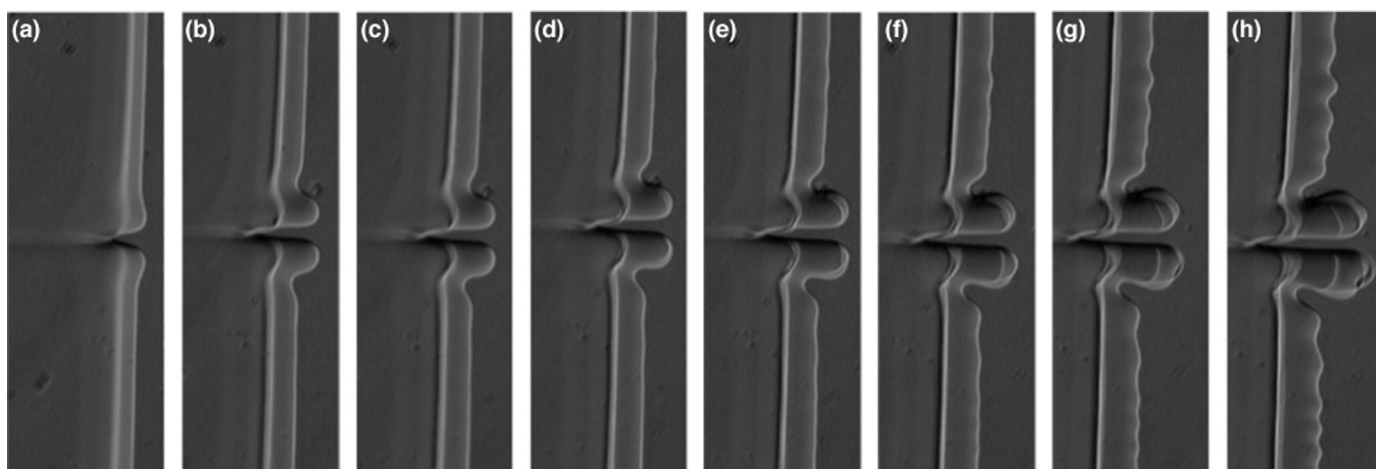


Fig. 1. Temporal evolution of solid-liquid interface near the grain boundary of SCN-0.9 wt.%DCB (succinonitrile-p-dichlorobenzene) alloy. The time elapsed during evolution (a–h) is 7 s.

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