STATIONARY KINETIC MODEL OF A DENDRITE TWO-PHASE ZONE

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The theoretical investigation of crystallization processes for metal alloys is associated with the need to describe the phase transformation regularities in the two-phase zone. Either volume nucleation and growth of the solid phase [1], or the dendritic nature of the development of the two-phase zone (the theory of a quasiequilibrium two-phase zone) [2] is assumed in the mathematical models presently in existence. It is assumed in the latter that the two-phase zone is sufficiently finely dispersed and its development is realized in such a way that supercooling of the melt would be zero during the whole crystallization process.

It is known that the dendritic form of crystallization is characteristic for the majority of metal alloys, where the dendrites grow in the supercooled melt. Despite the smallness of its magnitude, this supercooling is the basic motive force of crystal growth, and therefore, of the development of a two-phase zone, where formation of the ingot structure occurs. Hence, an investigation of the kinetics of dendrite growth in the two-phase zone is of considerable interest. This kinetics is determined both by the thermal and diffusion phenomena as well as the kinetic processes on the surface of the growing crystals. The influence of supercooling on the kinetics of the development of a two-phase binary alloy zone is performed in [3] without taking account of diffusion processes and considering the dendrite shape.

To find the means for optimal control of the formation, physical and mechanical properties of the cast metal, aquantitative description of the regularities of dendrite growth, their shape and impurity the distribution during crystallization is necessary.

A one-dimensional stationary model of the two-phase zone taking account of the kinetics of dendrite growth and the distribution of the soluble impurity in the solid phase is assumed in this paper.

1. Let us consider the steady-state process of crystallization of a binary alloy moving along the z axis at a constant velocity v in an external cooling system (Fig. 1). Let us consider the two-phase zone to consist of homogeneous plane-symmetric dendrites of variable section. The number of dendrites n per unit cross section of ingot does not vary during the crystallization. The rate of dendrite growth in a normal direction to their surface R(z) is a function of the local supercooling ΔT

$$v_n = F_1(\Delta T). \tag{1.1}$$

The relation of the velocity \boldsymbol{v}_n to the velocity \boldsymbol{v} in the steady-state mode is determined by the expression

$$v_n = vR'(z)/\sqrt{1 + [R'(z)]^2}, \qquad (1.2)$$

analogous to the relationship used in determining the rate of crystallization in the theory of continuous casting [4]. Here the prime denotes the derivative with respect to z and 2R(z) is the dendrite dimension in the cross section at a certain point z. From (1.1) and (1.2) we have

$$vR'(z)/\sqrt{1+[R'(z)]^2} = F_1(\Delta T).$$
(1.3)

The rate of dendrite vertex growth in the case under consideration equals the velocity of melt motion and is also a function of the appropriate local supercooling. Taking account of the possibility of anisotropy in the growth of crystals in the longitudinal and transverse directions, we write

$$v = F_0(\Delta T). \tag{1.4}$$

Furthermore, for definiteness we take

714

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$$F_i(\Delta T) = K_i \Delta T^m, \ m \ge 1, \ i = 0, 1, \tag{1.5}$$

where K_{i} is the kinetic factor whose magnitude is considered constant in the considered range of the change in ΔT . The anisotropy of dendrite growth can be taken into account by the difference between the magnitudes of the factors K_{1} and K_{0} .

The magnitude of the supercooling ΔT taking account of the influence of the local dendrite surface curvature on the liquidus temperature is determined by the expression

$$\Delta T = T_l(C) \left(1 - \frac{2\sigma k_r}{\varkappa \rho} \right) - T; \qquad (1.6)$$

$$k_r = \frac{R''}{(1+R'^2)^{3/2}},\tag{1.7}$$

where k_r is the value of the local dendrite surface curvature, σ is the surface tension, \varkappa is the latent heat of fusion, ρ is the density, $T_{\mathcal{I}}(C)$ is the equilibrium value of the liquidus temperature for $k_r = 0$, and C is the concentration of soluble impurity.

