NONSTATIONARY TEMPERATURE FIELDS FOR GROWING LAMINATED LEUCOSAPPHIRE

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The influence of temperature fluctuations of the heater on the temperature field is investigated in a melt–leucosapphire crystal system. It is shown that the crystallization front is a thermal damper. The necessary accuracy of the automatic regulation system is determined.

A mathematical model is represented in [1], which was used to perform a number of temperature-field (T-field) calculations in leucosapphire horizontal directional crystallization apparatus. Comparison of the results obtained with experiment showed that the mathematical model developed for the apparatus corresponds with sufficient accuracy to the real physical processes occurring therein. Results were presented there for a computation of T-fields for the quasistationary heat-transfer regime and different discrete positions of the container relative to the thermal unit of the apparatus. The influence of the spatial location of the container on the T-field being formed in the melt–crystal system is shown in [2].

No less important is the investigation of the nonstationary temperature fields during crystal growth.

It is known that quite rigid requirements on the stability of the thermal conditions are imposed on the technological crystal growing regime (and therefore on the crystallization equipment) during the growth process. However, the requirements on the stability of the temperature regime rely, as a rule, on deductions made by means of different indirect parameters, and do not have a sufficiently clear foundation, and are often purely intuitive in nature. At first glance, this is related to difficulties in measuring the temperature generally, and the nonstationary temperature fields during the growth of optical crystals, in particular. Consequently, the stability of the temperature conditions in specific technological crystal growth processes remains not studied and the requirements on this parameter during the development of the apparatus are, as a rule, unjustifiedly exaggerated.

An attempt is made in this paper for a computational investigation of the influence of temperature fluctuations of the heater on the process of T-field formation in the melt–leucosapphire crystal system by the method of horizontal directional crystallization (HDC) during growth. All the computations were performed according to a program described in detail in [1-3] in application to the thermal unit of serial installations of the SGVK–"Sapphire" type which are used extensively in our country.

The heater of the apparatus under examination is fabricated from a tungsten bar of 10-mm diameter, and has significant specific heat; $C_{p\gamma} = 3.5 \cdot 10^6$ J/(m^3·K) at 2500°K, which permits early elimination of high-frequency power oscillations (with a period less than 1 sec) from consideration, which are related to instability of the power grid. Consequently, henceforth heater temperature fluctuations are considered that can be caused by either a time instability in automatic control system operation, or by defects of the thermal unit which unexpectedly occur (destruction of the shields, change in heater resistance, etc.). These reasons can cause temperature fluctuations of a different form at the heater. In all, twelve different kinds of temperature perturbations were investigated (Fig. 1) for different relationships between τ_0; τ_t; τ_d and ΔT.

The following were the main questions posed during execution of the computations: passage of the heater temperature perturbations into the melt–leucosapphire crystal system, change in the crystallization rate under the influence of the heater temperature perturbation, change in the temperature gradient field in the domain of the crystallization front as

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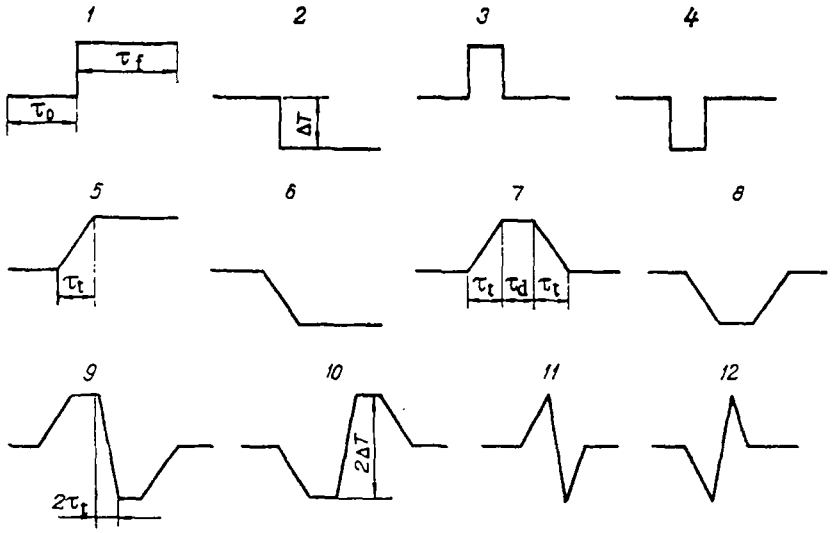

Fig. 1. Nature of the heater temperature perturbations: 1-12) possible kinds of temperature fluctuations given in the program.

a function of the absolute value of the crystallization front, the influence of the latent heat of crystallization on the change in the temperature field in the phase transition domain.

