MATHEMATICAL MODELS OF HEAT TRANSPORT IN PROCESSES TO OBTAIN REFRACTORY SINGLE CRYSTALS

L. A. Goryainov

UDC 536.421.4

Simplified mathematical models are considered for horizontal and vertical directional crystallization methods, as are programs to compute the process on an electronic computer, and the regularities disclosed.

Methods of horizontal and vertical directional crystallization are used extensively at this time to obtain single crystals of refractory materials. The initial material in the form of crumbs is loaded into a cylindrical or plane container when obtaining single crystals by these methods. The container is inserted into the zone of a resistance heater and the material is fused partially or fully. The container is then extracted slowly from the heater zone, the elimination of heat from the melt is increased, and its crystallization is started in the given direction. In connection with the high temperatures in the apparatus (up to 2600°K) the heat-transport processes have substantial influence on the quality of the single crystals obtained, which indeed raises the need for a detailed investigation.

The following fundamental simplifying hypotheses were taken in the mathematical model variations considered below. The process is considered quasistationary in a one-dimensional version. This latter is explained by the low rate of crystal growth (1.5-10 mm/h), which is verified experimentally [1]. It is assumed that transport of the heat can be described by the heat-conduction laws with the introduction of effective values of the transport coefficients taking into account all other kinds of heat transfer. The container was located close to its surrounding surfaces, with which it is in a state of radiant heat exchange, in which connection the angular coefficients were not taken in the computation. The temperature along the length of the heater was given in the form of a step function with known k, and for the remaining surfaces surrounding the container by $T_0(x)$.

The mathematical model of the heat-transport process for the method of horizontal directional crystallization (HDC) applied to the system represented in Fig. 1 has the form

$$\frac{d}{dx}\left(\lambda_i f_i \frac{dT_i}{dx}\right) = \sigma_0 \varepsilon_{\text{re}i}(T_i)\, u' \,[T_i^4 - T_0^4(x)], \quad i = 1, 2, \ldots, 8, \tag{1}$$

$$\left.\frac{dT_1}{dx}\right|_{x=x_0-s} = \frac{\sigma_0 \varepsilon_{\text{re}1}\,[T_1^4|_{x=x_0-s} - T_{\text{en}}^4]}{\lambda_1}. \tag{2}$$

The conditions

$$\lambda_3 \left.\frac{dT_3}{dx}\right|_{x=x_3} - \lambda_4 \left.\frac{dT_4}{dx}\right|_{x=x_3} = \rho L W_{\text{cr}}, \tag{3}$$

$$T_3|_{x=x_3} = T_4|_{x=x_3} = T_L, \tag{4}$$

$$\lambda_6 \left.\frac{dT_6}{dx}\right|_{x=x_6} - \lambda_7 \left.\frac{dT_7}{dx}\right|_{x=x_6} = \rho L W_{\text{me}}, \tag{5}$$

$$T_6|_{x=x_6} = T_7|_{x=x_6} = T_L, \tag{6}$$

are given on the desired phase transition boundaries x_3 and x_6, and on the rear endface of the boat

$$\left.\frac{dT_8}{dx}\right|_{x=x_8} = \frac{\sigma_0 \varepsilon_{\text{re}8}\,[T_{\text{en}}^4 - T_8^4|_{x=x_8}]}{\lambda_8} \quad \text{at} \quad x_8 > H, \tag{7}$$

Moscow Institute of Railroad Transport Engineers. Translated from Inzhenerno-Fizicheskii Zhurnal, Vol. 40, No. 2, pp. 359-363, February, 1981. Original article submitted January 2, 1980.

0022-0841/81/4002-0229$07.50

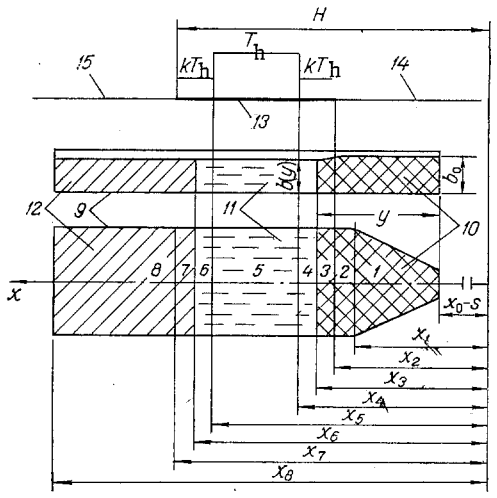

Fig. 1.

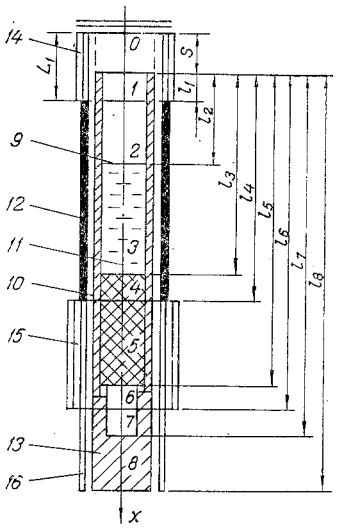

Fig. 2.