Taking account of (1.5)-(1.7), we obtain a kinetic equation to determine the dendrite shape in the two-phase zone from (1.3)

$$R' = \frac{K_1}{v} \sqrt{1 + R'^2} \left\{ T_1(C) \left[1 - \frac{\sigma R''}{\varkappa \rho (1 + R'^2)^{3/2}} \right] - T \right\}^m.$$
(1.8)

Taking account of (1.5) and (1.6), the relationship (1.4) sets up a connection between the velocity of two-phase zone motion and the temperature of the start of crystallization (or the magnitude of the supercooling on the two-phase zone front)

$$v = K_0 \{ T_1(C_s) [1 - \sigma k_r(z_s) / \kappa \rho] - T_s \}^m, \tag{1.9}$$

where the letter s denotes quantities corresponding to the start of the two-phase zone. Equations governing the changes in the temperature T and the concentration C during melt solidification must be appended to (1.8) and (1.9). Let us assume that the crystallizing ingot has plane or axial symmetry, its dimension in the transverse direction is sufficiently small, and the thermophysical parameters and diffusion coefficient are constants. The conditions

$$\frac{\partial T}{\partial r}\Big|_{r=r_0} = -\frac{\alpha}{\lambda} \left(T\Big|_{r=r_0} - T_c\right), \quad \frac{\partial C}{\partial r}\Big|_{r=r_0} = 0, \quad \frac{\partial T}{\partial r}\Big|_{r=0} = \frac{\partial C}{\partial r}\Big|_{r=0} = 0$$

are valid on the side surface of the ingot and on the axis of symmetry, respectively, where α is the coefficient of heat elimination from the ingot to the cooling medium, λ is the coefficient of heat conduction, T_c is the temperature of the cooling medium, r_o is the radius (half-thickness of the ingot). Forming the heat and mass balance for a certain layer dz (Fig. 1), we obtain the heat and mass transfer equations which we write after appropriate manipulation in the form

$$T'' - \frac{v}{a} T' - \frac{(1+v)\alpha}{r_0\lambda} (T - T_c) + \frac{\kappa\rho v}{\lambda} \psi' = 0; \qquad (1.10)$$

$$C'' + \left\{ \left[\ln (1 - \psi) \right]' - \frac{v}{D} \right\} C' - \frac{(1 - k)v}{D} \left[\ln (1 - \psi) \right]' C = 0,$$

$$\psi = 0 \text{ for } T \ge T_s, \psi \equiv 1 \text{ for } T < T_\kappa,$$
(1.11)

where α is the thermal diffusivity, ψ is the solid phase section in the two-phase zone, D is the diffusion coefficient in the liquid phase, k is the impurity distribution factor, T_K is the crystallization end temperature, $\nu = 0$ in the case of a plane ingot, and $\nu = 1$ in the case of a circular ingot. Equations (1.10) and (1.11) are obtained under the condition of rapid equilibration of the impurity temperature and concentration over the ingot section, and the absence of diffusion in the solid phase since for metal alloys $D_T/D \sim 10^{-4}$, where D_T is the diffusion coefficient in the solid phase.

The relation between the magnitude of the solid phase section Ψ and the transverse dimension of the dendrite 2R is determined by the relation

$$\psi(z) = 2nR(z),$$

which is valid for a plane-symmetric ingot. To obtain the appropriate dependence in the case of a circular ingot, we consider a certain annular interval dr >> R in a plane of the ingot cross section. The area of the ring is $f_o = 2\pi r_i dr$, where r_i is the distance between

(1.12)



Fig. 1

the ingot axis and the i-th dendrite. Therefore, the relative solid phase section is $f = 4\pi nR(R + r_i)f_0$. Replacing the discrete dendrite distribution by a continuous distribution and taking the average of the expression obtained for $\psi_1 = 4\pi nR(R + r_i)$ relative to the ingot radius ψ_1 , we find

$$\psi = 4\pi n R (R + 2r_0/3). \tag{1.13}$$

We express the dendrite density n by spacing between the dendrite axes d_1

$$n = 1/d_1.$$
 (1.14)

On the other hand, the dependence [5, 6]

$$d_1 = b_1(G_1 v)^{-s} \tag{1.15}$$

holds for the quantity d_1 , where the exponent s is almost 0.5, G_1 is the value of the temperature gradient at the front of the two-phase zone, and b_1 is a factor characterizing the alloy under consideration.

From (1.14) and (1.15) we have

$$n = b_1^{-1} (G_1 v)^s. (1.16)$$

Therefore, the differential equations (1.8), (1.10), (1.11) obtained determine the desired functions, the changes in impurity temperature and concentration, the dendrite shape, and the solid phase section in the two-phase zone, in combination with the relationship (1.12) or (1.13) and with (1.16) taken into account for appropriate boundary conditons.