Computations executed for temperature perturbations of the form 1, 2, 5, 6 (Fig. 1) showed that a new stationary regime sets in in the melt–leucosapphire system after 270-310 sec (τ_f) depending on the absolute value of the temperature perturbation (ΔT varied from 1 to 20°C). The magnitude of the temperature perturbation was 40-60% of the heater ΔT near the crystallization front in the crystal and depended on the sign and magnitude of the ΔT. It was also established that the 95% change of the T-field from the new stationary regime sets in in the melt–crystal system after a time period of $\sim\tau_f/5$.

Results of a computation of the time change in the T-field are represented as an example in Fig. 2 for a +20°C heater perturbation, which is 0.68% of its initial temperature level. The melt–crystal system is in the quasistationary regime shown by the dashed curves (τ = 0 sec) up to the time of the beginning of the temperature perturbation. The crystal grew at the constant rate of~9 mm/h. Precisely the fact that the container was shifted at a very low velocity during growth permits speaking about the quasistationarity of the process, i.e., at each instant there was a quasiequilibrium state (in the thermodynamic sense) between the melt and the crystal. Despite the fact that the temperature perturbation was realized in conformity with the mode 1 (see Fig. 1), the T-field in the melt–crystal system started to change substantially only after 18 sec and reached a value after 48 sec that comprises 93% of the new steady thermal mode. The system arrived totally in this state after 308 sec.

The location of the crystallization front shifted during formation of the T-field, and the temperature gradient field changed along the length of the crystal, where there is a domain that stands 25-30 mm off from the crystallization front, where the relative change of dT/dx is maximal (the absolute value of dT/dx also has a maximum here). This domain agrees with the position of the diaphragm that separates the crystallization and annealing zones of the apparatus in which the shields are perpendicular to the plane of the container with the crystal. Such a shield arrangement hinders incidence of direct radiation from the heater on the crystal in this domain, on one hand, and assures a significant radial heat flux outflow from the crystal, on the other, since the diaphragm is a set of narrow deep slots formed by the shields. The emissivity of such a set of slots is close to 1, i.e., at this location there is a surface opposite to the crystal that does not, in practice, reflect the radiation incident on it from the surface from the bulk of the crystal.

The change in the temperature gradient in the crystal in the domain separating the diaphragms will occur with a 3-5-sec time delay relative to the beginning of change of dT/dx on the crystallization front, which is related to the finite heat flux propagation velocity over the crystal.

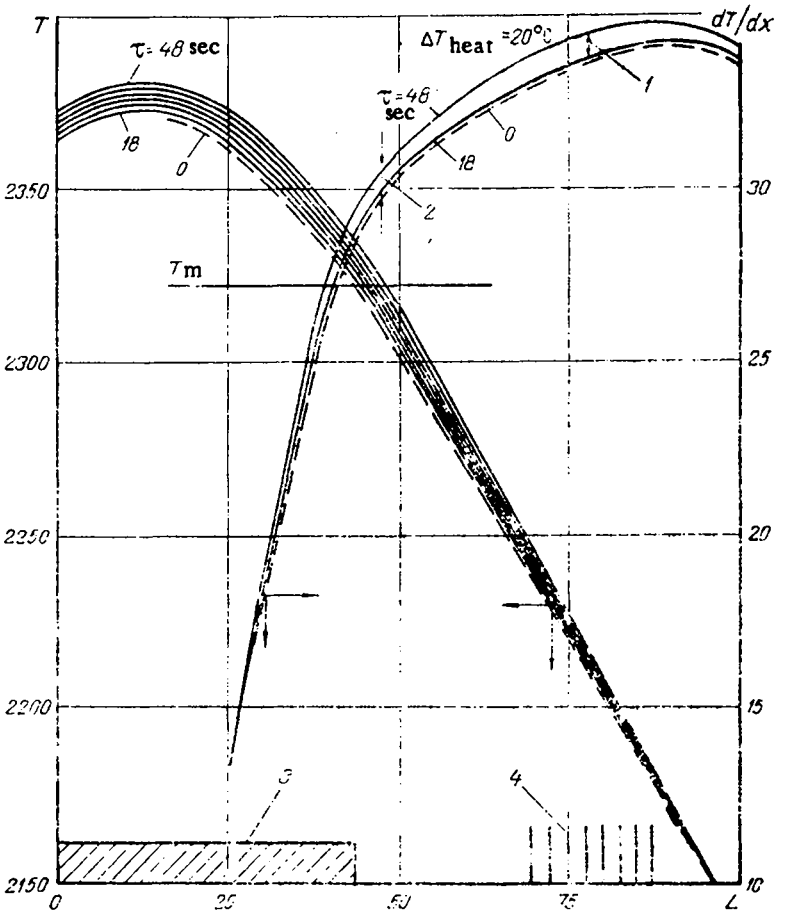

Fig. 2. Change in the T-field and temperature gradient field upon insertion of the heater perturbation ΔT: 1) ΔdT/dx maximal; 2) the same, crystallization front; 3) heater; 4) diaphragm; T, °K; L, mm; dT/dx, %.

