HEAT TRANSFER IN A COMPRESSIONAL CRYSTAL-GROWTH UNIT

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UDC 548.55:536.33

A two-dimensional model of the heat transfer in a furnace chamber with excess argon pressure for the growth of A_2B_6 crystals by the Shtober method is proposed.

In developing the design of thermal elements of crystallization units, it is necessary to determine how a temperature field of complex configuration, corresponding to the technological requirements in all stages of the process, may be created in the melt–crystal system. As a rule, temperature fields are investigated on mockups of the thermal elements, and then the results are transferred to the industrial design. Another effective method of analyzing the thermal conditions is mathematical modeliing of the heat transfer, permitting the solution of a whole series of problems in the design of a thermal element and the development of a technological program. To obtain satisfactory results in mathematical modeling, two conditions must be satisfied: adequacy of the mathematical model to the real physical object; and reliability of the data on the thermophysical and optical properties of all the bodies involved in heat transfer. In practice, these conditions are met fairly rarely.

This is absolutely the case in investigating the heat transfer in units for growing A_2B_6 crystals. Since these methods are highly aggressive at high temperature, contact methods of measuring the temperature directly in the melt–crystal system cannot be used, and the growth technology in the closed graphite containers is optical.

The presence of gas (usually argon) at high pressure (20 atm) in the chambers entails taking account of the convective component of heat transfer [1, 2], which prevents the use of the models employed earlier in calculating such equipment [3]. In addition, fundamentally new equipment is considered in the present case: an apparatus based on the Shtober method, which has not been used previously in growing A_2B_6 but is now more promising in view of the more stringent size requirements – primarily on the crystal diameter.

Consequently, a two-dimensional model is used for the heat transfer in the furnace with radiational heating in the presence of volume absorption and radiation in the component and with the possibility of specifying the convective boundary conditions at the surface of parts of the thermal element.

The formulation of the problem is as follows. The component to be treated is placed in a closed space (axisymmetric and plane-parallel versions are possible). In axial cross section, the chamber is a polygon of arbitrary shape, consisting of elements in which each side is parallel to one of the coordinate axes. These elements are massive bodies with a thermal capacity. In addition, it is possible to specify bodies with no thermal capacity in the working space – screens and heaters.

In bodies with thermal capacity, the two-dimensional Fourier heat-conduction equation is solved; in some of them, the problem of radiative–conductive heat transfer is solved. All the thermophysical properties are specified as a function of the temperature. The optical properties – the absorption coefficient, the refractive index for a semitransparent element, and the radiative properties of the other bodies – are assumed to be constant in the whole temperature range. The spectral region of the radiation (λ_0, λ_n) is divided into n intervals $(\lambda_0; \lambda_1); (\lambda_1; \lambda_2);\ldots; (\lambda_{n-1}; \lambda_n)$; λ_0 and λ_n are chosen so that the proportion of the radiant energy emitted in the intervals $(0; \lambda_0)$ and $(\lambda_n; \infty)$ is small at the working temperatures. Two values from the set $(\lambda_0, \ldots, \lambda_n)$ – λ_i and λ_j – are the boundaries of the transparency region of the object. In the spectral intervals $(\lambda_i; \lambda_{i+1}),\ldots,(\lambda_{j-1}; \lambda_j)$ the absorption co-

All-Union Scientific-Research, Design, and Technological Institute of Electrothermal Equipment, Moscow. Translated from Inzhenerno-Fizicheskii Zhurnal, Vol. 62, No. 3, pp. 473-479, March, 1992. Original article submitted June 17, 1991.

