PHYSICS OF CONDENSED STATE OF MATTER

X-Ray Heating of Perfect Crystals: Problem Statement and Analytical Solution

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Abstract—Analytical expressions are found that in the most general form describe the space—time distribution of the thermal field in an anisotropic crystal during heat exchange with the environment under the influence of synchrotron X-ray radiation or X-ray free-electron laser pulses with an arbitrary space-time structure.

Keywords: X-ray free-electron laser heating, X-ray heating, heat conductivity, anisotropic media.

INTRODUCTION

Powerful sources of X-ray radiation, that is, specific third-generation synchrotron sources and X-ray free-electron lasers, find increasing application for studying the structure of various systems. The brightness of these sources leads to a substantial increase in thermal load on both forming X-ray optics components and studied objects themselves.

In spite of the relatively low intensity of radiation of X-ray tubes, the experimental technique for determination of objects heating by X-ray radiation was developed as early as the 1940s (for example, [1, p. 408]). However, in classical works, i.e., "bibles" on the physics of X rays and X-ray structural analysis [2—7], X-ray heating was not considered.

The first work known to the author of this paper that was devoted to X-ray heating was published in 2008 [8]. In [8], based on a numerical solution to the heat conductivity equation, the thermal field profile in a silicon crystal with a size of $30 \times 10 \times 2$ mm, which was at 293 K and was irradiated by X-ray synchrotron radiation with an energy of 10 keV and energy density 0.23 W/mm^2, was calculated. It was shown that the crystal surface heated to a maximum temperature of approximately 296 K.

The next step was made in [9, 10], where, based on an analytical solution to the heat conductivity equation with boundary conditions of the first kind, the space—time distribution of temperature in the crystal under the influence of X-ray free-electron laser was analyzed. In this case, thermal properties of a model

diamond crystal were described not by a tensor, but by the heat conductivity factor, i.e., the crystal had isotropic thermal properties. This approach is justified for evaluation of the thermal influence on X-ray optics components, which are equipped with a cooling system, but is not applicable in other cases.

Since, crystals have substantially anisotropic thermal properties [11] the description of their thermal properties by a single scalar heat conductivity factor is a rather rough simplification.

Unfortunately, the author of this paper is not aware of other papers that are devoted to the study of X-ray heating of crystals that have anisotropic thermal properties. At the same time, as mentioned above and separately noted in [9, 10], this problem is of significant interest.

1. PROBLEM STATEMENT

When X rays fall on a substance part of the radiation is reflected from the surface, part of the radiation is scattered on the atoms of the substance, part of the radiation passes through the substance, and the remaining part is absorbed. The X-ray absorption is described by the law

$$I(x) = I_0 \exp(-\mu x), \qquad (1)$$

where I_0 is the X-ray intensity on the surface, $\mu = \tau + \sigma$ is the linear attenuation factor, τ is the true absorption factor, which corresponds to the extinction of the initial X-ray photon, σ is the scattering factor, which corresponds to changing the direction of the initial X-ray photon, and x is a coordinate that is directed deep into the material.

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The X-ray photon extinction during true absorption occurs due to the photoelectric effect, when the photon energy is spent on atomic ionization. As a result of the true absorption, the radiation energy is transformed into the energy of photo- and Auger electrons and the energy of the secondary radiation. Electrons that hit the irradiated substance, when interacting with atoms of this substance, give them their energy, which is transformed into other forms of energy (depending on the properties of the absorbing body, thermal, chemical energy, energy of radiation, and ionization).

