It should be noted that all cases of determining heat flux considered here give good results, while the proposed method of flux determination is distinguished by simplicity and can be recommended for practical use.

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TWO-PHASE ZONE DURING CRYSTALLIZATION OF A BINARY MELT

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A method is developed for calculating the solid–liquid zone, which is intermediate between the regions of the liquid and the solid phases, of a solidifying binary melt. Melts of Fe–C with different initial carbon contents were chosen as the binary melt.

The thermal and diffusional processes occurring in the two-phase zone have considerable importance in the formation of the micro- and macrostructures of ingots and castings.

The study of the kinetics of the movement of the zone under different conditions of crystallization and the question of the extent of the two-phase zone have great importance, since they determine the main technological properties of the metals.

The processes of a two-phase zone were studied in a region for which a diagram (of half) is presented in Fig. 1a.

The two-phase state of the medium at each point η is conveniently characterized by the function $l(\eta, \mathrm{Fo})$, representing the fraction of the solid phase in the liquid melt at the isotherm with the coordinate η at the time Fo [1, 2]. All the isotherms are assumed to be parallel planes perpendicular to the $O\eta$ axis. The coefficients of thermal conductivity λ and heat capacity c_p are the same and are equal for the solid and liquid phases. The concentration $C(\eta, \mathrm{Fo})$ of the admixture at one isotherm is the same at all points of the melt [3]. The character of the occurrence of diffusional processes allows one to assume that the rate of diffusion of the admixture into the solid phase is small in comparison with the rate of diffusion of the same admixture into the liquid melt. Crystals develop in the liquid phase in the process of crystallization. As this happens, the latent heat of fusion is released, depending on the rate of change of the amount of solid melt. It is expedient to treat the effect of the developing crystals on the fields of temperature $T(\eta, \mathrm{Fo})$ and concentration $C(\eta, \mathrm{Fo})$ as the action of additional sources of heat and admixture. Moreover, we assume that concentration supercooling is absent within the two-phase zone. Mathematically, this means that the concentration and temperature are connected by the equation for the liquidus line on the equilibrium diagram of state [1, 2].

With allowance for the foregoing and for simple transformations of the equations of the quasiequilibrium theory of a two-phase zone [1, 2], the processes of mass and heat transfer

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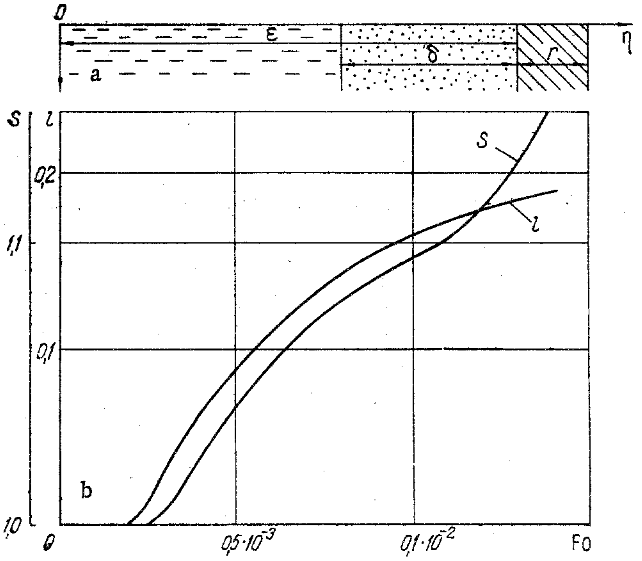

Fig. 1. Diagram of crystallizing region (a) and time variation of the concentration and the fraction of the solid phase at the local point $\eta = 0.6$ of the crystallizing region (b).