1062-0125/92/6203-0353 $12.50

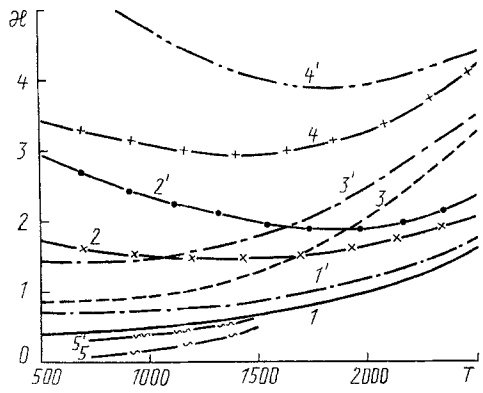

Fig. 1

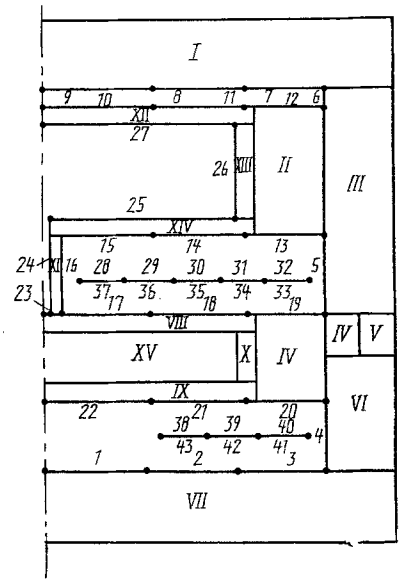

Fig. 2

Fig. 1. Thermal conductivity of fibrous carbon materials in vacuo (1-5) and in argon (1'-5'): 1) TKM-0.14 (perpendicular to the fiber direction); 2) TKM-0.3 (perpendicular); 3) TKM-0.14 (parallel to the fiber direction); 4) TKM-0.3 (parallel); 5) VVP-2500 felt. $\varkappa$, W/m·K; T, K.

Fig. 2. Calculation scheme for thermal element of apparatus: I-VII) heat-insulation blocks; VIII-X) crucible; XI) bunker holder; XII-XIV) loading bunker; XV) melt—crystal; the points denote the vertices of the radiant heat-transfer sections; 1-43) numbers of the sections.

efficients and reflective indices are specified; these parameters are constant within each interval. It is evident from this formulation that the grey-selective problem is considered here; this is the internal heat-transfer problem in the furnace, in the present case. The corresponding calculation method will not be outlined here, since it was described in detail in [4], which is a development of [5-7].

The external problem includes the calculation of the heat transfer between structural elements and the heat loss to the atmosphere through the heat insulation. The heat transfer between the elements is by conduction through the contacting surfaces and radiation. It is possible to specify convective heat-transfer conditions. At the external wall, boundary conditions of the third kind are specified. In calculating the radiant heat transfer, the total matrix of angular coefficients is calculated [8].

To specify the conditions of convective heat transfer, the whole working volume is divided into zones of convective heat transfer. Within the limits of each zone, the heat transfer of the gas with the structural elements is schematized according to one of the given models of convective heat transfer: for example, free convection at a horizontal plate in upward flow, free convection between two horizontal (vertical) plates, free convection between two vertical coaxial cylinders, etc.

Within the limits of each convective zone, the local heat-transfer coefficients $\alpha = f(T; T_b)$ to the solid wall are specified, on the basis of literature data on the dependences $Nu = f(Gr; Pr)$.

In the general case, the boundary condition at the boundary of the heat-conducting body is written in the form

$$-\varkappa_M \frac{\partial T_M}{\partial l_M} = q_j + \alpha_k (T_M;\ T_{b,k})(T_M - T_{b,k}), \qquad (1)$$

where j is the number of the radiational heat-transfer zone which includes boundary point M of the body; k is the number of the convective heat-transfer zone including point M: ℓ is the normal to the body surface at point M.

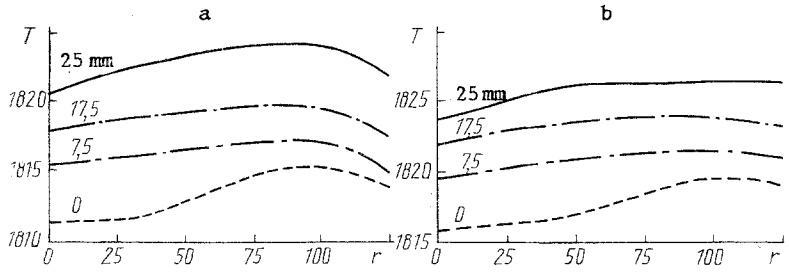

Fig. 3. Radial temperature distribution in the crucible at the stage of melt holding, specifying purely radiative (a) and radiational–convective (b) heat transfer in the working space; the figures on the curves give the coordinate over the height of the crucible. T, K; r, mm.