Following (1), in a layer of the substance with a thickness x the energy

$$W(x) = W_0\{1 - [1 - R]\exp(-\mu x)\}$$

is absorbed, where R is the X-ray reflection factor: the specular reflection under sliding angles of the incidence of the radiation on the crystal surface (in the region of the total external reflection), away from the diffraction conditions, the diffraction reflection, at large angles of the radiation incidence on the surface under the diffraction conditions, and the specular-diffraction reflection when conditions of diffraction for atomic crystalline planes and the specular reflection for the surface are simultaneously fulfilled for incident X rays. In the most general case, the reflection factor will be a function of two spatial coordinates y, z, as well as time t: $R(y, z, t)$ [12–14]. A linear attenuation factor can be represented in the form [1, 6]

$$\mu = (\tau_e + \tau_S) + (\sigma_e + \sigma_S),$$

where the coefficient τ_e takes the energy that is transformed into the energy of photoelectrons into account, τ_S takes the energy of a characteristic X-ray that occurs upon ionization of atoms into account, σ_e takes the energy that is transformed into the kinetic energy of recoil electrons into account, and σ_S takes the energy of the scattered X rays into account.

Therefore, the part of the absorbed energy of the incident X rays that is transformed into the energy of electrons is characterized by a linear coefficient of electron transformation $\gamma = \tau_e + \sigma_e$ [1].

In the absence of chemical and ionization processes in the substance, as well as phase transitions, the entire energy of electrons $W_0\{1 - [1 - R]\exp(-\gamma x)\}$ heats the irradiated substance and is transferred deep into the substance by the heat conductivity. The kinetics of this process are described by an inhomogeneous heat conductivity equation with an internal thermal source [15–19]:

$$c(\mathbf{r})\rho(\mathbf{r})[\partial T(\mathbf{r}, t)/\partial t]$$
$$= \text{div}[\Lambda(\mathbf{r}, t) \times \text{grad}T(\mathbf{r}, t)] + F(\mathbf{r}, t), \quad (2)$$

where $c(\mathbf{r})$ is the specific heat capacity, $\rho(\mathbf{r})$ is the density, $T(\mathbf{r}, t)$ is the temperature field, $\Lambda(\mathbf{r}, t)$ is the heat conductivity tensor, $F(\mathbf{r}, t)$ is the density of internal thermal sources, $\mathbf{r}$ is the spatial coordinate, and t is time. In the framework of this model, it is assumed that the specific heat capacity and heat conductivity tensor do not depend on temperature. In a real situation, this, in fact, implies the approximate solution to the problem only within a certain temperature interval ΔT, in which, one can neglect the change of $c(T)$ and $\Lambda(T)$. In this case, it is of particular note that Eq. (2) itself was obtained in the following approximations [19].

1. The deformation of the considered volume, which is related to the change of temperature, is very small compared to the volume itself.

2. Macroscopic particles of the body are motionless with respect to each other.

Moreover, the heat conductivity equation (2) is the general mathematical model for a set of heat conductivity phenomena and by itself, is not indicative of development of the heat transfer process in the body. This is explained by the nonuniqueness of the solution to partial differential equations. In order to derive a single partial solution, which corresponds to a certain problem, one needs to have additional data that are not contained in the initial equation. These data include:

1. Geometric conditions that give the shape and size of the body in which heat exchange processes take place;

2. Physical conditions that give not only the heat and temperature conductivity but also the density of internal thermal sources;

3. Boundary conditions that give the thermal interaction of the surface of the body with the environment;

4. Initial conditions that give the distribution of teh temperature at any point of the body at a certain initial time.

We will consider ideal dielectric or semiconductor crystals as the objects of study, where, following [20, 21], one can consider the specific heat capacity and the density to be independent of the coordinate and the heat conductivity components to be independent of the coordinate and time.