The fundamental results presented in Table 1 display the substantial difference in the changes in the main thermal parameters of the growth process of crystal being formed because of the action of the temperature perturbations. In the area of small temperature perturbations (to ±3-4°C) the greatest relative changes arrive at the magnitude of the temperature gradient in the domain of the separating diaphragm, and at the location of crystallization front for more than 7-8°C temperature perturbations, where the difference in the change of dT/dx on the crystallization front and in the domain of its maximum value diminishes as the absolute value of the temperature perturbation grows. For example, $dT/dx|_{max}$ is 3.3-3.5 times greater than $dT/dx|_{cryst}$ for ΔT = ± 1-2°C, while it diminishes to 1.7-1.8 for ΔT = ±20-25°C.

The temperature change at different points of the crystal due to the action of the temperature perturbation ±ΔT is shown in Fig. 3. It can be noted that the T-field in the crystal reacts differently to the increase and decrease in the heater temperature. The diverse nature of the T-field reaction is caused by the presence of a phase transition in the material at which the heat of crystallization is liberated, where this quantity is quite substantial for leucosapphire even for relatively low crystallization rates.

Analogous computations performed for a lower temperature level yielded completely symmetric pattern of T-field changes for positive and negative values of ΔT. It must be noted that in this case the maximal temperature change at the "hottest" point of the crystal was ±12.8, 7.3, 3.4, 1.42°C, respectively, for the temperature perturbations ±20, 10, 5, 2°C. Therefore, a stronger influence of the heater temperature fluctuations is seen in the crystal in the absence of latent heat liberation despite the lower temperature level (2100°K).