in a solid—liquid region in the absence of convection are described by the following system of equations in dimensionless form:

$$\frac{\partial l}{\partial \mathrm{Fo}} = \frac{\varphi}{W + S\,\dfrac{\varphi(1-k_0)}{1-l}}\left[\frac{1}{1-l}\,\frac{\partial l}{\partial \eta}\,\frac{\partial S}{\partial \eta} + \left(\frac{1}{\mathrm{Le}} - 1\right)\frac{\partial^2 S}{\partial \eta^2}\right],$$

$$\frac{\partial S}{\partial \mathrm{Fo}} = \frac{1}{l-1}\,\frac{\partial l}{\partial \eta}\,\frac{\partial S}{\partial \eta} + \frac{\partial^2 S}{\partial \eta^2} + \frac{1-k_0}{1-l}\,S\,\frac{\partial l}{\partial \mathrm{Fo}}\,;\quad \Theta = -\varphi S.$$

For the liquid region of the crystallizing melt the system of equations of diffusion and heat transfer has the form

$$\frac{\partial S}{\partial \mathrm{Fo}} = \frac{\partial^2 S}{\partial \eta^2}\,,\quad \frac{\partial \Theta}{\partial \mathrm{Fo}} = \frac{1}{\mathrm{Le}}\,\frac{\partial^2 \Theta}{\partial \eta^2}\,.$$

To obtan an unambiguous solution to the problem we supplement the initial equations by the boundary conditions.

Initial conditions (Fo = 0):

$$S = 1,\ \Theta = 1,\ l = 0.$$

Conditions at boundary:

$$\eta = 0:\quad \frac{\partial S}{\partial \eta} = 0,\quad \frac{\partial \Theta}{\partial \eta} = 0;$$

$$\eta = \varepsilon:\quad \frac{\partial S}{\partial \eta} = -(1-k_0)\,S\,\frac{d\varepsilon}{d\,\mathrm{Fo}}\,,\quad \Theta = -\varphi S,\ l = \mathrm{const}\ (\mathrm{const} < 1);$$

$$\eta = \varepsilon - \delta:\ l = 0.$$

In the formulated problem it is desirable to change to new variables, which are introduced with the purpose of converting the region in question with boundaries (liquid and solid—liquid) which move with time into regions of unit dimensions. The two-phase zone is converted into a unit region with the help of the coordinates

$$x = \frac{\eta - (\varepsilon - \delta)}{\delta} \quad (0 \leqslant x \leqslant 1),$$

while for the liquid zone

$$x_1 = \frac{\eta}{\varepsilon - \delta} \quad (0 \leqslant x_1 \leqslant 1).$$

Performing the appropriate transformations, and assuming that the dimensionless time Fo' in the new coordinate system is identically equal to the time Fo in the old system, we obtain the systems of initial equations in the new variables:

$$\frac{\partial l}{\partial \mathrm{Fo}} \left[\frac{x\delta' + (\varepsilon' - \delta')}{\delta} + \frac{\varphi \dfrac{\partial S}{\partial x}}{(1-l)\left(W + S = \dfrac{\varphi(1-k_0)}{1-l}\right)\delta^2} \right] \frac{\partial l}{\partial x} + \frac{\varphi\left(\dfrac{1}{\mathrm{Le}} - 1\right)}{\delta^2\left(W + S\dfrac{\varphi(1-k_0)}{1-l}\right)} \frac{\partial^2 S}{\partial x^2}, \tag{1}$$

$$\frac{\partial S}{\partial \mathrm{Fo}} = \left[\frac{x\delta' + (\varepsilon' - \delta')}{\delta} + \frac{\dfrac{\partial l}{\partial x}}{(l-1)\delta^2} \right] \frac{\partial S}{\partial x} +$$

$$+ \frac{1}{\delta^2} \frac{\partial^2 S}{\partial x^2} + \frac{1-k_0}{1-l} S \left[\frac{\partial l}{\partial \mathrm{Fo}} - \frac{x\delta' + (\varepsilon' - \delta')}{\delta} \frac{\partial l}{\partial x} \right], \tag{2}$$

$$\Theta = -\varphi S; \tag{3}$$

$$\frac{\partial \Theta}{\partial \mathrm{Fo}} = \frac{x_1(\varepsilon' - \delta')}{\varepsilon - \delta} \frac{\partial \Theta}{\partial x_1} + \frac{1}{\mathrm{Le}(\varepsilon - \delta)^2} \frac{\partial^2 \Theta}{\partial x_1^2}, \tag{4}$$

$$\frac{\partial S}{\partial \mathrm{Fo}} = \frac{x_1(\varepsilon' - \delta')}{\varepsilon - \delta} \frac{\partial S}{\partial x_1} + \frac{1}{(\varepsilon - \delta)^2} \frac{\partial^2 S}{\partial x_1^2}. \tag{5}$$

