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Cellular tip splitting instability during transient growth

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ABSTRACT

In this work, cellular growth under transient conditions is investigated by using a developed quantitative phase-field model in which both the pulling speed and thermal gradient are time-dependent variables. Cellular tip shapes during transient growth are first characterized using the three-dimensional Saffman-Taylor viscous finger shape equation. Simulation results show that cellular tip and shoulders under non-steady-state conditions can be described by this simple mathematical model even at large Peclet number. The problem of cellular pattern evolution during directional solidification in the laser molten pool is possibly that of viscous finger in fluid mechanics. Previous tip splitting criterion is not applicable in our work. The mechanism of cellular tip splitting and later tip crack deepening under transient conditions is first studied, this interesting phenomenon may result from the coupling effect between morphological instabilities which can be measured by the shape factor and cellular spacing, and non-equilibrium of tip solute concentration which provides the driving force for deepening of the bifurcation.

1. Introduction

Interface dynamical instability has fascinated many metallurgists and physicists for years, and today the field of pattern forming instabilities elicit interest from distinctly different disciplines, ranging from alloy solidification to medicine and biology [1–3]. The investigation of dynamical instabilities has achieved noteworthy progresses in the several past decades due to theoretical advances [4–6], developments of computational techniques [7] and utilizations of precise experimental techniques such as real-time synchrotron X-ray radiography [8,9].

Cellular shapes are tightly related to cellular spacing which is one of the foremost characteristics of directional solidification. Previous studies have shown that there exists a selection mechanism of cellular spacing [10]: After planar instability, the spacing adjustment of the cellular pattern is determined by the tip splitting and submerging mechanism to keep the cellular spacing within the stable range. If the spacing is too small, the cell submerging mechanism works to increase the spacing; otherwise, the tip splitting mechanism works to narrow the spacing.

The cellular tip splitting mechanism is an unsolved question requiring further investigations. Two distinctively different theories have been proposed to tackle this noteworthy phenomenon. One is the noise induced perturbation theory. This theory suggests that the thermal fluctuation in the liquid phase near the cellular tip could be amplified, which would further cause tip splitting instability. Johann Nittmann et al. [11] studied tip splitting without considering interfacial tension through the experiment in which a fluid pushes into another miscible fluid of higher viscosity. In the experiment they related this growth form to a single statistical mechanical model, finding that noise reduction arising from suppression of fluctuations does introduce a characteristic finger thickness. Based on the noise induced perturbation theory, Chen et al. [9] carried out a thorough numerical simulation aiming at answering the question of tip splitting mechanism responsible for the seaweed pattern transition under steady-state conditions. Another theory was recently proposed by Wang et al. [12]. They believe that a deterministic dynamic mechanism for tip splitting may exist, i.e., the cellular tip splitting is deterministic rather than noise-induced.

The steady-state solidification conditions were used in most experimental and simulation works. However, the steady-state conditions of a fixed temperature gradient and a fixed pulling speed is just an ideal process in the lab through careful control of the experimental procedure. Although steady-state solidification is an important academic issue, it is far from representing conditions really occur in industrial manufacturing, such as in the laser melt pool during wire and laser additive manufacturing (WLAM) conducted in the current work. The growth conditions during WLAM process are complex and often varying spatially within a build due to the variable thermal histories. The

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WLAM is a potentially disruptive manufacturing technique in which large metallic materials can be fabricated layer by layer [13–15]. Solidification in this process controls the size of the grains, the dendritic/cellular morphology, the extent of microsegregation, and ultimately the mechanical properties of the product. Therefore, understanding of the melt pool solidification behavior under transient conditions is essential.

To date, no comprehensive studies of cellular tip splitting under non-steady-state conditions have been reported yet. In this work, a quantitative thin-interface phase-field model is used to simulate the cellular pattern evolution during wire and laser additive manufacturing under transient conditions where the thermal gradient and pulling speed are time-dependent. Cellular tip shapes under transient conditions are first characterized using the three-dimensional Saffman-Taylor viscous finger shape equation. The mechanism of cellular tip splitting and later tip crack deepening are investigated by combining the shape factor, cell spacing and tip solute concentration.

2. Phase-field model description and convergence study

The phase-field method has emerged as promising candidate of a fundamental and self-consistent theory for modeling microstructure evolution including cellular growth in recent years [16–23]. In this work, a quantitative phase-field model is used to simulate the cellular pattern evolution during non-steady-state growth based on the thin interface analysis which was proposed by Karma and co-workers [24–26] and further developed by Nikolas Provatas [27,28]. Alloy solidification in the laser melt pool during WLAM can be regarded as two-dimensional directional solidification in an externally imposed time-dependent temperature gradient $G(t)$, with surface-tension anisotropy γ moving in the z direction at a time-dependent pulling velocity $V_p(t)$. The relative orientation of preferential crystal growth is supposed to be parallel to the heat flow direction.

