Growth of an acicular crystal near a wall

E. A. Brener
Institute of Solid State Physics, Russian Academy of Sciences, 142432 Chernogolovka, Russia

Y. Saito
Department of Physics, Keio University, 223 Yokohama, Japan

H. Müller-Krumbhaar
Institut für Festkörperforschung, D-52425 Jülich, Germany

D. E. Temkin
Institute of Physical Metallurgy and the Physics of Metals, 107005 Moscow, Russia

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The growth of a 2D needle in a supercooled melt near a heat-insulating wall is analyzed. The capillary length d_0 is assumed to be isotropic. A model in which the system is divided into a "free" part, away from the wall, and a part at the wall is proposed. The first part is described in a boundary-layer model, while the second is described in the approximation of a constant thickness of the gap between the wall and the crystal. Conditions for joining the diffusion fields and the two parts of the crystallization front are formulated. These conditions determine the growth velocity v and the gap thickness δ as a function of the supercooling Δ: $v \simeq 0.4(D/d_0)\Delta^5$, $v\delta/D \simeq 0.8$.© *1995 American Institute of Physics.*

Let us examine the growth of an asymmetric dendrite initiated by a heat-insulating wall, along which the dendrite grows. As we know (see some reviews[1,2]), in free growth of a symmetric dendrite the velocity and direction of the growth are determined by the anisotropy of the surface tension, as is the length scale of the tip of the dendrite. During growth in a channel, on the other hand, these factors may be governed by the channel wall, even in the absence of a surface-tension anisotropy.[3] An asymmetric dendrite (more precisely, a "finger") has been observed in a numerical study of the growth of 2D crystals in a channel.[4] At channel widths above a certain critical value, a symmetric finger is unstable with respect to a splitting of the tip. This effect first results in the formation of two fingers; as these fingers subsequently grow congruently, an asymmetric, steadily growing finger forms. In very wide channels, only a single wall has a substantial effect. A numerical analysis[5,6] for this case has also revealed that there can be a steady-state growth of an asymmetric dendrite along a wall in a situation with an isotropic surface tension. In this case the growth rate is independent of the width of the channel.

We will discuss the growth of a 2D dendrite near a wall in a supercooled single-component melt. The crystal growth is controlled by the diffusion of the latent heat of fusion. We will discuss the steady-state regime, in which a crystal, at a certain distance from a heat-insulating wall, grows at a velocity v along this wall (Fig. 1). In the coordi-

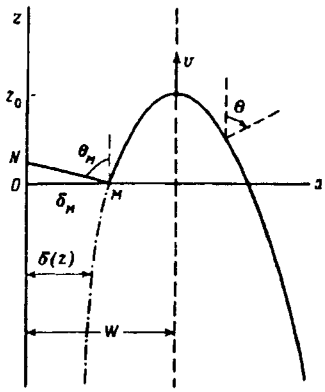

FIG. 1.

nate system which is moving at this velocity along the z axis, the steady-state diffusion field in the melt obeys the equation

$$\nabla^2 U + V\partial U/\partial z = 0. \qquad (1)$$

Here U is the temperature difference calculated from the melting point far from the crystal and the dimensionless quantity L/c, where L is the latent heat of crystallization, and c is the specific heat; $V = v d_0/D$ is the dimensionless growth velocity; d_0 is the capillary length, assumed isotropic; and D is the thermal diffusivity of the melt. All lengths in Eq. (1) and the equations below are expressed in units of d_0. The condition

$$(\partial U/\partial x)_{x=0} = 0 \qquad (2)$$

holds at the heat-insulating wall. At the interface, the field U_i satisfies the Gibbs–Thomson equilibrium condition

$$U_i = \Delta - K, \qquad (3)$$

and the heat-balance condition

$$V\cos\theta = -\mathbf{n}\cdot\nabla U \qquad (4)$$

holds. Here K is the curvature, put in dimensionless form with the help of the capillary length d_0, Δ is the dimensionless supercooling of the melt, and θ is the angle between the z axis and the normal to the boundary, $\mathbf{n}$. For simplicity, we adopt the so-called single-sided model.[7]

The problem formulated above has no exact solution. One might propose various versions of this solution. One is that no selection occurs, and there is a continuous spectrum of solutions characterized by, for example, the dependence $V = V(\delta,\Delta)$, where δ is the thickness of the layer of melt (or gap) far from the tip of the needle. Another version is that the wall has a selective effect such that for a given supercooling Δ there are certain values of the growth velocity, $V = V(\Delta)$, and certain values of the layer thickness, $\delta = \delta(\Delta)$. We assume that the latter version is realized. Even in this case, there are two possibilities: Either a selection occurs at any supercooling $\Delta > 0$, or it occurs only at a supercooling greater than a certain critical value, as in (for example) the growth of a symmetric finger in a channel.[3] The purpose of the model description proposed below in place of exact equations (1)–(4) is to explore the problem formulated above. The interface and the melt region are divided into two parts: a "free" part (to the right of line MN in Fig. 1), which does not sense the wall, and a near-wall part (to the left of MN). These parts are described by different models, and the results are then joined.