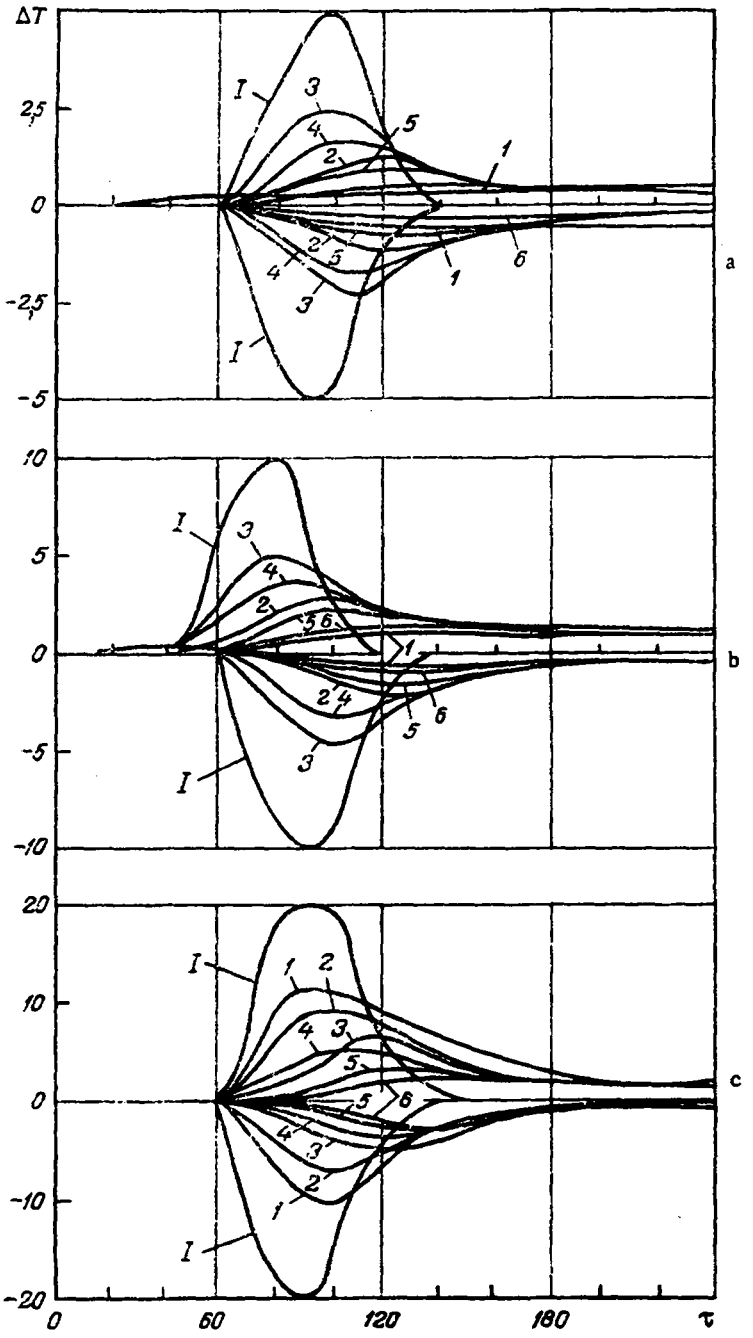

Fig. 3. Temperature change at different points of a growing crystal as a function of the sign and magnitude of ΔT: a, b: 1) 1382°K; 2) 2027; 3) 2368; 4) 2307; 5) 2178; 6) 1697; c: 1) 2368°K; 2) 2307; 3) 2027; 4) 2178; 5) 1381; 6) 1697; I) heater temperature perturbation; ΔT, °C; τ, sec.

Estimates performed showed that for a 25 × 100 mm crystal cross section, from 17.63 W at V_{cr} = 6 mm/h to 30 W at V_{cr} = 10 mm/h is liberated at the front. The heat flux eliminated from the crystallization front in the solid phase is around 25 W for dT/dx = 10 K/cm and 130 W for dT/dx = 50 K/cm. Therefore, the crystallization front can exert substantial influence on the passage of the temperature perturbation from the heater to the growing crystal.

Depending on the magnitude of the temperature perturbation, five different versions of the crystallization front behavior (Fig. 4) can occur. Let us consider the case when the velocity of container motion (V_{con}) relative to the heater and the velocity of crystallization front motion (V_{fr}) relative to the container are opposite and equal, i.e., the crystallization front "stands" at a fixed location. For an abrupt diminution in the heater

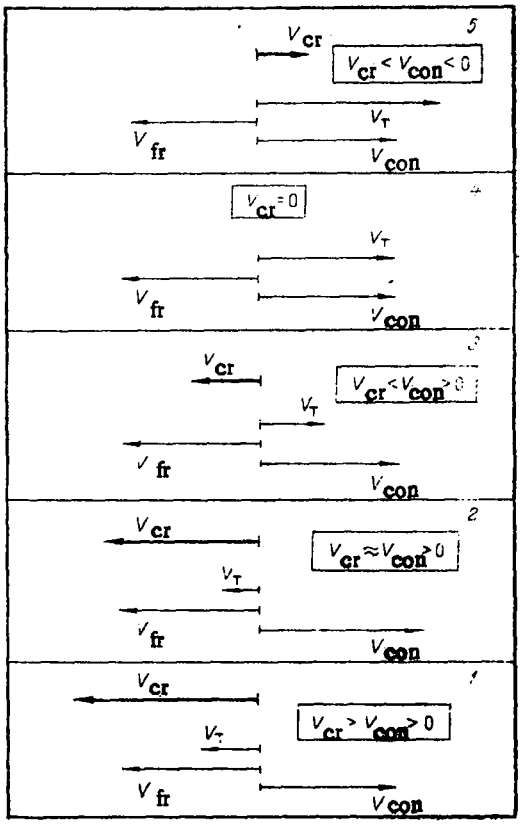

Fig. 4. Influence of the magnitude and sign of ΔT on the rate of material crystallization: 1) $V_{cr} > V_{con}$; 2) $V_{cr} = V_{con}$; 3) $V_{cr} < V_{con}$; 4) $V_{cr} = 0$; 5) melting of the crystal.

TABLE 1. Influence of Temperature Perturbations on the Main Thermal Parameters on the Crystallization Front