Suppose that

$$\psi_i = \pi \int_{\lambda_i}^{\lambda_{i+1}} I_{P,\lambda}(T)\, d\lambda$$

is the density of blackbody radiation in the frequency range $[\lambda_i; \lambda_{i+1}]$; $I_{p,\lambda}(T)$ is the Planck intensity of the equilibrium radiation in vacuum at temperature T. Then in Eq. (1)

$$q_j = \sum_{[\lambda_i;\lambda_{i+1}]\in \mathrm{rtr}} \bar{\varepsilon}^{s,0}_{\lambda_i,j}\left[E^{s,0}_{\mathrm{inc}_i,j} - \psi_i(T_j)\right], \tag{2}$$

where subscript s denotes surface flow; 0 denotes that the flux corresponds to the external radiation problem; rtr denotes the region of transparency of the component.

For bodies with no thermal capacity, in equilibrium with the other elements (the purely radiational case), the heat-balance equation is solved. For a section of a heater (screen) with two sides S_{j_1} and S_{j_2}

$$S_{j_1}\sum_{\lambda_i}\bar{\varepsilon}^{s,0}_{i,j_1}\left[E^{s,0}_{i,j_1} - \psi_i(T_j)\right] + S_{j_2}\sum_{\lambda_i}\bar{\varepsilon}^{s,0}_{i,j_2}\left[E^{s,0}_{i,j_2} - \psi_i(T_{j_2})\right] = W(j_1,\ j_2) \tag{3}$$

(in the case of a passive screen, W = 0). The sum in Eq. (3) and in all cases where no spectral region is indicated extends over all the spectral intervals $\lambda \in [0; \infty)$.

On the basis of Eq. (2)

$$S_{j_1} q_{j_1} + S_{j_2} q_{j_2} = W(j_1,\ j_2). \tag{4}$$

In addition, the condition of a thermally thin screen (heater) is assumed: $T_{j_1} = T_{j_2}$.

If

$$Y_j(T) = \sum_{[\lambda_i;\lambda_{i+1}]} \bar{\varepsilon}^{0}_{i,j}\psi_i(T)$$

is the flux density of intrinsic radiation of the zone S_j, a one-dimensional nonlinear equation of the following form is obtained from Eq. (3) for determining the temperature T_{j_1} of a thermally thin heater (screen), assuming that the incident flux E_{inc} is known from the preceding iteration and the radiative properties of both sides of the heater (screen) are the same

$$A_j\tilde{T} + B_j Y_j(\tilde{T}) = C_j, \tag{5}$$

where

$$A_{j_1} = 0;\ B_{j_1} = S_{j_1} + S_{j_2};\ C_{j_1} = S_{j_1}\sum_{[\lambda_i;\lambda_{i+1}]}\bar{\varepsilon}^{s,0}_{i,j_1}E^{s,0}_{i,j_1} + S_{j_2}\sum_{[\lambda_i;\lambda_{i+1}]}\bar{\varepsilon}^{s,0}_{i,j_2}E^{s,0}_{i,j_2} - W(j_1,\ j_2).$$

In the program, equations of the form in Eq. (5) are solved by inverse interpolation on the basis of tables of the function AT + BY(T).

The energy balance at the two-sided section of the screen is written in the following form, taking account of convective heat transfer

$$S_{j_1}(\alpha_{1,k_1}(\tilde{T}_{j_1} - T_{r,k_1}) + q_{j_1}) + S_{j_2}(\alpha_{2,k_2}(\tilde{T}_{j_2} - T_{r,k_2}) + q_{j_2}) = W(j_1;\ j_2). \tag{6}$$

Equation (6) takes the form in Eq. (5) if the incident radiation is separated from the intrinsic radiation at temperature $\tilde{T}$ in the expression for q.

In the grey case – $\varepsilon \neq f(\lambda)$ – Eq. (5) reduces to the form $D_1T^4 + D_2T = D_3$, which may be solved by Newton's method or by the accurate formula containing radicals.