Boundary conditions for the unknown functions in the new variables: at Fo = 0

$$S = 1, \ \Theta = 1, \ l = 0;$$

conditions at the boundary $x_1 = 0$:

$$\frac{\partial S}{\partial x_1} = 0, \quad \frac{\partial \Theta}{\partial x_1} = 0;$$

at the boundary x = 1:

$$\frac{1}{\delta} \frac{\partial S}{\partial x} = -(1-k_0) S \frac{d\varepsilon}{d\mathrm{Fo}}, \ \Theta = -\varphi S, \ l = \mathrm{const} \ (\mathrm{const} < 1);$$

at the boundary x = 0: $l = 0$.

The problem formulated in such a way presumes the presence of a two-phase zone at the investigated time. Only in this case must one analyze the total system of equations for the two-phase region and the liquid zone. But if the two-phase zone is absent up to some time, then only the processes occurring in the liquid phase are investigated. In this case the conversion to a unit region is accomplished by the substitution $x = \eta/\varepsilon$.

Then the system of equations describing the transfer of mass and heat in the liquid melt will have the form

$$\frac{\partial \Theta}{\partial \mathrm{Fo}} = \frac{x\varepsilon'}{\varepsilon} \frac{\partial \Theta}{\partial x} + \frac{1}{\mathrm{Le}\,\varepsilon^2} \frac{\partial^2 \Theta}{\partial x^2}, \tag{6}$$

$$\frac{\partial S}{\partial \mathrm{Fo}} = \frac{x\varepsilon'}{\varepsilon} \frac{\partial S}{\partial x} + \frac{1}{\varepsilon^2} \frac{\partial^2 S}{\partial x^2}. \tag{7}$$

This system is supplemented by the following boundary conditions: initial conditions (Fo = 0):

$$S = 1,\ \Theta = 1;$$

conditions at the boundary x = 0:

$$\frac{\partial S}{\partial x} = 0,\ \ \frac{\partial \Theta}{\partial x} = 0;$$

at the boundary x = 1:

$$\frac{1}{\varepsilon}\,\frac{\partial S}{\partial x} = -(1 - k_0)\,S\,\frac{d\varepsilon}{d\,\mathrm{Fo}},\ \ \Theta = -\varphi S.$$

For the numerical realization of the formulated problem we use a finite-difference explicit scheme and an implicit scheme of construction of the solution [4]. The first is used to find the solution of (1), while the implicit scheme is used to construct the solutions of (2)-(7).

The numerical investigation of the two-phase zone was carried out on a Dnepr-21 computer for the following initial data: equilibrium coefficient of distribution $k_0 = 0.5$; specific latent heat of crystallization $L = 268 \cdot 10^3$ J/kg; coefficient of diffusion of melt $D = 0.14 \cdot 10^{-7}$ m²/sec; specific heat of melt $c_p = 0.725 \cdot 10^3$ J/(kg•deg); Lewis number $Le = 0.24 \cdot 10^{-2}$; superheat of melt $\Delta T = T_0 - T_c = 1$°K; tangent of slope angle of liquidus line, determined from the diagram of state, $\alpha = 0.414 \cdot 10^2$ °K.

In studying the formation of the solid—liquid region we investigated the influence of: 1) the law of distribution of the fraction of solid phase at a time one step removed from the initial time on the development of the two-phase zone; 2) the value of the fraction of the solid phase at the boundary between the solid and solid—liquid regions on the characteristics of the two-phase region; 3) the value of the initial concentration of the admixture on the distribution of the admixture itself and the fraction of the solid phase over the width of the transitional region.

