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Spatial–temporal stability analysis of faceted growth with application to horizontal ribbon growth

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ABSTRACT

Spatial–temporal stability analysis has been applied to a solidification model that includes both isotropic and non-isotropic kinetics. In agreement with previous temporal stability analyses, it was shown that the kinetics associated with the propagation of steps across a facet can stabilize solidification processes that would normally be thermally unstable. In cases where the solidification is unstable, it was also shown that pulling the solid with a tangential velocity can cause a transition from "absolute" instability where perturbations cause growth at all locations to "convective" instability where a perturbation grows as it propagates, but at any fixed location disturbances decay away after the perturbation passes. These results were applied to understand instabilities in the floating silicon method (FSM), which is a particular type of horizontal ribbon growth. It was shown that increasing pull-speeds in FSM leads to increasingly unstable thermal growth conditions, but the combination of the kinetics of faceted growth and the tangential pull velocity can stabilize the process. As the pull speed increases, however, the process becomes increasingly sensitive to perturbation.

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1. Introduction

Recently, we have reported experimental and numerical studies [1,2] of the production of single-crystal silicon sheets using the floating silicon method (FSM). FSM is a form of horizontal ribbon growth where the solid silicon sheet floats on molten silicon before being removed from the furnace. A schematic of the FSM process is shown in Fig. 1. The solid sheet of silicon grows because of heat removal caused by a helium jet, and then floats on the melt surface before being removed from the furnace. One of the interesting findings from our previous studies was that there was a {111} facet at the growing edge of the sheet and that solidification kinetics must be considered to predict the horizontal position of the growth front as a function of pull speed. Previous studies of horizontal ribbon growth did not consider these effects [3–14]. In [1], it was shown that facet kinetics limit the maximum growth rate attainable by FSM. This limitation manifested itself in the numerical results as a turning point in the response of the growth front position versus the pull speed; beyond a limiting pull speed no steady solutions could be found. Although the growth front position predicted numerically agreed well with the experiment, the numerically predicted pull speed limits were often higher than those attained in the experiment. In the experiment, a transition to dendritic growth was often observed before reaching the predicted pull speed limit.

The goal of this paper is to perform a stability analysis of solidification including solidification kinetics and apply the results to understand the transition to dendritic growth seen in the FSM experiments. The most relevant previous stability analyses are those of Coriell et al. [15,16] who analyzed the solidification of binary alloys [15] and pure substances [16] including step propagation kinetics. They showed that for growth on a vicinal plane, step propagation can stabilize growth conditions that would normally be thermally unstable. In this work, we extend their analysis by including the effect of a tangential solid motion on the growth process. To understand this effect, spatial–temporal stability analysis is used [17,18]. Not to be confused with a spatial–temporal instability such as cellular growth, spatial–temporal stability analysis predicts the system response to a *localized* disturbance. Using the spatial–temporal stability analysis algorithm described in [18], unstable growth conditions are classified as either "absolutely" or "convectively" unstable based on this response. Absolute instability corresponds to the case where the disturbance amplitude at any fixed location grows in time. Convective instability corresponds to growth of a disturbance as it propagates, but decay at any fixed location after the initial disturbance passes. To our knowledge, this is the first time this type of analysis has been applied to solidification. The distinction turns out to be critical for understanding

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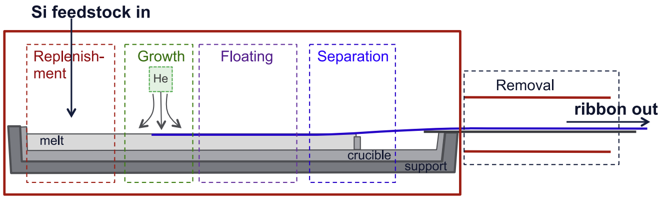

Fig. 1. Schematic of the experimental configuration.

FSM because there is a velocity tangential to the growth direction that causes disturbances to propagate as they grow.

2. Formulation

This is a spatial–temporal stability analysis of the faceted growth of silicon at some misalignment angles from the [111] direction. The basic problem is the same as that analyzed in [15] except that segregation effects are not included; only pure substances are considered and a uniform tangential velocity, u, is imposed on both the solid and liquid. A schematic of the assumed geometry and boundary conditions is shown in Fig. 2. The misalignment angle between the vertical propagation direction and the [111] direction is θ_0. The wavelength of the perturbation, λ, is used to define a perturbation wavenumber, $k = 2\pi/\lambda$. The perturbation itself is assumed to be small enough in amplitude such that the misalignment angle is bounded away from zero. The height of the domain is given by L, which is typically assumed to be much larger than λ and will be taken to the limit $L \to \pm\infty$. At the bottom of the domain, liquid is assumed to enter with a velocity v such that the unperturbed solidification front remains stationary even though liquid is being solidified. The total energy flux in and out of the domain is specified as f_s and f_l respectively where the subscripts s and l respectively indicate solid and liquid in all of the following. The domain is assumed to be infinite in the horizontal direction because spatial–temporal stability analysis relies on the continuous Fourier transform.