We describe the *free part* of the interface on the basis of the boundary-layer model,[8] using the equation[9]

$$V(1-U_i)\cos\theta-\frac{KU_i^2}{\cos^2\theta}-2\tan\theta\times KU_i\frac{dU_i}{d\theta}+\frac{K}{V}\frac{d}{d\theta}\left(\frac{KU_i}{\cos\theta}\frac{kU_i}{d\theta}\right)=0,\quad \theta_M<\theta<\pi/2. \tag{5}$$

Here U_i is given by Eq. (3). The profile of this part of the boundary can be found through a numerical integration of Eq. (5) from the point $\theta=\pi/2$, near which we have the following expansion of K in powers of $\cos\theta$:

$$K=V\frac{1-\Delta}{\Delta^2}\cos^3\theta+V^2\frac{(1-\Delta)(5\Delta-4)}{\Delta^5}\cos^6\theta+\dots\ . \tag{6}$$

The boundary is assumed to be free as long as the distance to the wall, $-\delta(z)/\sin\theta$, is greater than the effective width of the boundary layer, which we estimate to be $\Delta/V\cos\theta$. At the end of the free region, $\theta=\theta_M$, these quantities are equal. We thus have

$$\tan\theta_M=-V\delta_M/\Delta. \tag{7}$$

For an approximate description of the *near-wall region* we make use of the circumstance that the interface here, $x=\delta(z)$, is nearly parallel to the wall, and we formulate conditions (3) and (4) not at the actual wall but at $x=\delta_M$ (Fig. 1):

$$U(\delta_M,z)=\Delta,\quad V\delta'(z)=(\delta U/\partial x)_{x=\delta_M}. \tag{8}$$

Here we are ignoring the contribution of the curvature in Eq. (3). The beginning of the near-wall region, which coincides with the end of the free region, is on line MN (Fig. 1). However, we specify the "initial" distribution not on this line but on line $0M$, and we assume that it is linear:

$$U(x,0)=\Delta x/\delta_M. \tag{9}$$

This condition reflects in a qualitative way the continuity of the diffusion fields; this continuity must prevail on the line at which these fields are joined, MN. From Eqs. (1), (2) and (8), (9), we find the profile of the interface:

$$x=\delta(z)=\delta+\frac{4\Delta}{\pi V\delta_M}\sum_{n=1}^{\infty}(-1)^{n+1}\frac{\exp(s_nz)}{(2n-1)s_n}\quad (z\leqslant 0), \tag{10}$$

where $\delta\equiv\delta(-\infty)$, $\delta_M\equiv\delta(0)$, and

$$s_n=-V/2+[(V/2)^2+\pi^2(2n-1)^2/4\delta_M^2]^{1/2}. \tag{11}$$

It follows from Eq. (10) that at the joining point the quantity $\tan\theta\equiv-1/\delta'(0)$ is the same as $\tan\theta_M$ from condition (7). Profile (10) thus automatically satisfies the condition for continuity of the angles at the joining point.

We also impose two auxiliary joining conditions. The joining of the diffusion fields requires continuity of these fields and of the fluxes (or the first derivatives of the fields) on the joining line, MN. The first of these conditions is already satisfied. Instead of the second condition we require satisfaction of the condition of a global balance in the band $0<x<W$, which is parallel to the heat-insulating wall (in Fig. 1, the dashed line $x=W$ passes through the tip of the needle):

$$Q+V(W-\delta)=VW\Delta, \quad Q=\int_{z_0}^{\infty}\left(\frac{\partial U}{\partial x}\right)_{x=W} dz.$$

Here Q is the total heat flux into this band from the rest of the melt. In the boundary-layer model,[8] this flux is estimated to be $Q=-[\Delta-K(0)]K(0)K'(0)/V$. The condition for global balance thus takes the form

$$V\left\{\int_{\theta_M}^{0}\frac{\cos\theta d\theta}{K(\theta)}+\delta_M-\delta-\frac{\Delta\delta}{1-\Delta}\right\}-\frac{\Delta-K(0)}{V(1-\Delta)}K(0)K'(0)=0. \tag{12}$$

Finally, we require continuity of the curvature of the profile at the joining point:

$$-\left[\frac{\delta''}{[1+(\delta')^2]^{3/2}}\right]_{z=0}=K(\theta_M).$$

Using expressions (10) and (11) for $\delta(z)$, we find, under the condition $V\delta_M\ll\pi$,

$$2\Delta/\pi V\delta_M^2[1+\Delta^2/(V\delta_M)^2]^{3/2}=K(\theta_M), \tag{13}$$

where

$$\delta_M=\delta+8\Delta G/\pi^2 V, \tag{14}$$

and $G=0.916...$ is the Catalan constant.

Equation (5), along with Eqs. (7) and (12)–(14), determines the needle growth velocity V and the thickness (δ) of the gap between the needle and the wall as a function of the supercooling Δ. This behavior has been determined numerically. At a fixed value of Δ we specified some trial values of V and δ. From Eqs. (7) and (14) we found θ_M and δ_M. Equation (5) was integrated, with the help of expansion (6), from $\theta=\pi/2$; the quantities $K(0)$, $K(\theta_M)$, etc., in Eqs. (12) and (13) were found. The two latter equations were used to determine V and δ for the given Δ. The numerical results for small values of Δ are

$$V\simeq 0.4\Delta^5, \quad \delta\simeq 2\Delta^{-5}, \quad V\delta\simeq 0.8. \tag{15}$$

The tail of the dendrite far from the wall is described in this case by the equation of a parabola, $K(\theta)=(V/\Delta^2)\cos^3\theta$, with a tip radius $\rho\equiv 1/K(0)\simeq 2.5\Delta^{-3}$.

In summary, the model discussed here yields the same dependence of the velocity of the dendrite growth along the wall on the supercooling, $v\sim(D/d_0)\Delta^5$, as is predicted by the boundary-layer model for a free dendrite[9] (we recall that the velocity of a free dendrite in the rigorous theory is proportional to Δ^4; Refs. 1 and 2). There is, on the other hand, a fundamental difference. The velocity of a free dendrite depends on the anisotropy of the surface tension, vanishing in the isotropic case,[1,2,9] while a dendrite near a wall grows at a finite velocity even when the surface tension is isotropic. In conclusion we wish to stress that the problem of the growth of an asymmetric dendrite, which we have examined here on the basis of a crude model, requires further study, by subtler analytic methods.

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