The necessity of studying the first question is connected with a certain arbitrariness in the choice of the law of distribution of the fraction of solid phase over the width of the two-phase region at the indicated time. Knowledge of this law is needed to find the solution of the diffusion equation (2) at this same time. The investigation of the formation of the two-phase zone was begun with the solution of this equation, since it was assumed that the concentration of the admixture is responsible for the value of the fraction of solid phase in the solid—liquid region.

We analyzed three laws of distribution of the fraction of solid phase:

1) linear ($l = l_0 x$),

2) parabolic ($l = l_0 x^2$),

3) $l = l_0 x^{12}$.

An analysis of the results shows that for a region with a characteristic size $x_0 = 0.6$ m the chosen laws of distribution of the fraction of solid phase do not have a significant effect on the characteristics of the two-phase zone after 9 min from the start of the process of solidification of the melt and up to its end.

In studying the second question we chose the following boundary values of the fraction of solid phase: $l_0 = 0.2$ and $l_0 = 0.5$. For both cases we took a linear law of distribution of the fraction of solid phase at a time one step removed from the initial time.

An analysis of Fig. 2 shows that with an increase in the boundary value of the fraction of solid phase its value within the two-phase region also increases.

An increase in the fraction of solid phase within the transitional region leads to an increase in the content of the admixture in its liquid phase (Fig. 3a). This is explained by the fact that by virtue of the lower solubility of the admixture in the solid phase than in the liquid phase one can treat the solid phase as an internal source of the admixture whose power increases with an increase in the fraction of the solid phase.

Varying the value of the initial content of the admixture showed that the higher the initial concentration of the admixture, the larger the fractions of solid phase within the

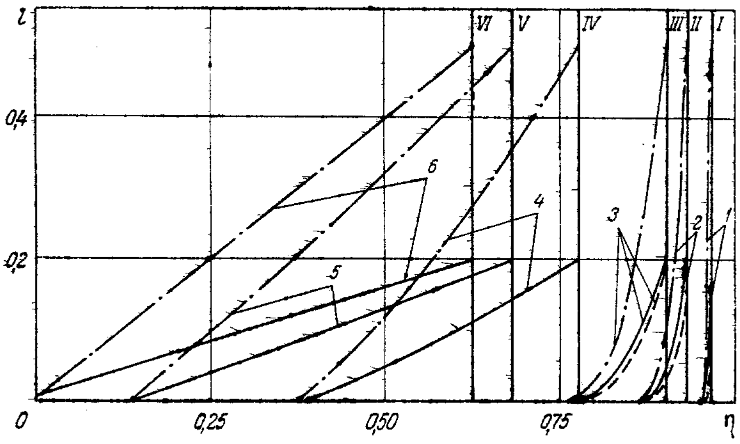

Fig. 2. Distribution of fraction of solid phase over width of test region for different times: 1) Fo = $0.1\cdot10^{-4}$; 2) $0.5\cdot10^{-4}$; 3) $0.1\cdot10^{-3}$; 4) $0.5\cdot10^{-3}$; 5) $0.1\cdot10^{-2}$; 6) $0.14\cdot10^{-2}$; solid curves) C_0 = 1%, l_0 = 0.2; dashed-dot curves) C_0 = 1%, l_0 = 0.5; dashed curves) C_0 = 0.3%, l_0 = 0.2. Straight lines I-VI) positions of solidus boundary at the same respective times.