2. In order to obtain analytical dependences, we consider the approximate solution of the problem of crystallizing a supercooled binary alloy. We assume that the crystallizing ingot has a plane symmetric shape, its motion velocity is along the z axis, and the origin of coordinates coincides with the beginning of the two-phase zone. The liquid phase occupies the half-space z < 0 (domain 1), and the two-phase zone z > 0 (domain 2), For $z = -\infty$ the melt temperature equals the temperature of the cooling medium T_{C_1} . At the end of the two-phase zone the alloy is cooled to the temperature of the external medium, or T_{C_2} . For generality, it is here assumed that the temperature of the cooling medium and the heat transfer coefficient in domains 1 and 2 can have different values, respectively, which are constants within the limits of their domains. Moreover, by considering that a normal growth mechanism is valid for dendrites, we set m = 1 [7, 8]. Going over to dimensionless variables and taking account of the assumptions made above, we write the system (1.8)-(1.12) in the form

$$Y'(x) = \frac{\operatorname{Pe}_{\mathbf{R}1}}{\operatorname{Pe}_{\mathbf{R}0}} \left[\Theta_{\mathbf{i}} - \Theta(x)\right], \quad 0 \leqslant Y \leqslant \psi_{\mathbf{R}}/N;$$
(2.1)

$$\Theta_{i}^{''}(x) - \operatorname{Pe}\Theta_{i}^{'}(x) - \operatorname{Bi}_{i}\Theta_{i}(x) = - \varkappa \operatorname{Pe}NY^{\prime}(x) - \operatorname{Bi}_{i}\Delta\Theta_{ci}; \qquad (2.2)$$

$$X(x) = [1 - NY(x)]^{k-1}, Y = 0 \text{ for } z < 0;$$
(2.3)

$$\Theta_t = \varphi(X); \tag{2.4}$$

$$Pe = Pe_{R0}(\Delta \Theta - \Theta_{s}), \qquad (2.5)$$

where
$$\Theta_{j} = (T_{j} - T_{c1})/T_{10}; \Theta_{1} = (T_{1} - T_{c1})/T_{10}; \Delta \Theta = 1 - T_{c1}/T_{10}; X = C/C_{0}; Y = R/r_{0}; Pe = vr_{0}/a; Bi = \alpha r_{0}(1 + v)/\lambda; Pe_{K1} = K_{1}T_{10}r_{0}/a; Pe_{K0} = K_{0}T_{10}r_{0}/a; \varkappa = \varkappa_{0}/cT_{10}; N = 2r_{0}n; x = z/r_{0}; \Delta \Theta_{c1} = (T_{c1} - T_{c1})/T_{10}.$$

The subscript j = 1 denotes the temperature and the heat transfer coefficient in the domain 1, and the subscript j = 2 in the domain 2. The quantity ψ_{K} determines the section of the solid phase at the end of the two-phase zone, T_l is the value of the liquidus temperature corresponding to the concentration C = C₀. Equation (2.3) follows from (1.11) for D = 0, k = const, and agrees with the Schale equation [5].

We solve the system (2.1)-(2.4) under the boundary conditions:

$$\Theta_1|_{z=-\infty} = 0, \ \Theta_1|_{z=0} = \Theta_2|_{z=0} = \Theta_3;$$
 (2.6)

$$\Theta_1|_{z=0} = \Theta_2|_{z=0}, \quad \Theta_2|_{z=\infty} = \Theta_{c2};$$
 (2.7)

$$Y|_{z=0} = 0 (2.8)$$

taking (2.5) into account. The liquidus equation (2.5) is hence determined by the phase diagram. Considering the latter linear, we write

$$\Theta_l = \Theta_A - \beta X, \tag{2.9}$$

where $\Theta_A = (T_A - T_{C1})/T_{lo}$, T_A is the melting point of the pure component, $\beta = (T_A - T_{lo})/T_{lo}$ is the slope of the liquidus line. Linearizing (2.3), we obtain

$$X = 1 + (1 - k)NY.$$

Substituting this latter into (2.9) with the expression for β taken into account, we find

$$\Theta_l = \Delta \Theta - \beta (1-k) NY. \qquad (2.10)$$

The problem therefore reduces to integrating two linear differential equations

$$\Theta_{j}^{"} - \operatorname{Pe}\Theta_{j}^{'} - \operatorname{Bi}_{j}\Theta_{j} = -\varkappa \operatorname{Pe}NY' - \operatorname{Bi}_{j}\Delta\Theta_{cj}; \qquad (2.11)$$

$$Y' = (\operatorname{Pe}_{\kappa 1}/\operatorname{Pe})(\Delta \Theta - \Theta_2 - \beta N(1-k)Y),$$

$$Y \equiv 0 \text{ for } \Theta \ge \Theta_{S_k} Y \equiv 1 \text{ for } \Theta < \Theta_{\kappa}$$
(2.12)

with the boundary conditions (2.6)-(2.8). Equations (2.12) follows from (2.1) with (2.10) taken into account. The solution of the system (2.11)-(2.12) can be written in the form of analytic expressions. The dependence of the rate of crystallization on the supercooling of the melt at infinity

$$\Delta\Theta = \frac{\operatorname{Pe} A \left(\gamma - \gamma_1 - \gamma_2 - A \right)}{\operatorname{Pe}_{\kappa_0} \left(A\gamma + \gamma_1 \gamma_2 \right)}$$
(2.13)

is of interest, where A = N $Pe_{K_1}\beta(1-k)/Pe$, γ_1 and γ_2 are the negative roots of the equation

 $\gamma^3 - p\gamma^2 - q\gamma - ABi_2 = 0,$

where p = Pe - A, $q = Bi_2 + \varkappa Pe_{K_1}N + A$.