Changing to the principal axes (x', y', z') of the heat conductivity, the components of a symmetric

second rank tensor $\Lambda(\mathbf{r}, t)$ take the diagonal form [13, 16, 19, 22]:

$$\Lambda'(\mathbf{r}') = \begin{pmatrix} \lambda_1 & 0 & 0 \\ 0 & \lambda_2 & 0 \\ 0 & 0 & \lambda_3 \end{pmatrix},$$

and the heat conductivity equation (2), in view of this, is simplified:

$$c\rho\frac{\partial T}{\partial t} = \lambda_1\frac{\partial^2 T}{\partial x'^2} + \lambda_2\frac{\partial^2 T}{\partial y'^2} + \lambda_3\frac{\partial^2 T}{\partial z'^2} + F.$$

Further, we will work in the system of principal axes of the heat conductivity and omit the symbol $'$ at coordinates, and present the studied crystal itself in the form of a rectangular parallelepiped with a size of $l_1 \times l_2 \times l_3$ along the principal axes of the heat conductivity.

In most X-ray experiments the studied sample is small, and the time of mounting, adjustment, and equipment alignment is large. In this case, if temperature experiments are not performed, then the sample is under conditions of convective and radiative heat exchange with the environment. Consequently, the temperature distribution of the studied sample at the initial instant of time can be considered uniform and equal to the environment temperature, which is a constant and does not depend on time:

$$T(\mathbf{r}, t) = T_0 = \text{const}.$$

In the most general case, the boundary conditions of the formulated problem are inhomogeneous boundary conditions of the third kind [16, 17, 22]:

$$\alpha(T_0 - T)|_S + \lambda_n\frac{\partial T}{\partial n}\bigg|_S = \Psi(\mathbf{r}, t), \qquad (3)$$

where n is the unit outer normal to the surface (boundary) S of the body, α is the heat exchange factor, and $\Psi(\mathbf{r}, t)$ is the energy density of thermal sources on the surface. Thus, in [8], it is assumed that $\Psi(\mathbf{r}, t) = \mu_a q_r - \sigma\mu_e T^4$, where μ_a and μ_e are surface factors of absorption and emission, q_r is the surface density of the incident heat flux, σ is the Stefan–Boltzmann constant, and T is the surface temperature. Following [8, 17], we neglect changing the heat exchange factor α on time and its dependence on the thermophysical properties of the body, i.e., we will assume $\alpha = \text{const}$ on all edges of the sample.

Therefore, the problem is reduced to solving the third inhomogeneous boundary-value problem for the heat conductivity equation with a source in an orthotropic parallelepiped:

$$\frac{\partial T}{\partial t} = a_1\frac{\partial^2 T}{\partial x^2} + a_2\frac{\partial^2 T}{\partial y^2} + a_3\frac{\partial^2 T}{\partial z^2} + \frac{F(\mathbf{r}, t)}{c\rho},$$

$$\mathbf{r} \in V, \ t > 0; \qquad (4)$$

$$T(\mathbf{r}, t = 0) = T_0 = \text{const}, \quad \mathbf{r} \in V; \qquad (5)$$

$$\alpha(T_0 - T)|_x + \lambda_1\frac{\partial T}{\partial x}\bigg|_x = \Psi_1(\mathbf{r}, t),$$

$$x = 0, \quad 0 < y < l_2, \quad 0 < z < l_3, \quad t > 0; \quad (6.1)$$

$$\alpha(T_0 - T)|_x + \lambda_1\frac{\partial T}{\partial x}\bigg|_x = \Psi_2(\mathbf{r}, t),$$

$$x = l_1, \quad 0 < y < l_2, \quad 0 < z < l_3, \quad t > 0; \quad (6.2)$$

$$\alpha(T_0 - T)|_y + \lambda_2\frac{\partial T}{\partial y}\bigg|_y = \Psi_3(\mathbf{r}, t),$$

$$y = 0, \quad 0 < x < l_1, \quad 0 < z < l_3, \quad t > 0; \quad (6.3)$$

$$\alpha(T_0 - T)|_y + \lambda_2\frac{\partial T}{\partial y}\bigg|_y = \Psi_4(\mathbf{r}, t),$$

$$y = l_2, \quad 0 < x < l_1, \quad 0 < z < l_3, \quad t > 0; \quad (6.4)$$

$$\alpha(T_0 - T)|_z + \lambda_3\frac{\partial T}{\partial z}\bigg|_z = \Psi_5(\mathbf{r}, t),$$

