# DETERMINATION OF FLUCTUATIONS OF TEMPERATURE SUPERCOOLING AND THE SOLIDIFICATION FRONT IN THE DIRECTIONAL CRYSTALLIZATION OF A MELT UNDER CONTROLLED CONDITIONS

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Relations are obtained to calculate transient temperature supercooling at the solidification front in the directional crystallization of a melt. Relations are also obtained to calculate fluctuations in the front with arbitrary perturbations of a prescribed thermal regime.

Various modifications of directional crystallization, which includes zone refining, are widely used to obtain an oriented structure (columnar and monocrystalline) in ingots. Other conditions being equal, the degree of perfection of the crystal structure of the resulting material is determined by the stability of heat transfer in the solidification zone. Convenient parameters for analyzing and optimizing the prescribed thermal regime are temperature supercooling at the crystallization front and the position of the front due to this supercooling.

The goal of the present study is to obtain relations to calculate these parameters with arbitrary known perturbations of the prescribed thermal regime. We also want to develop a method to evaluate the effect of the perturbing factors on the value of these parameters.

We will analyze the conditions under which single crystals of magnetic alloys are grown.

The USSR has developed a technology and industrial equipment for producing permanent magnets with a monocrystalline structure on the basis of Fe–Co–Ni–Al [1]. Here, monocrystalline ingots are obtained in special units using inoculation and controlled directional crystallization (CDC) [2] in vertically positioned tubular containers. Figure 1 shows a diagram illustrating heat exchange in the formation of a monocrystalline structure in the dynamic regime of CDC, i.e., with the motion of the thermal component (the heater–cooler block) at a constant speed relative $v_0$ relative to the cylindrical container. The temperature field is assumed to be axisymmetric. The temperature distribution in the gap between the container and the tubular container located coaxially relative to it (for example, along the straight line $l_m$) can be described by a certain curve Q and a function approximating this curve. For the sake of determinateness, we assume that in the case of equilibrium solidification the crystallization front coincides with the isothermal surface corresponding to the solidus $t_{sol}$. The remaining assumptions used in constructing the mathematical model of CDC are contained in [3].

The main factors affecting steady-state heat exchange are fluctuations in the power supplied to the heater and mechanical vibrations of the drive of the thermal component. The power oscillations correspond to sinusoidal oscillations of the curve Q in a direction perpendicular to the ingot axis, while the mechanical vibrations of the drive are along the axis [3].

Temperature supercooling at the crystallization front will be represented in the form of the sum of two components: $\delta t = \delta t_m + \delta t_t$.

We will examine the case of crystallization of a unidimensional rod. The derivation of the equation of interest to us is based on the following assumptions: a) there is the normal mechanism of crystal growth [4]: $dx/d\tau = v = K(\delta t)$; b) the magnitude of the temperature gradient G at the crystallization front remains the same during oscillations of the front.

The validity of the last assumption becomes obvious after comparing the scales of a typical curve Q [5] and the range of its oscillations as determined experimentally. It fol-

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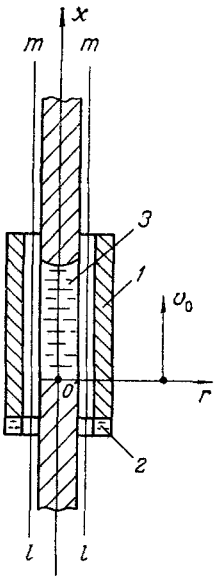


Fig. 1. Analysis of heat exchange during the growing of single crystals of magnetic alloys: 1) heater; 2) cooler; 3) molten zone.

lows from the calculations that in the case of oscillations of heater power, the gradient G, with deliberately exaggerated oscillations of the curve describing the temperature distribution along the ingot axis, can be considered constant with a relative error less than 2%. The vibrations of the drive correspond to simple shifting of these curves along the ingot axis, and the validity of assumption (b) is obvious in this case.