In our model, the Ni-Nb alloy system is in the dilute alloy limit. The solidus and liquidus lines are straight and with slopes of m/k and m, respectively. The partition coefficient k (assume $k < 1$) is the ratio of the equilibrium concentration on the solid side of the interface to that on the liquid side. In addition, the solute transport is assumed to be diffusive, with diffusion in the solid and attachment kinetics neglected. Besides, the latent heat of fusion is supposed to be sufficiently small, and the thermal conductivities of the liquid and solid are sufficiently large and close to each another. The temperature field is defined by the modified "frozen temperature approximation,"

$$T(z,t) = T_0 + G(t)\left(z - z_0 - \int_0^t V_P(t')dt'\right), \tag{1}$$

where $T(z_0, 0) = T_0$ is the reference temperature and z the heat-flow direction. The interface is assumed to be in local equilibrium given by the Gibbs–Thomson relation:

$$T = T_m - |m|c_l - \Gamma\kappa - v_n/\mu_k, \tag{2}$$

where T_m is the bulk melting temperature of the pure material, c_l is the concentration on the liquid side of the interface, $\Gamma = \gamma T_m/L$ is the Gibbs–Thomson coefficient, L is the latent heat of fusion per unit volume, κ is the interface curvature, v_n is the normal interface velocity and μ_k is the atomic mobility at the interface. Under the above assumptions, the sharp-interface equations can be derived:

$$\frac{\partial c}{\partial t} = D\nabla^2 c - \vec{\nabla}\cdot\vec{J_c}, \tag{3}$$

$$c_l(1-k)v_n = -D\partial_n c|^+ + \hat{n}\cdot\vec{J_c}, \tag{4}$$

$$\frac{c_l}{c_l^0} = 1-(1-k)d_0\kappa a(\hat{n}) - (1-k)\beta v_n - \frac{(1-k)(z-\int_0^t V_P(t')dt')}{l_T}, \tag{5}$$

where D is the solute diffusion coefficient in the liquid and $\partial_n c|^+$ is the normal gradient of concentration on the liquid side of the interface, $d_0 = \Gamma/\Delta T_0$ is the chemical capillary length, and $\Delta T_0 = |m|(1-k)c_l^0$ is the freezing range, $l_T = \Delta T_0/G = |m|(1-k)c_l^0/G$ is the thermal length, and $\beta = 1/(\mu_k \Delta T_0)$ is the kinetic coefficient. c_l^0 is the equilibrium concentration on the liquid side of the interface at T_0 defined as $c_l^0 = c_\infty/k$, where c_∞ is the background concentration in the liquid phase far away from the advancing interface. In addition, the fourfold anisotropy function with anisotropy strength ε_4 in two dimensions can be described as:

$$a(\hat{n}) = 1-3\varepsilon_4 + 4\varepsilon_4(\hat{n}_x^4 + \hat{n}_y^4 + \hat{n}_z^4), \tag{6}$$

where $\hat{n} = -\vec{\nabla}\phi/|\vec{\nabla}\phi|$ is the unit vector normal to the interface.

The current $\vec{J_c}$ is introduced to embody thermal noise-induced concentration fluctuations in the liquid phase whose components are random variables obeying a Gaussian distribution with variance [29]

$$\langle J_c^m(\vec{r},t)J_c^n(\vec{r}',\vec{t}')\rangle = 2DF_c\delta_{mn}\delta(\vec{r}-\vec{r}')\delta(\vec{t}-\vec{t}'), \tag{7}$$

where the noise magnitude F_c is determined through the fluctuation-dissipation relation

$$\langle(\delta c)^2\rangle = \frac{c}{(N_A/v_0)\Delta V} = \frac{F_c}{\Delta V}, \tag{8}$$

where $\langle(\delta c)^2\rangle$ is the equilibrium average of the square of the departure of the concentration from its equilibrium value in a microscopically large but macroscopically small volume ΔV, N_A is Avogadro's number while v_0 the molar volume of solvent atoms. This term is critical since it provides the possibility to investigate the noise amplification mechanism on side branching or tip splitting [30].

A phase-field parameter ϕ is employed here, which takes the value $\phi = 1(-1)$ in the solid (liquid), varying sharply but smoothly across a diffuse interface. The complete set of the phase-field equations including anisotropy are given by

$$\tau_0 a(\hat{n})^2\left[1-(1-k)\frac{z-\int_0^t V_P(t')dt'}{l_T}\right]\frac{\partial\phi}{\partial t} = W^2\vec{\nabla}[a(\hat{n})^2\vec{\nabla}\phi] + \phi-\phi^3 - \lambda(1-\phi^2)^2\left(U + \frac{z-\int_0^t V_P(t')dt'}{l_T}\right), \tag{9}$$

$$\left(\frac{1+k}{2} - \frac{1-k}{2}\phi\right)\frac{\partial U}{\partial t} = \vec{\nabla}\left[Dq(\phi)\vec{\nabla}\,U + \frac{1}{2\sqrt{2}}W(1+(1-k)U)\frac{\partial\phi}{\partial t}\frac{\vec{\nabla}\phi}{|\vec{\nabla}\phi|}\right] + \frac{1}{2}[1+(1-k)U]\frac{\partial\phi}{\partial t} - \vec{\nabla}\cdot\vec{J_u}, \tag{10}$$

where U is the supersaturation field defined as

$$U = \frac{1}{1-k}\left[\frac{c/c_l^0}{(1-\phi)/2 + k(1+\phi)/2} - 1\right], \tag{11}$$

$q(\phi) = (1-\phi)/2$ is the interpolation function which governs diffusivity across the interface. The fluctuating current term $\vec{J_u}$ obeys the same correlation as in Eq. (10),

$$\langle J_u^m(\vec{r},t)J_u^n(\vec{r}',\vec{t}')\rangle = 2Dq(\phi)F_u\delta_{mn}\delta(\vec{r}-\vec{r}')\delta(\vec{t}-\vec{t}'), \tag{12}$$

which depends on the order parameter ϕ via the solute diffusivity $Dq(\phi)$. The magnitude F_u is defined via the relation

$$\langle(\delta U)^2\rangle = \frac{\langle(\delta c)^2\rangle}{(\Delta c_0)^2} = \frac{F_u}{\Delta V}, \tag{13}$$

combining Eqs. (12) and (13), the following relation can be obtained:

$$F_u = F_u^0[1+(1-k)U], \tag{14}$$

and the constant noise magnitude,

$$F_u^0 = \frac{kv_0}{(1-k)^2 N_A c_\infty}, \tag{15}$$