In the case of weak heat elimination $(\text{Bi}_2 \rightarrow 0)$ this relationship can be written explicitly

$$\Delta\Theta = \frac{\operatorname{Pe}}{\operatorname{Pe}_{\mathrm{R0}}} \frac{\sqrt{\operatorname{Pe}^{2} + 4\operatorname{Bi}_{1}} + \sqrt{(\operatorname{Pe} - A)^{2} + 4Ag\operatorname{Pe} - A}}{\operatorname{Pe} + \sqrt{\operatorname{Pe}^{2} + 4\operatorname{Bi}_{1}}}, \qquad (2.14)$$

where $g = 1 + \varkappa/\beta(1 - k)$. The shape of the dendrites and the temperature distributions in the domains 1 and 2 are determined, respectively, by the formulas

$$Y = (\operatorname{Pe}_{\mathrm{R}1}/\lambda \operatorname{Pe}_{\mathrm{R}0}) (e^{\lambda z} - 1), \, \Theta_1 = \Theta_{\mathrm{S}} e^{\gamma z}, \\ \Theta_2 = \Delta \Theta + (\operatorname{Pe}/\lambda \operatorname{Pe}_{\mathrm{R}0}) [A - (A + \lambda) e^{\lambda z}],$$

$$(2.15)$$

where $\Theta_s = \Delta \Theta - Pe/Pe_{K_0}$, $\gamma = Pe/2 + (Pe^2/4 + Bi_1)^{1/2}$, $\lambda = (Pe - A)/2 - \sqrt{(Pe - A)^2/4 + AgPe}$, $\Delta \Theta$ is determined from (2.14). The relationship setting up a connection between the number of dendrites in the ingot section N = 2ron, where n is determined by (1.16) and the crystallization parameters, should be added to these expressions. Omitting intermediate computations, we write this relation for s = 1/2 in the form



$$N = \left(\sqrt{2} \operatorname{Pe}/b \operatorname{Pe}_{R_0}^{1/2}\right) \left(\sqrt{(\operatorname{Pe} - A)^2 + 4Ag \operatorname{Pe}} - A - \operatorname{Pe}\right)^{1/2},$$
(2.16)

where $b = b_1 \sqrt{aT_{lo}/r_0^2}$. The expression (2.16) characterizes the dependence of the dendrite density on the crystallization rate. This dependence is almost linear for sufficiently high values of the quantity Pe (crystallization rate).

The first formula in (2.15) determines the relative size of the dendrite grain Y_K at the end of the two-phase zone as $z \rightarrow \infty$ as a function of the dimensionless crystallization rate Pe. It follows from this relationship that Y_K decreases with the increase in Pe. This corresponds to known experimental data about breakage of the ingot structure as the crystallization rate increases [9]. As an analysis of (2.13) and (2.14) shows, as Pe $\rightarrow \infty$ the relation between the crystallization rate and the supercooling of the melt at infinity becomes linear $(v = K_0 (T_{i_0} - T_{c_1}))$ which can be used in experiments to determine the kinetic coefficient K₀ by means of the slope of the curve of the dependence $v = f(\Delta T)$ for large values of ΔT .

Theory is compared with known experimental results obtained on the binary alloys Sn + 0.5 wt.% Bi [10] (curve 1), Sn + 0.5 wt.% Pb and Sn + 1 wt.% Pb [11] (curves 2 and 3, respect-tively). Since the influence of the external the heat removal is essential (Bi_j << 1) for sufficiently high crystallization rates (Pe \geq 1), the computations were performed by using (2.14) for Bi₁ = 0. Moreover, starting from the dependence of N on Pe found, the quantity A was considered independent of Pe, and its value was determined at one of the points of the appropriate experimental curve for a given value of Pe_{Ko}. The following values of the physical parameters were used for the computations: for the first alloy T_A = 505, T_{Zo} = 504, 225, $\alpha = 0.288$, $\varkappa/c = 219.6$, ro = 0.2, g = 404.75, Pe_{Ko} = 6542, A = 7.38, and for the second and third alloy, respectively, T_A = 505, T_Z = 504.25, 503.5, $\alpha = 0.236$, $\varkappa/c = 249.57$, ro = 0.2, g = 386, 194.4, Pe_{Ko} = 4361, 3840, A = 5.2, 9.27, where T, K, α , cm²/sec, \varkappa/c , K, ro, cm. The theoretical curves (the solid lines) agree well enough with the appropriate experimental results.