Figure 2 shows theoretical schemes used to determine the components of temperature supercooling.

Let temperature oscillations described by the function $\Delta t(\tau)$ arise at $\tau = 0$ on the crystallization front in a movable coordinate system (x, t). At an arbitrary moment of time $\tau_1$ on the axis corresponding to the initial position of the front (at $\tau = 0$), the temperature deviation is equal to $\Delta t_1$ (or $\Delta t_2$), while the front is shifted to the position denoted by the coordinate $x = x_1$ (or $x = x_2$) (Fig. 2a).

Taking assumptions (a) and (b) into account and considering that $\tan \alpha = G$, for any moment of time we have:

$$\delta t_t = \Delta t - xG. \tag{1}$$

Differentiating (1), we obtain:

$$\frac{d(\delta t_t)}{d\tau} = \frac{d(\Delta t)}{d\tau} - G\frac{dx}{d\tau}$$

or

$$\frac{d(\delta t_t)}{d\tau} + KG(\delta t_t) = \frac{d(\Delta t)}{d\tau}. \tag{2}$$

For convenience of analysis, we will represent the solution of Eq. (2), with the initial condition $\delta t_T(0) = 0$ (and, hence, $\Delta t(0) = 0$) in the form

$$\delta t_t = \Delta t - KG\exp(-KG\tau)\int_0^\tau (\Delta t)\exp(KG\xi)\,d\xi. \tag{3}$$

We will examine the transient CDC regime, i.e., the start and development of the process during a certain time interval from the moment when the thermal component begins to move with a constant velocity $v_0$ relative to the ingot. In the absence of perturbing factors, the deviation $\Delta t$ is caused only by shifting of the thermal component. In this case, at an arbitrary moment of time, $\tau$, $\Delta t = v_0\tau G$ (Fig. 2b), while $\delta t_t = \delta t_m$. Using (3), we obtain

$$\delta t_m = \frac{v_0}{K}[1 - \exp(-KG\tau)]. \tag{4}$$

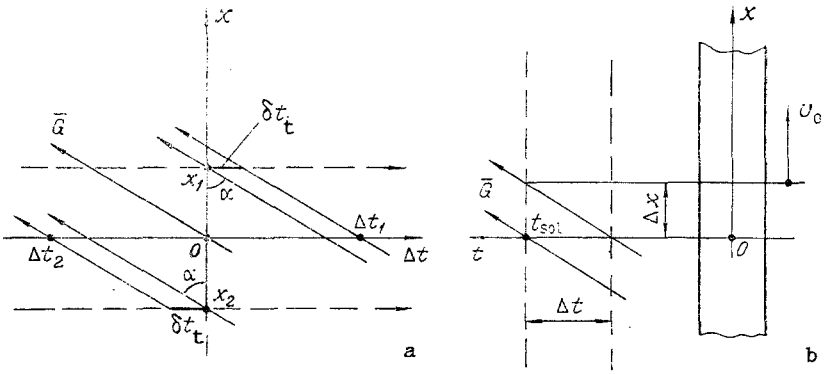


Fig. 2. Scheme for determining temperature supercooling: a) component $\delta t_t$; b) component $\delta t_m$.

In the steady-state dynamic regime of CDC, i.e., with a sufficiently large value of $\tau$, $\delta t_m = v_0/K$.

Equation (2) agrees with the equation derived in [6] for the special case when at the crystallization front there is a limited transient deviation $\Delta t$ only in one direction from the prescribed temperature value. Equation (4), which follows from (3), also agrees with the corresponding expression in [6]. This confirms the possibility of using (2), (3) to solve a broad range of problems.