$$z = 0, \quad 0 < x < l_1, \quad 0 < y < l_2, \quad t > 0; \quad (6.5)$$

$$\alpha(T_0 - T)|_z + \lambda_3\frac{\partial T}{\partial z}\bigg|_z = \Psi_6(\mathbf{r}, t),$$

$$z = l_3, \quad 0 < x < l_1, \quad 0 < y < l_2, \quad t > 0, \quad (6.6)$$

where $a_i = \lambda_i/(c\rho)$ are temperature conductivity factors ($i = 1, 2, 3$) and V is the parallelepiped volume. An attempt to solve problem (4)–(6) was made in [22]; however, in the course of solution, boundary conditions were changed from third-kind boundary conditions to second-kind boundary conditions.

Let X rays propagate along the x axis and fall on the input surface $x = 0$. Then, the density of internal thermal sources $F(\mathbf{r}, t)$ can be presented in the form

$$F(\mathbf{r}, t)$$
$$= W_0(y, z, t)\{1 - [1 - R(y, z, t)]\exp(-\gamma x)\},$$

where $W_0(y, z, t)$ determines the time dependence of the X-ray intensity on the surface.

2. ANALYTICAL SOLUTION TO THE PROBLEM

In view of the linearity of problem (4), we present the function $T(\mathbf{r}, t)$ in the form of a sum:

$$T(\mathbf{r}, t) = v(\mathbf{r}, t) + w(\mathbf{r}, t),$$

we substitute this expression into (3)–(5) and select problems for functions $w(\mathbf{r}, t)$:

$$a_1\frac{\partial^2 w}{\partial x^2} + a_2\frac{\partial^2 w}{\partial y^2} + a_3\frac{\partial^2 w}{\partial z^2} = 0,$$

$$\mathbf{r} \in V, \quad t > 0; \qquad (7.1)$$

$$\lambda_n \frac{\partial w}{\partial n}\bigg|_S - \alpha w|_S = \Psi(\mathbf{r}, t) - \alpha T_0,$$

$$\mathbf{r} \in S, \quad t > 0, \qquad (7.1)$$

and $v(\mathbf{r}, t)$:

$$\frac{\partial v}{\partial t} = a_1 \frac{\partial^2 v}{\partial x^2} + a_2 \frac{\partial^2 v}{\partial y^2} + a_3 \frac{\partial^2 v}{\partial z^2} + \frac{F(\mathbf{r}, t)}{c\rho} - \frac{\partial w}{\partial t},$$

$$\mathbf{r} \in V, \quad t > 0; \qquad (8.1)$$

$$v(\mathbf{r}, t = 0) = T_0 - w(\mathbf{r}, t = 0), \quad \mathbf{r} \in V; \qquad (8.2)$$

$$\lambda_n \frac{\partial v}{\partial n}\bigg|_S - \alpha.v|_S = 0, \quad \mathbf{r} \in S, \quad t > 0. \qquad (8.3)$$

In fact, this implies that we presented the temperature field $T(\mathbf{r}, t)$ inside the studied sample as a superposition of "stationary" (since boundary conditions depend on time) $w(\mathbf{r}, t)$ and nonstationary with sources $v(\mathbf{r}, t)$ temperature fields.