Fig. 1. Diagram to obtain single crystals by the horizontal directional crystallization method: 1-8) domains under consideration in the boat; 9) boat; 10) crystal; 11) melt; 12) crumbs; 13) heater; 14) forward crystallizer; 15) rear crystallizer.

Fig. 2. Diagram to compute the process to obtain single crystals by the method of vertical directional crystallization: 1-8) domains to be considered in the system; 9) container; 10) crystal; 11) melt; 12) heater; 13) heat eliminating rod; 14) upper module of screens; 15) lower module of screens-I; 16) lower module of screens-II.

$$\left.\frac{dT_8}{dx}\right|_{x=x_8} = 0 \quad \text{at} \quad x_8 < H. \tag{8}$$

On the remaining domain boundaries

$$T_i|_{x=x_i} = T_{i+1}|_{x=x_i}, \quad \lambda_i \left.\frac{dT_i}{dx}\right|_{x=x_i} = \lambda_{i+1} \left.\frac{dT_{i+1}}{dx}\right|_{x=x_i}, \tag{9}$$

$$i = 1, 2, 4, 5, 7.$$

Eight domains, which are distinguished by the values of the effective coefficients of heat conduction, the geometric and radiation characteristics, or the heat-transfer characteristics to the surrounding surfaces, are considered in the boat. In connection with the different densities of the melt and the crystal ($\rho_{cr} > \rho_m$), the latter has a height b variable over the length, which can be obtained from an examination of the processes of melt crystallization and fusion of the initial material in the boat.

The height of the forward conical part of the crystal was taken constant, while the rectangular part was approximated by a linear dependence. The height of the melt layer diminished as the crystal length increased, and is constant over the length of the boat for the system state under consideration. In a first approximation, the height of the crystal, melt, and crumbs can be taken constant.

The mathematical model of the heat-transport process for the vertical directional crystallization (VDC) method applied to the state of the system represented in Fig. 2 has the form

$$\frac{d}{dx}\left[\lambda_i(T_i)\frac{dT_i}{dx}\right] = \frac{\sigma_0 \varepsilon_{re\,i}(T)\,u}{f}[T_i^4 - T_0^4(x)] + \frac{du}{f}(T_i - T_{en}) + \frac{q_l(x)}{f}, \tag{10}$$

$$\left.\frac{dT_1}{dx}\right|_{x=s} = \frac{\sigma_0 \varepsilon_{re1}(T)[T_1^4|_{x=s} - T_{en}^4]}{\lambda_1} \quad \text{at} \quad s \leqslant L_1, \tag{11}$$

$$\left.\frac{dT_2}{dx}\right|_{x=s} = \varphi\,[T_2|_{x=s},\ s - L_1] \quad \text{at} \quad s \geqslant L_1, \tag{11a}$$

$$\left.\frac{dT_8}{dx}\right|_{x=s+l_8} = -\frac{T_8|_{x=s+l_8} - T_{en}}{\lambda_8 R_{hr}}, \tag{12}$$

$$\lambda_i \left.\frac{dT_i}{dx}\right|_{x=s+l_i} = \lambda_{i+1} \left.\frac{dT_{i+1}}{dx}\right|_{x=s+l_i}, \quad i = 1,\ 2,\ 4,\ 5,\ 6,\ 7, \tag{13}$$

$$T_i|_{x=s+l_i} = T_{i+1}|_{x=s+l_i}, \quad i = 1,\ 2,\ 4,\ 5,\ 6,\ 7, \tag{14}$$

$$T_3|_{x=s+l_3} = T_4|_{x=s+l_3} = T_L, \tag{15}$$

$$-\lambda_3 \left.\frac{dT_3}{dx}\right|_{x=s+l_3} + \lambda_4 \left.\frac{dT_4}{dx}\right|_{x=s+l_3} = \rho L w_{cr}. \tag{16}$$

Programs for computation on an electronic computer were compiled to solve the problems (1)-(8) and (10)-(16). The computation was executed by successive approximations. As a result of the computations, that temperature was selected for the forward container endface for which the boundary condition on its rear endface (7) or (12) would be satisfied. The position of one or two phase transition boundaries was hence determined. The state of the system was computed during crystal growth as a function of its displacement s from the initial position. That state of the system was taken as initial for which the melt temperature in the domain of crystal origination was equal to the phase transition temperature, while the crystallization process had still not occurred. Mathematical models and a computation program on an electronic computer were produced for its determination. The maximum melt temperature without fixing its coordinates was given in the computation of the initial state in the form of the condition

$$T_m = T_{max} \quad \text{for} \quad \frac{dT_m}{dx} = 0, \quad s = 0. \tag{17}$$