Thus, for example, in the production of ingots of magnetic alloys with a monocrystalline structure, it is possible to evaluate the change in thermal conditions in the solidification zone under the influence of each perturbing factor individually, as well as together. Here, the following sequence should be observed. First, we solve the quasi-steady heat-conduction equation with the corresponding boundary conditions in the movable system (r, x, t) without consideration of perturbations [7]. The resulting solution t(r, x) makes it possible to determine the position and form of the crystallization front, with constant thermal conditions, from the equation

$$t_{sol} - \frac{v_0}{K} = t(r, x). \tag{5}$$

Then inserting a function corresponding to the perturbing factor [3] into the boundary conditions and solving the transient heat-conduction equation, we obtain an expression $t_1(r, x, \tau)$ describing temperature oscillations inside the cylinder. Then, to find the component $\delta t_t$ in the neighborhood of any point $(r_0, x_0)$ on the crystallization front, it is necessary to replace $\Delta t$ in solution (3) by the function $t_1(r, x, \tau)$, where $r = r_0$, $x = x_0$. This substitution can be justified by one of the main requirements of the technology: in growing crystals, the temperature profile is prescribed so that it ensures a solidification front which is either planar or slightly convex in the direction of the melt. Thus, using unidimensional solution (3), it is possible to assume that in a sufficiently small neighborhood of the point $(r_0, x_0)$ the form of the front is close to being a plane normal to the cylinder axis.

The temperature deviations $\Delta t$ in both directions from the prescribed value cause a change in the sign of the component $\delta t_t$ (in the coordinate system used in Fig. 2a). Thus, the motion of the crystallization front, together with the system (r, x, t), will occur with the superposition of the corresponding oscillations relative to the position determined by (5). The magnitude of the oscillations of each fairly narrow ring, determined on the front by the coordinate $r_0$, in a direction parallel to the cylinder axis is calculated from the formula

$$\Delta x = K \int_0^\tau (\delta t_t)\, d\xi, \tag{6}$$

which follows from assumption (a) with the initial condition $x(0) = 0$.

If the value of $\delta t$ of the resulting temperature supercooling on the annular element of the front remains positive in the dynamic CDC regime

$$\delta t = \frac{v_0}{K} + \delta t_t > 0,$$

then solidification of the melt zone adjacent to the elementary ring continues, and its translational motion is pulsative in character.

When there is a sudden, temporary increase in heater power, the component $\delta t_t$ may exceed $v_o/K$ in absolute value, since its sign is negative (in the chosen coordinate system) and this in turn causes a temporary melting of the solid phase. If the mechanism of melting of the material satisfies assumption (a), then the superheating of the phase boundary and the displacement of the boundary will also obey laws (3) and (6).

When $v_o = 0$, $\delta t = \delta t_t$, i.e., the instability of thermal conditions at the crystallization front is determined only by a single transient component of temperature supercooling. In the transitional regime, the behavior of the component $\delta t_m$ is described by function (4).

In sum, evaluating the effect of each perturbing factor or their aggregate effect on thermal conditions in the solidification zone reduces to variation of the boundary conditions of the investigated heat-conduction problem.

Knowing the permissible temperature supercooling in the solidification zone and using the proposed method, it is possible (for example) to formulate the accuracy requirements for a heater temperature control system and requirements for smooth operation of the drive of the thermal component in a unit for growing crystals by the CDC method.

## NOTATION

$t$, temperature; $t_{sol}$, solidus temperature; $\tau$, time; $x$, $r$, spatial coordinates: length and radius; $v_o = \text{const}$, speed of thermal component along container with ingot; $v$, speed of solidification front; Q, curve describing the temperature distribution in the gap between the thermal component and the container (along the straight line $l_m$); G, temperature gradient on the solidification front; $\delta t$, temperature supercooling on the solidification front; $\delta t_m$, "necessary" supercooling due to mechanical displacement of the thermal component; $\delta t_t$, transient supercooling due to temperature fluctuations on the front; K, kinematic constant dependent on the physical properties of the crystallizing substance; $\Delta t(\tau)$, function describing fluctuations in temperature on the solidification front; $\Delta x(\tau)$, function describing fluctuations of the front.

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