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NUMERICAL SOLUTION OF THE TWO-DIMENSIONAL PROBLEM OF DIRECTED CRYSTALLIZATION

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UDC 518.3

In [1-4] mathematical models of the process of directed crystallization were constructed and investigated in a one-dimensional approximation. However, these models do not explain such experimentally observed phenomena as the inhomogeneity of the distribution of an impurity over a transverse cross section of the ingot. To clarify the structure of the concentration profile, the present article considers a mathematical model of the process of directed crystallization in a two-dimensional approximation, taking account of diffusion in the melt. Integral balance relationships are used to construct two difference schemes and to obtain evaluations of the error of the difference solutions. On the basis of numerical calculations an analysis is made of radial inhomogeneity for different configurations of the crystallization front, depending on different values of the crystallization rate v and the equilibrium coefficient k_0 [5].

We assume that the thermal characteristics of the substance depend only slightly on the concentration of the impurity and that the diffusion coefficient depends on the temperature. The problem of the redistribution of the impurity can then be considered separately from the thermal Stefan problem, assuming that the configuration of the front at every moment of time $z = z(r, t)$ and the rate of displacement v are known.

We consider an ingot of cylindrical form of radius R and finite length L_s. The interface between the two phases and the boundary conditions are assumed to be symmetrical with respect to the axis. We shall assume that the principal mechanism of mixing in the melt is diffusion. Then the distribution of the concentration of the impurity in the region $z(r, t) < z < L_s$ $(0 < r < R)$ obeys the diffusion equation

$$\frac{\partial u}{\partial t} = \frac{D}{r}\frac{\partial}{\partial r}\left(r\frac{\partial u}{\partial r}\right) + D\frac{\partial^2 u}{\partial z^2} \tag{1}$$

and the initial condition

$$u(r, z, 0) = u_0 = \text{const}.$$

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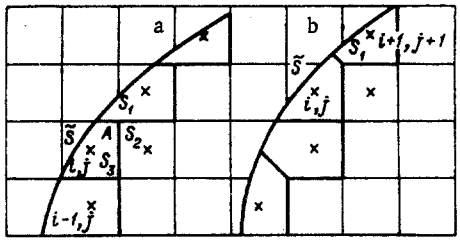

Fig. 1

At the lateral and end surfaces and the axis of symmetry we give the condition of absence of flow:

$$\partial u/\partial \mathbf{n} = 0. \tag{2}$$

In the crystallizing phase in the absence of diffusion the concentration of the impurity is determined from the condition of equilibrium of the phases at the front:

$$u_s(r, t, z(r, t)) = k_0 u(r, t, z(r, t)), \tag{3}$$

where k_0 is the equilibrium distribution coefficient.

At the surface of the crystallization front, by virtue of the nonequilibrium crystallization conditions [5], we have the boundary condition

$$-D\partial u/\partial \mathbf{n} + v_N(1 - k_0)u = 0, \tag{4}$$

where $\mathbf{n}$ is an external normal to the surface $\tilde{S}$ of the crystallization front; v_N is the normal component of the velocity.

Methods for the difference approximation of the problems under consideration have been investigated by a number of authors (see [6] and the literature cited therein). The present article considers a somewhat different approach, based on the approximation of balance relationships.

We introduce in the ingot the uniform fixed grid $z_j = jhz + hz/2$, $r_i = ihr + hr/2$, $hr = R/(M + 1/2)$, $hz = L_s/(N + 1/2)$, where M and N are the numbers of points over the radius and length of the ingot, respectively. The calculating region here will include the internal cells and the boundaries, arranged along the lateral and end surfaces, the axis of symmetry, and the crystallization front.