The equation for gas heating (cooling) in the k-th convective heat-transfer zone takes the form

$$c_k m_k \frac{dT_{b,k}}{d\tau} = \sum_i S_{i,k}\alpha_k (T_{b,k} - T_i) + Q_k, \tag{7}$$

where $S_{i,k}$ are the gas-immersed surfaces in the k-th convective heat-transfer zone; m_k is the gas mass in the k-th zone (assumed to be proportional to the volume of the zone); Q_k is the heat influx to the gas on account of convection

$$Q_k = \sum_j Q_{\text{conv}_{j,k}}.$$

The summation in Eq. (7) is taken over all the zones adjacent to the k-th

$$Q_{\text{conv}_{j,k}} = F_{j,k} f(T_j;\ T_k), \tag{8}$$

where $F_{j,k}$ is the surface area of intersection of zones j and k; $f(T_j; T_k)$ takes account of the mutual position of zones j and k.

In taking approximate account of convection using Eq. (8), $Q_{\text{conv}j,k} = Q_{\text{conv}k,j}$. The computer time required in this case is not greatly different from that required when convection is ignored, since the number of convective zones is small and combined solution of Eq. (7) with the equations of radiative and conductive heat transfer is not particularly difficult.

Note that the results given by the program in modeling the heat transfer in a unit where gallium–scandium–gadolinium garnet is grown by the Czochralski method (only radiant heat transfer) are in good agreement with experimental data [9].

Thus, this program permits the calculation of the temperature field in units with radiant heat transfer in the presence of a single semitransparent element, and allows the convective heat transfer to be taken approximately into account by specifying the local heat-transfer coefficients.

The basic problem in thermal calculations with such equipment is the lack of data on the thermophysical and optical properties of the crystal being grown and the materials of the structural elements.

The lack of literature data on the thermal conductivity $\varkappa$, absorption coefficient k, and refractive index of A_2B_6 materials – the most common of which, ZnSe, is chosen for modeling here – at temperatures above 600 K is evidently explained in that such materials are highly aggressive and volatile. The situation is similar for the heat-insulation material: the graphite composite TKM, for which $\varkappa$ depends significantly not only on the temperature, but also on the density, the direction of fiber packing ($\varkappa_\perp$, transverse to the fibers; $\varkappa_\parallel$, along the fibers), and the presence or absence of gas in the working space.

To date, this topic has only been addressed in [10], which found the dependence $\varkappa(T)$ in vacuo for various densities of the material when $\varkappa_\parallel/\varkappa_\perp = 2$, which was assumed to be the case for the whole of the temperature and density range.

In the present work, these problems are solved empirically, on the basis of the similarity of heat transfer in the materials being studied and others, and so on.

The choice of $\varkappa(T)$ for ZnSe on the basis of the model material – high-porosity molybdenum foam – was described in [1, 2]. For 1750-1800 K, $\varkappa$ is around 6 W/m·K; 100% variation of $\varkappa$ at T = 1800 K is specified in modeling the phase transition: from 6 to 3 W/m·K. Measurements of the absorption coefficient of ZnSe show that it loses transparency in the near-IR range at 1000 K [11]. This suggests that both the crystal and the ZnSe melt are completely nontransparent to IR radiation close to 1800 K, which is characteristic for semiconductor materials overall. In the present case, $k = 5 \cdot 10^3$ cm^{-1} is assumed for ZnSe. The data on $n(\lambda)$ are taken from [12]; on the basis of the dependence $(dn/DT)(\lambda)$ in [12], $n(\lambda)$ is calculated for ZnSe at 1600-1800 K.

The thermal conductivity of TKM in the presence of argon is calculated on the basis of the structural similarity of this material and VVP-2500 graphite felt, for which $\varkappa$ is known in argon and in vacuo [13]

$$\varkappa(T)_{\text{TKM, Ar}} = \varkappa(T)_{\text{TKM, vacuum}} \frac{\varkappa(T)_{\text{VVP, Ar}}}{\varkappa(T)_{\text{VVP, vacuum}}}.$$

The calculation results for $\varkappa$ are shown in Fig. 1, together with literature data for these metals.

Taking account of the graphite base and the porous structure, the emissivity of TKM is assumed to be 0.95.