In order to solve problem (7), we present the sought function in the form of a sum $w(\mathbf{r}, t) = w_1(\mathbf{r}, t) + w_2(\mathbf{r}, t) + w_3(\mathbf{r}, t)$, each term of which satisfies the initial equation (7.1) and one-dimensional boundary conditions of the third kind. In this case, for function $w_1(\mathbf{r}, t)$, homogeneous boundary conditions of the third kind are given on the edges $y = 0$, $y = l_2$, $z = 0$, $z = l_3$, for function $w_2(\mathbf{r}, t)$, on edges $x = 0$, $x = l_1$, $z = 0$, $z = l_3$, and for function $w_3(\mathbf{r}, t)$, on edges $x = 0$, $x = l_1$, $y = 0$, $y = l_2$:

$$a_1 \frac{\partial^2 w_1}{\partial x^2} + a_2 \frac{\partial^2 w_1}{\partial y^2} + a_3 \frac{\partial^2 w_1}{\partial z^2} = 0,$$

$$\mathbf{r} \in V, \quad t > 0; \qquad (9.1)$$

$$\lambda_1 \frac{\partial w_1}{\partial x}\bigg|_{x=0} - \alpha w_1|_{x=0} = \Psi_1(\mathbf{r}, t) - \alpha T_0,$$

$$0 < y < l_2, \quad 0 < z < l_3, \quad t > 0; \qquad (9.2)$$

$$-\lambda_1 \frac{\partial w_1}{\partial x}\bigg|_{x=l_1} - \alpha w_1|_{x=l_1} = \Psi_1(\mathbf{r}, t) - \alpha T_0,$$

$$0 < y < l_2, \quad 0 < z < l_3, \quad t > 0; \qquad (9.3)$$

$$\lambda_2 \frac{\partial w_1}{\partial y}\bigg|_{y=0} - \alpha w_1|_{y=0} = 0,$$

$$0 < x < l_1, \quad 0 < z < l_3, \quad t > 0; \qquad (9.4)$$

$$-\lambda_2 \frac{\partial w_1}{\partial y}\bigg|_{y=l_2} - \alpha w_1|_{y=l_2} = 0,$$

$$0 < x < l_1, \quad 0 < z < l_3, \quad t > 0; \qquad (9.5)$$

$$\lambda_3 \frac{\partial w_1}{\partial z}\bigg|_{z=0} - \alpha w_1|_{z=0} = 0,$$

$$0 < x < l_1, \quad 0 < y < l_2, \quad t > 0; \qquad (9.6)$$

$$-\lambda_3 \frac{\partial w_1}{\partial z}\bigg|_{z=l_3} - \alpha w_1|_{z=l_3} = 0,$$

$$0 < x < l_1, \quad 0 < y < l_2, \quad t > 0. \qquad (9.7)$$

The problems for functions $w_2(\mathbf{r}, t)$ and $w_3(\mathbf{r}, t)$ are similar and we will not write them separately.

Using the method of separation of variables to solve the problem (9) $w_1(x, y, z, t) = X(x, t)P(y, z)$, we derive the following eigenfunction $P(y, z)$ and eigenvalue λ^2 problem:

$$a_2 \frac{\partial^2 P}{\partial y^2} + a_3 \frac{\partial^2 P}{\partial z^2} + \lambda^2 P = 0,$$

$$0 < y < l_2, \ 0 < z < l_3; \qquad (10.1)$$

$$\lambda_2 \frac{\partial P}{\partial y}\bigg|_{y=0} - \alpha P|_{y=0} = 0,$$

$$\lambda_2 \frac{\partial P}{\partial y}\bigg|_{y=l_2} + \alpha P|_{y=l_2} = 0; \qquad (10.2)$$

$$\lambda_3 \frac{\partial P}{\partial z}\bigg|_{z=0} - \alpha P|_{z=0} = 0,$$

$$\lambda_3 \frac{\partial P}{\partial z}\bigg|_{z=l_3} + \alpha P|_{z=l_3} = 0. \qquad (10.3)$$

We will again solve the problem (10) by the method of separation of variables $P(y, z) = Y(y)Z(z)$:

$$a_2 Y'' + \beta_2^2 Y = 0,$$

$$\lambda_2 Y'|_{y=0} - \alpha Y|_{y=0} = 0,$$

$$\lambda_2 Y'|_{y=l_2} + \alpha Y|_{y=l_2} = 0; \qquad (11.1)$$

$$a_3 Z'' + \beta_3^2 Z = 0,$$

$$\lambda_3 Z'|_{z=0} - \alpha Z|_{z=0} = 0,$$

$$\lambda_3 Z'|_{z=l_3} + \alpha Z|_{z=l_3} = 0; \qquad (11.2)$$

$$\beta_2^2 + \beta_3^2 = \lambda^2, \qquad (11.3)$$

where the primes traditionally denote teh derivatives.