We integrate Eq. (1) over the cell $D_{i,j}$ in the interval of time $(t_n, t_n + \tau)$; we apply the Gauss–Ostrogradskii formula and, as a result, obtain the balance relationship

$$\iiint\limits_{V_{i,j}(t_n+\tau)} [u(t_n + \tau) - u(t_n)]\, dV = \int\limits_{t_n}^{t_n+\tau} dt \iint\limits_{S_{i,j}(t)} D\frac{\partial u}{\partial \mathbf{n}}\, ds, \tag{5}$$

where $V_{i,j}(t)$ is the volume and $S_{i,j}(t)$ the surface area of the cell. If a mesh point of the grid is located near a curved front we use two methods for forming the cell, depending on the arrangement of the adjacent mesh points (Fig. 1a, b). The implicit difference scheme approximating (5) has the form

$$(y_{i,j}^{n+1} - y_{i,j}^{n})\, V_{i,j}^{n+1} - \tau \sum_{k=1}^{m} \int\limits_{S_k^{n+1}} \left[D\frac{\partial u}{\partial \mathbf{n}}\right]^{n+1} ds = 0, \tag{6}$$

where S_k^{n+1} is one of the surfaces of revolution forming the elementary cell $D_{i,j}$; m is their number. Here, near the curved front we use the first method for forming the cells. The other scheme is based on an explicit approximation of the diffusional terms

$$(y_{i,j}^{n+1} - y_{i,j}^{n})\, V_{i,j}^{n+1} - \tau \sum_{k=1}^{m} \int\limits_{S_k^{n+1}} \left[D\frac{\partial u}{\partial \mathbf{n}}\right]^{n} ds = 0 \tag{7}$$

and the use of the second method for forming the cells near the curved front. In formulas (6) and (7) the integral terms are approximated by finite differences of the first order, taking account of boundary conditions (2)–(4).

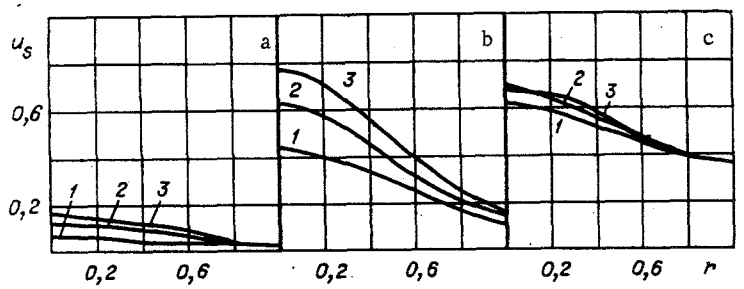

Fig. 2

For both differences schemes it can be shown that the error of the approximation of the difference schemes ψ_h satisfies the relationship $|\psi_h| < C_0 h$, where $h = \max\{hr, hz, \tau\}$; C_0 is some constant. With satisfaction of the conditions

$$l_N < \frac{D}{v_N |1 - k_0|} \quad \text{common for both schemes;} \tag{8}$$

$$V_{i,j} > \frac{\tau D}{l_N} \tilde{S}_{i,j} \frac{(1-\alpha)}{\alpha} \quad \text{for (6);} \tag{9}$$

$$V_{i,j} > \tau D \left\{ \sum_{k=1}^{m-1} \frac{S_k}{l_k} + \frac{\tilde{S}_{i,j}}{l_N} \frac{(1-\alpha)}{\alpha} \right\} \quad \text{for (7),} \tag{10}$$

where $\alpha = 1 - v_N l_N (1 - k_0)/D$; S_k, $\tilde{S}_{i,j}$ are the areas of the surfaces S_k^{n+1}; and l_k and l_N are the distance along the normal, on the basis of the principal of a maximum, the result can be obtained that the error of the difference solution $z_{i,j}^n = y_{i,j}^n - u_{i,j}^n$ with $0 < t < L_s/v$ for both schemes satisfies the evaluation $\max_{i,j,n} |z_{i,j}^n| < C_1 h$, where C_1 is some constant.