The calculation model of the thermal zone of the apparatus is shown schematically in Fig. 2. The massive bodies are the heat-insulation units, the loading bunker, the container, and the charge; the bodies with no heat capacity are the heaters. The division of the massive bodies into individual rectangles depends on their thermophysical properties and the requirements of the program regarding the configuration of the structural elements. The radiant sections of the heater correspond to their real electrical zones with different energy liberation. At the other surfaces, the radiant sections are specified on the basis of increase in accuracy of the calculation with simultaneous reduction in machine time. The total number of radiant sections is 43. To calculate the temperature field in the massive bodies, the whole model is divided into cells by means of a single grid. The number of grid points is 28 over the height and 16 over the radius.

Calculations are performed for conditions of melt holding, specifying both purely radiational and radiational–convective heat-transfer conditions in the working space. In the second case, in accordance with the recommendations of [14], the convective heat transfer is specified at vertical surfaces (the lateral heat-insulation blocks, the bunker holder) and at horizontal surfaces with the hot surfaces above the cold surfaces – for example, in the system of the upper heater, the floor of the loading bunker, etc. The heat-transfer coefficients are calculated for each case from the dependences in [14]. The data on the argon properties do not depend on the pressure, apart from the gas density, which is directly proportional to the pressure [15].

The calculation results show (Fig. 3) that the temperature field in the container volume does not depend on the presence of gas in the working chamber, in the absence of free cavities with a large temperature difference at the boundary surfaces and at a temperature level ensuring the predominant influence of the radiative component. Overall, the value of $\varkappa$ of the porous heat insulation and hence the power required by the apparatus depend on the presence of gas in such conditions.

The power of the heaters in the basic stages of the technological process has been determined by the given model and nonsteady conditions of melt crystallization have been found. The data obtained may be used to develop the design of thermal elements and a technological program to perform the corresponding process.

NOTATION

$\varkappa$, thermal conductivity; T, temperature; qR, radiative flux density; α, heat-transfer coefficient; ε, emissivity; E_{inc}, spectral density of radiative flux incident at the body; W, power; c, specific heat of gas; m, mass of gas; Q, heat influx to gas on account of convection; λ, wavelength.

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CALCULATION OF METAL PLATE FUSION BY A CONCENTRATED ENERGY FLUX

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UDC 536.421:539.211

The one-dimensional problem of heating and melting of a metal plate by a constant surface heat source is considered. The kinetics of fusion front motion are studied with consideration of absorption of the latent heat of phase transition up to temperatures close to the boiling point.

Studies of the processes of heating and formation of a melt under the action of concentrated energy sources on condensed media have been under way for quite some time. Interest therein has been stimulated by the need to develop laser, plasma, electron-beam, ion, and other forms of materials processing. In such technological processes as laser doping, surfacing, laser-plasma compound synthesis, etc. redistribution of components initially deposited on the target surface, gas saturation, chemical compound synthesis, and other processes take place in the liquid phase. To study and optimize the latter it is necessary to know the depth of the melt pool and the temperature distribution therein to a sufficient accuracy. In connection with this, a series of studies [1-9] has been dedicated to solution of the problem of fusion under the action of a concentrated energy source. In [8] the approximate Biot method was used to consider fusion of a semi-infinite target. The shortcomings of that technique are: the complexity of theoretical justification, insufficient accuracy (the error in determining pool depth reaches 15%), and the absence of any generalization to fusion of finite plates. Numerical calculation by a computer was used in [9] with a finite difference technique and explicit specification of the fusion front. The shortcoming of this method is the necessity of composing a complex program.

In the present study we will offer an approximate analytical solution of the problem of heating and fusing a metal plate of finite thickness, which is characterized by simplicity, high accuracy (error of about 1%), and ease of use. Major attention will be given to phase transition kinetics.

We will briefly describe the process to be considered. A constant energy flux is incident on a metallic target of finite thickness and is absorbed upon the surface. We will assume that the coefficient for absorption of the concentrated energy flux by the surface is approximately constant, which is valid, for example, for a low-energy electron beam. Moreover, we let the transverse dimension of the source action zone R be much greater than the target thickness H: $R \gg H$. The problem can then be considered in one-dimensional formulation.

A. A. Baikov Metallurgy Institute, Academy of Sciences of the USSR, Moscow. Translated from Inzhenerno-Fizicheskii Zhurnal, Vol. 62, No. 3, pp. 480-485, March, 1992. Original article submitted May 13, 1991.

 1062-0125/92/6203-0358 $12.50