The eigenfunction Y and eigenvalue β_2 problem (11.1) has the general solution

$$Y(y) = C_1 \cos\left(\frac{\beta_2}{\sqrt{a_2}}y\right) + C_2 \sin\left(\frac{\beta_2}{\sqrt{a_2}}y\right),$$

and integration constants C_1 and C_2 are determined from boundary conditions in (11.1) and connected by relation $C_1 = \frac{\lambda_2}{\sqrt{a_2}}\frac{\beta_2}{\alpha}C_2$. In this case, eigenvalues β_2 are determined from a numerical solution to a transcendental equation

$$\cot\left(\frac{\beta_2}{\sqrt{a_2}}l_2\right) = \frac{1}{2}\left[\frac{\lambda_2}{\sqrt{a_2}}\frac{\beta_2}{\alpha} - \frac{\sqrt{a_2}}{\lambda_2}\frac{\alpha}{\beta_2}\right], \qquad (12)$$

having an infinite number of roots $\beta_{2,m}$.

The problem (11.2) is also solved similarly. Moreover, solving problem (9) for functions $w_2(\mathbf{r}, t)$ and

$w_3(\mathbf{r}, t)$ in the same way, we obtain an analogous expression for function $X(x)$ as well. Therefore, we can write eigenfunctions of the problem (11) in the following most general form:

$$X_{i,m}(x_i) = D_i \left[\frac{\lambda_i}{\sqrt{a_i}} \frac{\beta_{i,m}}{\alpha} \cos \left(\frac{\beta_{i,m}}{\sqrt{a_i}} x_i \right) \right.$$
$$\left. + \sin \left(\frac{\beta_{i,m}}{\sqrt{a_i}} x_i \right) \right], \qquad (13)$$

where D_i are arbitrary, for example equal to unity, constants of integration, coordinates x, y, z are renamed as x_i $(i = 1, 2, 3)$, and eigencalues $\beta_{i,m}$ are roots of Eq. (12): $\cot \left(\frac{\beta_{i,m}}{\sqrt{a_i}} l_i \right) = \frac{1}{2} \left[\frac{\lambda_i}{\sqrt{a_i}} \frac{\beta_{i,m}}{\alpha} - \frac{\sqrt{a_i}}{\lambda_i} \frac{\alpha}{\beta_{i,m}} \right].$

It is easy to show that eigenfunctions X_i (13) are orthogonal on segments $0 < x_i < l_i$ and their squared norm is determined by expression

$$||X_{i,m}(x_i)||^2 = \frac{1}{2} \left[l_i + \frac{2\lambda_i a_i \alpha}{\beta_{i,m}^2 \lambda_i^2 + a_i \alpha^2} \right].$$

In turn, eigenfunctions of the problem (10), which are determined by expression

$$P_{nk}(x_2, x_3)$$
$$= D_{nk} \left[\frac{\lambda_2}{\sqrt{a_2}} \frac{\beta_{2,n}}{\alpha} \cos \left(\frac{\beta_{2,n}}{\sqrt{a_2}} x_2 \right) + \sin \left(\frac{\beta_{2,n}}{\sqrt{a_2}} x_2 \right) \right]$$
$$\times \left[\frac{\lambda_3}{\sqrt{a_3}} \frac{\beta_{3,k}}{\alpha} \cos \left(\frac{\beta_{3,k}}{\sqrt{a_3}} x_3 \right) + \sin \left(\frac{\beta_{3,k}}{\sqrt{a_3}} x_3 \right) \right],$$