Heater temp. perturbation	Change in T after $\tau_k/5$, %			Displacement of crystallization front	Change in temp. gradient		Stationary regime build-up time	Maximal melt temp. °K
	in melt (maximal value)	on crystallization front	in domain of maximal gradient		on crystallization front	in domain of maximal gradient		
+20	0,42	0,43	0,27	+10,74	+1,3	+2,35	308	2381
—20	0,4	0,38	0,28	—9,43	—1,36	—2,51	296	2357
+10	0,22	0,15	0,11	+4,82	+0,83	+1,92	287	2378
—10	0,21	0,14	0,112	—4,2	—0,87	—2,02	280	2358
+5	0,1	0,077	0,06	+1,8	+0,47	+1,56	274	2374
—5	0,09	0,073	0,063	—1,51	—0,51	—1,63	268	2363
+2	0,036	0,027	0,021	+0,71	+0,31	+1,07	267	2370
—2	0,034	0,024	0,022	—0,62	—0,34	—1,12	259	2366

temperature (Fig. 4, No. 1), a component of the crystallization front motion velocity occurs due to the change in the temperature conditions (V_T), which is directed to the same side as V_{fr}. The crystallization front starts to shift toward the heater and V_{cr} becomes greater than V_{con}, and the heat-of-crystallization liberation increases correspondingly, tending to cancel the action of the temperature perturbation. For a small negative value $-\Delta T$ (Fig. 4, No. 2), the velocity component V_T is also small and V_{cr} remains practically equal to V_{con}, i.e., the front shift from the initial position is insignificant.

There can be three cases for a positive perturbation $+\Delta T$. If ΔT is small (Fig. 4, No. 3), the component V_T is also small, but directed oppositely to V_{fr}, and the crystallization rate diminishes ($V_{cr} < V_{con}$); here the liberation of the heat of crystallization diminishes on the front. Increase of $+\Delta T$ can result in V_T becoming equal to V_{fr}, and in this case

crystallization of the material ceases. Finally, the perturbation can be so large that $V_T > V_{fr}$, and submelting of the material being crystallized starts with absorption of the heat of the phase transition.

Therefore, in all cases the crystallization front exerts a damping action on the originating temperature perturbations, weakening them significantly. For this reason, positive and negative ΔT differently exert influence on the change in the T-field in the crystal. Checking computations executed at a lower temperature level (no crystallization front) confirmed the validity of the statements expressed. In these cases the pattern of the T-field change would be independent of the sign of ΔT.

Estimates performed on the power for installations of the type SKBK-"Sapphire" showed that in the nominal regime power fluctuations within the limits ±0.35% result in a not more than 0.08-0.1 mm crystallization front shift; here the heater temperature fluctuations are about ±0.85-0.95°C.

The analysis performed on the temperature conditions for leucosapphire crystallization by the HDC method showed that requirements on the automatic regulation systems are elevated without complete justification, and existing power, voltage, and other regulating systems possess sufficient accuracy for the maintenance of stable temperature conditions in the melt–crystal system. On the other hand, it can be assumed that the main source of instability in the conditions on the crystallization front for an installation of this kind is the work of the container displacement mechanism. Thus, for instance, a change in the velocity from 8 to 7 mm/h results in a 15-17% diminution in the liberation of the heat of crystallization, which is 5-10% of the internal heat flux from the liquid to the solid phase for small temperature gradients. Such a velocity fluctuation turns out to be equivalent to the temperature perturbation of 30-40°C at the heater, where it must be taken into account that the instability in driver operation is reflected on the crystallization front without any attenuating factors. Therefore, it can be considered that the transfer coefficient of the perturbing action from the heater on the crystallization front location is 0.4-0.6, and from the drawing mechanism is equal to one. In connection with this the requirements imposed on the stability of maintaining the heater temperature should be matched to the stability of operation of the mechanism, otherwise the increase in regulation accuracy is unjustified.

NOTATION

C_p, specific heat; γ, material density; τ_o, τ_t, τ_d, τ_f, time period of the initial section, the transition to the new temperature level, the holding, and the termination of the transient; dT/dx, derivative of the temperature with respect to the coordinate; ΔT, magnitude of the temperature deviation from the nominal value; V_{cr}, V_{con}, V_{fr}, V_T, crystallization, container motion, relative crystallization front displacement, and front displacement rates due to the action of the temperature perturbation.

LITERATURE CITED

1. Yu. K. Lingart and Ya. I. Shtipel'man, "Investigations of temperature fields in apparatus to grow leucosapphire single crystals by using mathematical modeling," Inzh.-Fiz. Zh., 43, No. 2, 306-314 (1982).
2. S. V. Bodyachevskii, Yu. K. Lingart, N. A. Tikhonova, et al., "Computation of temperature fields of laminated leucosapphire single crystals," Tr. VNIIETO, No. 10, 90-102, Energiya, Moscow (1979).
3. L. D. Boiko, Yu. K. Lingart, M. A. Mel'tser, and Ya. I. Shtipel'man, "Investigation of heat transfer during crystal growth by using an electronic computer," Manuscript Deposited in Informélektro No. 297-d/81, VINITI, "Deponir. ruk,"No. 1 (123), 154 (1982).