Moreover, for the HDC method it was assumed

$$T|_{x=x_0} = T_L, \quad s = 0, \tag{18}$$

and for the VDC method

$$T|_{x=l_5} = T_L, \quad s = 0. \tag{19}$$

Therefore, the mathematical model for the system initial state includes conditions (1), (2), (5), (6)-(8), (17), (18) for the HDC method and (10)-(14), (17), (18) for the VDC method. In both cases $w_{cr} = 0$, $w_{me} = 0$, $s = 0$. There is no crystal in which connection an appropriate change of subscripts should be made. The problems turn out to be overdefined when the two additional conditions (17) and (18) or (19) are introduced. For the possibility of solving them, the heater temperature T_h ($T_0(x)$ in the appropriate domain) and, moreover, the initial position of the boat x_0 for the HDC method and the heat-transfer condition on the lower endface of the part of the heat-eliminating rod under consideration R_{hr} are considered desired. Two successive approximation cycles were accomplished in the computation programs for the system initial state. For example, the heater temperature was varied to satisfy boundary condition (7) in the first cycle of approximations in the computation of the system initial state for the HDC case, and the boat position x_0 was varied in the second cycle to satisfy the boundary condition (17). Both approximation cycles were accomplished after each change in x_0.

The program to compute the processes on an electronic computer provides for correction of the initial mathematical model. Thus, e.g., the case when the crystallization front is in the heater is shown in Fig. 2. Two domains for the melt (inside and outside the heater) and one for the crystal are hence considered. The crystallization front can be shifted from the heater zone during crystal growth, and then two domains for the crystal (inside and outside the heater) and one for the melt will be considered. The computation program permits determination of the value of the effective heat transfer coefficients for specific conditions by comparing the computation results with test data. Thus, to determine the value of the effective heat conduction coefficient λ_{ef} for the melt when obtaining single crystals by the VDC method, the initial system state was computed for different values of λ_{ef}. The value of λ_{ef} determined by the agreement of the experimental and computational curves of the

temperature distribution over the container height turns out to equal 140 W/m·deg.

Numerous computations were performed by the programs developed in order to clarify the general regularities of the thermal aspect of obtaining refractory single crystals by directional crystallization. It is established that the crystallization front alters its position in space during crystal growth, in which connection the rate of crystal growth differs from the rate of container displacement. The expediency of shielding the container outside the heater zone is shown. The influence of the geometric and model factors on the process is clarified. Conclusions obtained from a computation by the programs are verified by results of an experimental investigation of the process. They are used to obtain refractory single crystals and their operating mode upon improvement of the apparatus.

NOTATION

T, temperature; x, space coordinate; u, perimeter; f, cross-sectional area; F, melt surface area; b, crystal height; l, crystal width; s, system shift from the initial position; y, position of the crystallization front measured from the forward endface of the boat; w, velocity; α, heat-exchange coefficient; ε_{re}, reduced coefficient of radiant exchange; ρ, density; L, heat of the phase transition; λ, heat-conduction coefficient. Subscripts: cr, crystallization; me, melting; en, surrounding medium (environment); m, melt; ef, effective.

LITERATURE CITED

1. Kh. S. Bagdasarov and L. A. Goryainov, "Experimental investigation of the temperature and heat flux distribution in apparatus to obtain single crystals by the vertical directional crystallization method," Inzh.-Fiz. Zh., 29, No. 6, 1109-1110 (1975).
2. Kh. S. Bagdasarov and L. A. Goryainov, "On an analytic investigation of heat-transport processes in an apparatus to obtain single crystals by the vertical directional crystallization method," Fiz.-Khim. Obrab. Met., No. 1, 73-78 (1978).

SOME FEATURES OF THE DISCHARGE IN AN ION SOURCE BASED ON A PENNING CELL

A. I. Lyapin and V. M. Gurov

UDC 537.523.74

Results of investigating the operating regimes of a Penning cell in the absence of a magnetic field are discussed.

The effect of a hollow cathode in a Penning cell type source is described in [1] and the dependence of the boundaries of its existence on the cavity length is investigated. In the interests of the possible application of this effect to obtain different polarity beams at the output, we investigated the dependence of the Penning cell operating regimes on the discharge intensity, the magnitude of the limiting resistance Rlim, and the electrode geometry.

Structurally, the source is executed in conformity with the recommendations in [1, 2]. Its schematic principle is presented in the figure. The anode and both cathodes are fabricated from tungsten. The working gas Ar was delivered by a metallic pipe of length $l = 0.15$ and diameter $d = 3 \cdot 10^{-3}$ m. In contrast to [2], a negative potential was given to the cathode 2 from a separate supply source. There was no magnetic field. The length of the cavity in the cathode (actually the length of the gas delivery tube) was selected to be greater than required to maintain the relationship between cavity length and cross section necessary for stable operation.

Analysis of the current-voltage characteristics of the discharge from the extended zone of the anode ($l = 2 \cdot 10^{-2}$, $d = 8 \cdot 10^{-3}$ m) obtained for the values $R_{lim} = (2\text{-}10) \cdot 10^5$ Ω and $p = 1.3\text{-}4$ Pa showed that high-voltage, weak-current ($I_p = (1\text{-}10) \cdot 10^{-3}$ A; $U_p = (1.5\text{-}5.0) \cdot 10^3$

Mogilev Machine Construction Institute.

Translated from Inzhenerno-Fizicheskii Zhurnal, Vol. 40, No. 2, pp. 364-365, February, 1981. Original article submitted January 15, 1980.

0022-0841/81/4002-0232$07.50