For the solution of (6) we use an iteration method of the upper relaxation with successive fittings at the lines r_i [6]. It can be verified that with the conditions (8)-(10) the schemes (6) and (7) will be stable.

With the aim of verification of the algorithms in the case of a flat front, methodological calculations were made in accordance with an implicit scheme for the following initial data: L_s = 10 cm, R = 1 cm, D = 0.1 cm^2/h, v = 0.1 cm/h, k_0 = 0.1, and M = 20.

The number of points along the length of the ingot N was taken equal to 100 and 200, and the values of the time spacing τ used were 0.125, 0.5, and 1.0. Experiments showed that the change in the spacing hz gives only an inconsiderable difference in the results (on the order of 0.1%). The effect of a change in the time spacing was more considerable. A decrease in the value of τ leads to a decrease in the number of iterations and to a change in the results by approximately 1%. We note that test calculations in accordance with an implicit scheme with a somewhat greater calculating time gave approximately identical results to the explicit scheme.

A calculation of processes with a curved front for the investigation of radial inhomogeneity was made using an explicit scheme; here the form of the front was given by the parabola $z = z_0 r^2 + vt - z_0 (3R/4)^2$ for the following values of the invariable parameters: L_s = 4 cm, R = 1 cm, D = 0.1 cm^2/h, M = 20, and N = 100. The values of the other parameters were taken as follows: equilibrium coefficient k_0 = 0.01, 0.1, and 0.5; crystallization rate v = 0.5 and 1 cm/h; and parameter of curvature of front z_0 = 0.5, 1.0, and 1.5.

Curves 1-3 of Figs. 2-4 show, for the above values of z_0, the dependence of the concentration of impurity on the radius r for the cross sections z = 0.6, 1.56, and 2.36, respectively.

As can be seen from the results, an increase in the curvature of the front leads to an increase of the inhomogeneity; the impurity is concentrated at the center of the ingot, while, in sections at a distance from the axis of symmetry, the concentration is close to the equilibrium value. An increase in the rate of crystallization (see Fig. 4a, b; v = 0.5 and 1 cm/h, respectively) also leads to an increase in the radial inhomogeneity. Depending on the value of the equilibrium concentration k_0, the distribution of the impurity is a nonmonotonic function. The effect of radial inhomogeneity comes out weakly with k_0 = 0.01 (Fig. 2a, Fig. 3a, and Fig. 4a) and is more sharply marked with k_0 = 0.1 (Fig. 2b and Fig. 3b). A further

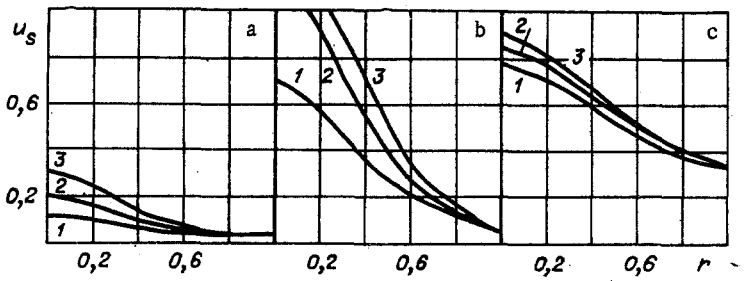

Fig. 3

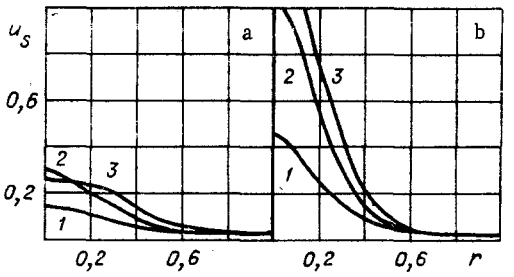

Fig. 4

increase in the equilibrium coefficient ($k_0 = 0.5$, Fig. 2c and Fig. 3c) weakens the inhomogeneity. This is qualitatively in agreement with experiment.

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