are orthogonal in rectangle $(0 < x_2 < l_2) \times (0 < x_3 < l_3)$, and their squared norm is

$$||P_{nk}(x_2, x_3)||^2 = ||X_{2,n}(x_2)||^2 ||X_{3,k}(x_3)||^2.$$

From (9), in addition to problem (10) on eigenfunctions $P(y, z)$ and eigenvalues λ^2, we also obtain equation

$$a_1 \frac{\partial^2 X(x_1, t)}{\partial x_1^2} - \lambda^2 X(x_1, t) = 0,$$

which solution at known eigenvalues λ_{nk} is a function

$$X_{nk}(x_1, t) = A_{nk}(t) \exp \left\{ \frac{\lambda_{nk}}{\sqrt{a_1}} x_1 \right\}$$
$$+ B_{nk}(t) \exp \left\{ -\frac{\lambda_{nk}}{\sqrt{a_1}} x_1 \right\}.$$

Consequently, the solution to problem (9) has the form:

$$w_1(x_1, x_2, x_3, t) = \sum_{n,k=1}^{\infty} \left\{ \left[A_{nk}(t) \exp \left\{ \frac{\lambda_{nk}}{\sqrt{a_1}} x_1 \right\} \right. \right.$$
$$\left. + B_{nk}(t) \exp \left\{ -\frac{\lambda_{nk}}{\sqrt{a_1}} x_1 \right\} \right]$$
$$\times \left[\frac{\lambda_2}{\sqrt{a_2}} \frac{\beta_{2,n}}{\alpha} \cos \left(\frac{\beta_{2,n}}{\sqrt{a_2}} x_2 \right) + \sin \left(\frac{\beta_{2,n}}{\sqrt{a_2}} x_2 \right) \right]$$
$$\left. \times \left[\frac{\lambda_3}{\sqrt{a_3}} \frac{3,k}{\alpha} \cos \left(\frac{\beta_{3,k}}{\sqrt{a_3}} x_3 \right) + \sin \left(\frac{\beta_{3,k}}{\sqrt{a_3}} x_3 \right) \right] \right\}.$$
$$(14)$$

Coefficients $A_{nk}(t)$ and $B_{nk}(t)$ depend on time, since they are determined from inhomogeneous boundary conditions of the third kind (9.2), (9.3) with the right sides, which depend on time.

In order to find coefficients $A_{nk}(t)$ and $B_{nk}(t)$, we substitute $w_1(x_1 = 0, x_2, x_3, t)$ and $w_1(x_1 = l_1, x_2, x_3, t)$, which are expressed from (14), into (9.2) and (9.3). We multiply the obtained equalities by eigenfunctions $P_{qs}(x_2, x_3)$ with indices q, s and integrate over x_2 within limits from 0 to l_2, and over x_3 within limits from 0 to l_3. In view of the orthogonality of eigenfunctions, all terms of the obtained series, apart from the term at $n = q$ and $k = s$, will be zero. As a result, we obtain the system of equations to find the sought coefficients:

$$\begin{cases} A_{nk}(t) \left[\lambda_1 \frac{\lambda_{nk}}{\sqrt{a_1}} - \alpha \right] \\ + B_{nk}(t) \left[-\lambda_1 \frac{\lambda_{nk}}{\sqrt{a_1}} - \alpha \right] = \widetilde{\Psi}_1(t) \\ A_{nk}(t) \left[\lambda_1 \frac{\lambda_{nk}}{\sqrt{a_1}} - \alpha \right] \exp \left\{ \frac{\lambda_{nk}}{\sqrt{a_1}} l_1 \right\} \\ + B_{nk}(t) \left[-\lambda_1 \frac{\lambda_{nk}}{\sqrt{a_1}} - \alpha \right] \\ \times \exp \left\{ -\frac{\lambda_{nk}}{\sqrt{a_1}} l_1 \right\} = \widetilde{\Psi}_2(t), \end{cases} (15)$$