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WAVE FORMATION IN LIQUID FILM FLOW ON A VERTICAL WALL

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Theoretical and experimental investigations show that laminar vertical liquid film flow is unstable starting with the lowest Reynolds numbers Re. The instability results in the origination of periodic waves, which grow rapidly in amplitude with distance and emerge into the stationary mode for specific amplitudes. Linear stability of a smooth film was investigated in many papers [1-5]. The greatest successes have been achieved on the basis of numerical methods of calculating the Orr-Sommerfeld equation. Dependences have been obtained for the wave amplitude increment, for the phase velocity and wave number of neutral perturbations and maximum growth waves as a result of the computations.

Clarity in the nonlinear wave formation mechanism at high Reynolds numbers is substantially lower. Research on nonlinear waves can be divided into two provisional groups in which the cases of low and high numbers Re are examined, respectively. For the case Re ~ 1 (here Re = q_0/v , q_0 is the specific mass flow rate, and v is the kinematic viscosity), a nonlinear nonstationary equation is derived for long waves on the film surface by using the method of narrow bands [6-8]. For the moderate number range Re ~ 5-50, only a stationary equation is derived [9-11], and nonlinear nonstationary waves are analyzed on the basis of a system of equations of boundary layer type by using the integral relations method.

There is a definite objective need to derive a universal model equation for nonstationary nonlinear waves which would permit extension of existing approaches and which would be valid in a broad range of numbers Re. An attempt to derive such an equation is presented in this paper. Results of a linear analysis of this equation are compared with experimental results for growing linear waves and with results of other authors.

1. DERIVATION OF THE EQUATION FOR THE WAVES

Let us write the Navier Stokes equations and the boundary conditions for a fluid film flowing on a vertical wall (Fig. 1) in the dimensionless form

$$\frac{\partial u^*}{\partial t^*} + u^* \frac{\partial u^*}{\partial x^*} + v^* \frac{\partial u^*}{\partial y^*} = \frac{3}{\operatorname{Re} \varepsilon} + \frac{1}{\varepsilon \operatorname{Re}} \left(\frac{\partial^2 u^*}{\partial x^{*2}} \varepsilon^2 + \frac{\partial^2 u^*}{\partial y^{*2}} \right) - \frac{\partial p^*}{\partial x^*};$$
(1.1)

$$\varepsilon^{2}\left(\frac{\partial v^{*}}{\partial t^{*}} + u^{*}\frac{\partial v^{*}}{\partial x^{*}} + v^{*}\frac{\partial v^{*}}{\partial y^{*}}\right) = \frac{3}{\operatorname{Re}}\left(\frac{\partial^{2}v^{*}}{\partial y^{*2}} + \varepsilon^{2}\frac{\partial^{2}v^{*}}{\partial x^{*2}}\right) - \frac{\partial p^{*}}{\partial y^{*}};$$
(1.2)

$$\frac{\partial u^*}{\partial x^*} + \frac{\partial v^*}{\partial y^*} = 0; \tag{1.3}$$

$$\varepsilon^2 \frac{4\partial h^*/\partial x^*}{1-\varepsilon^2 (\partial h^*/\partial x^*)^2} \frac{\partial v^*}{\partial y^*} + \frac{\partial u^*}{\partial y^*} + \varepsilon^2 \frac{\partial v^*}{\partial x^*} = 0 \quad \text{for } y = h;$$
(1.4)

$$\Delta p^{*} = -\frac{3^{1/3} \mathrm{Fi}^{1/3} \varepsilon^{2}}{\mathrm{Re}^{5/3}} \frac{\partial^{2} h^{*} / \partial x^{*2}}{\left[1 + \varepsilon^{2} (\partial h^{*} / \partial x^{*})^{2}\right]^{3/2}} + \frac{2\varepsilon}{\mathrm{Re}} \frac{\partial v^{*}}{\partial y^{*}} \left[\frac{1 + \varepsilon^{2} (\partial h^{*} / \partial x^{*})^{2}}{1 - \varepsilon^{2} (\partial h^{*} / \partial x^{*})^{2}}\right]$$
(1.4)

for y = h;

$$u^* = 0, v^* = 0$$
 for $y = 0;$ (1.6)

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719

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