Looking ahead to the FSM analysis, the schematic shown in Fig. 2 is meant to represent a localized region in a coordinate system aligned with the solidification front. In the application to FSM, this analysis has some inherent assumptions. Because the domain is assumed infinite in the x-direction, only periodic temperature perturbations in the horizontal direction can be analyzed. In the FSM simulations, the temperature gradients normal to the growth front are generally significantly larger than those tangential to the front so this assumption is reasonable. Another assumption is that the liquid flow is uniform. This is also not a restrictive assumption. In the FSM simulations, a replenishment flow was added such that both the solid and the liquid were moving horizontally at a similar velocity. In some cases, Marangoni effects were included which caused non-uniform flows, but this did not significantly change the numerical results. This indicates that non-uniform flow effects are of secondary importance.

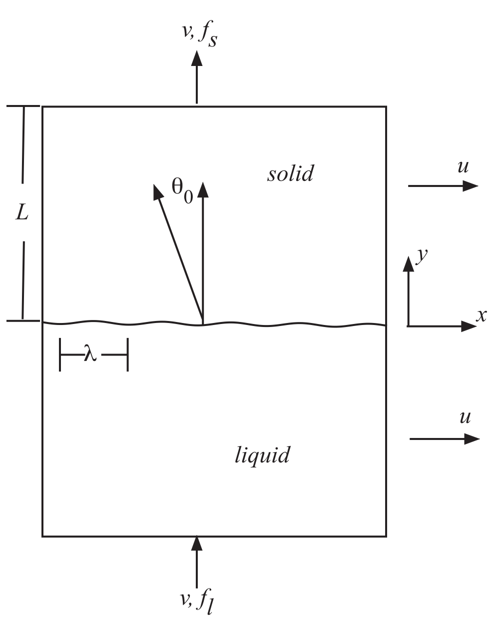

Fig. 2. Geometry and boundary conditions for the linear stability analysis of faceted growth.

3. Governing equations

The liquid and the solid are assumed to be incompressible with equal density, ρ, and specific heat, c. In this case, mass conservation ensures that the velocity of the solid and liquid are everywhere v in the vertical direction and u in the horizontal direction. The equations governing the temperature, T, in the solid and liquid are then given by

$$\frac{\partial \rho cT}{\partial t} + \frac{\partial}{\partial x}\left(\rho cuT - k_i\frac{\partial T}{\partial x}\right) + \frac{\partial}{\partial y}\left(\rho cvT - k_i\frac{\partial T}{\partial y}\right) = 0 \tag{1}$$

where k_i is the thermal conductivity and $i = s, l$. Note that k is the wavenumber, while k_s and k_l are thermal conductivities.

The boundary conditions at the bottom and top of the domain are given by

$$\left.\left(\rho cvT - k_i\frac{\partial T}{\partial y}\right)\right|_{y=L_i} = f_i \tag{2}$$

where for convenience we define $L_l = -L$ and $L_s = L$.

At the interface between the solid and the liquid, conservation of energy gives

$$[\![-k_i\nabla T\cdot\vec{n}]\!] = \rho L_f v_g \tag{3}$$

where double brackets indicate a jump in a quantity across the interface. The normal to the interface, $\vec{n}$, is taken to point from the liquid towards the solid and jumps are defined as the solid quantity minus the liquid quantity. The right side of the equation is the energy released by solidification. L_f is the heat of fusion of the material, and v_g is the solidification velocity. For the configuration given in Fig. 2, v_g is given by $\left(u\vec{i} + \left(v - h_t\right)\vec{j}\right)\cdot\vec{n}$ where $h(x)$ is the height of the interface relative to $y=0$, and h_t is the vertical velocity of the interface. In the following, subscripts of t and x denote differentiation with respect to that variable. The temperature at the interface is assumed to be continuous such that

$$[\![T]\!] = 0. \tag{4}$$

Lastly, it is assumed that the interface propagates according to the kinetic solidification model of Weinstein and Brandon [19]. This model includes mechanisms for nucleation of atoms onto a facet, step propagation along a facet, and roughened growth. The model constants are all taken from [19]. The model relates the supercooling to the growth velocity as

$$T_e - T = Kv_g \tag{5}$$

where all variables are evaluated on the interface, T_e is the equilibrium melting temperature, and K is the inverse of the more typically used kinetic coefficient β which relates the growth velocity to the amount of supercooling. This less standard form was

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