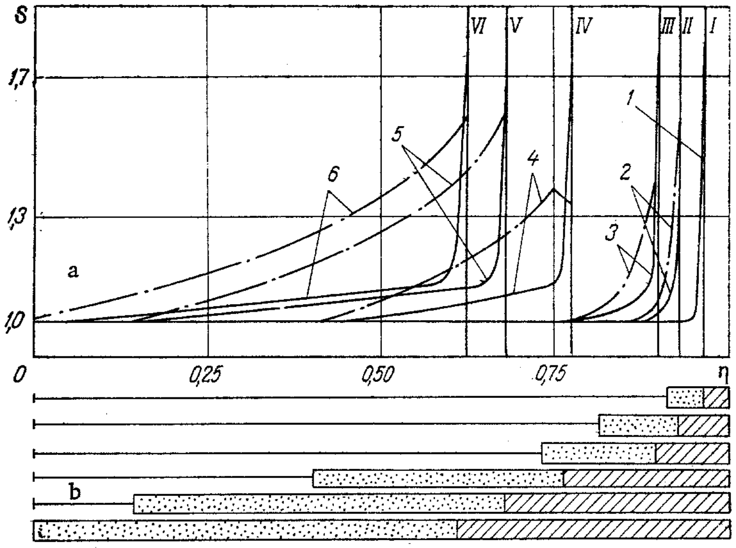

Fig. 3. a) Distribution of concentration of admixture over width of test region for different times: 1) Fo = $0.1\cdot10^{-4}$; 2) $0.5\cdot10^{-4}$; 3) $0.1\cdot10^{-3}$; 4) $0.5\cdot10^{-3}$; 5) $0.1\cdot10^{-2}$; 6) $0.14\cdot10^{-2}$; solid curves) C_0 = 1%, l_0 = 0.2; dashed-dot curves) C_0 = 1%, l_0 = 0.5; I-VI) positions of solidus boundary at the same respective times; b) diagram of crystallizing region.

two-phase region, which is especially pronounced in the initial period of solidification.

The differences in the character of the distribution of solid phase over the width of the transitional region practically disappear by the end of the solidification.

The development of the process of solidification of the melt with allowance for the two-phase zone is shown rather clearly in the diagram presented in Fig. 3b.

An analysis of Fig. 4 shows that the character of the advance of the liquidus boundary practically repeats the character of the advance of the solidus boundary, which is described by a square-root law. The variation of the fraction of solid phase and of the concentration of the admixture at a local point of the region is presented in Fig. 1b.

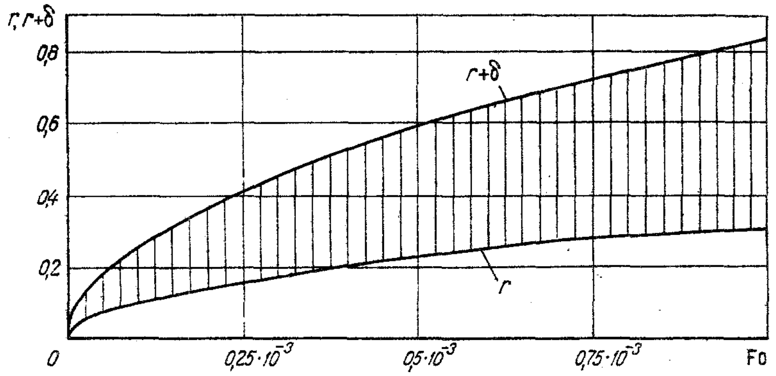

Fig. 4. Variation in position of boundaries of two-phase zone with time.

NOTATION

x_0, characteristic size, equal to half of width of region; $\eta = z/x_0$, dimensionless coordinate; z, dimensional coordinate; $Fo = Dt/x_0^2$, dimensionless time; t, dimensional time; $\Theta = (T - T_c)/(T_0 - T_c)$, dimensionless temperature; T, T_0, T_c, dimensional current temperature, initial temperature of melt, and crystallization temperature of pure melt; C, C_0, absolute and initial concentrations, respectively; $S = C/C_0$, dimensionless concentration; $\varphi = \alpha C_0/(T_0 - T_c)$, constant; $W = L/c_p(T_0 - T_c)$, crystallization criterion; $Le = D/a$, Lewis number; D, coefficient of diffusion of admixture in liquid phase of melt; a, coefficient of thermal diffusivity; ε, coordinate of solidus boundary; δ, width of two-phase zone; l_0, value of fraction of solid phase at solidus boundary; r, width of solidified crust; $\varepsilon' = d\varepsilon/dFo$, velocity of advance of solidus boundary; $\delta' = d\delta/dFo$, rate of change of width of two-phase zone.

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