where it is introduced the notation

$$\widetilde{\Psi}_{1,2}(t) = \frac{1}{||P_{nk}||^2}$$
$$\times \int\int_0^{l_2, l_3} \left\{ \left[\Psi_{1,2} \left(\begin{matrix} x = 0 \\ x = l_1 \end{matrix}, \xi_2, \xi_3, t \right) - \alpha T_0 \right] \right.$$
$$\times \left[\frac{\lambda_2}{\sqrt{a_2}} \frac{\beta_{2,n}}{\alpha} \cos \left(\frac{\beta_{2,n}}{\sqrt{a_2}} \xi_2 \right) + \sin \left(\frac{\beta_{2,n}}{\sqrt{a_2}} \xi_2 \right) \right]$$
$$\times \left[\frac{\lambda_3}{\sqrt{a_3}} \frac{\beta_{3,k}}{\alpha} \cos \left(\frac{\beta_{3,k}}{\sqrt{a_3}} \xi_3 \right) \right.$$
$$\left. \left. + \sin \left(\frac{\beta_{3,k}}{\sqrt{a_3}} \xi_3 \right) \right] \right\} d\xi_2 d\xi_3. \qquad (16)$$

The solution to system (15) has the following simple form:

$$A_{nk}(t), B_{nk}(t)$$

$$= \frac{\widetilde{\Psi}_1(t)\left[\lambda_1\frac{\lambda\lambda_{nk}}{\sqrt{a_1}} \mp \alpha\right]\exp\left\{\mp\frac{\lambda_{nk}}{\sqrt{a_1}}l_1\right\}}{-\left[\lambda_1\frac{\lambda_{nk}}{\sqrt{a_1}} + \alpha\right]^2\exp\left\{\frac{\lambda_{nk}}{\sqrt{a_1}}l_1\right\}}$$

$$\frac{+\widetilde{\Psi}_2(t)\left[\lambda_1\frac{\lambda_{nk}}{\sqrt{a_1}} \pm \alpha\right]}{+\left[\lambda_1\frac{\lambda_{nk}}{\sqrt{a_1}} - \alpha\right]^2\exp\left\{\frac{-\lambda_{nk}}{\sqrt{a_1}}l_1\right\}}. \quad (17)$$

Therefore, the solution $w_1(\mathbf{r}, t)$ of problem (9) is determined by expression (14), where the coefficients $A_{nk}(t)$ and $B_{nk}(t)$ are given by (17), $\lambda_{nk}^2 = \beta_{2,n}^2 + \beta_{3,k}^2$, and $\beta_{i,m}$ are roots of Eq. (12).

We recall that the solution to problem (7) is $w(\mathbf{r}, t) = w_1(\mathbf{r}, t) + w_2(\mathbf{r}, t) + w_3(\mathbf{r}, t)$. The procedure to find $w_2(\mathbf{r}, t)$ and $w_3(\mathbf{r}, t)$ is similar to finding $w_1(\mathbf{r}, t)$ and will not be performed separately. We only note that the results themselves can be obtained from (14), (17) by circular permutation of coordinates x_1, x_2, x_3.

Problem (8) will be solved by the reduction method, having presented $v(\mathbf{r}, t) = v_1(\mathbf{r}, t) + v_2(\mathbf{r}, t)$. The substitution of this expression into (8) leads to a homogeneous partial differential equation with inhomogeneous initial and homogeneous boundary conditions for function $v_1(\mathbf{r}, t)$:

$$\frac{\partial v_1}{\partial t} = a_1\frac{\partial^2 v_1}{\partial x_1^2} + a_2\frac{\partial^2 v_1}{\partial x_2^2} + a_3\frac{\partial^2 v_1}{\partial x_3^2},$$
$$\mathbf{r} \in V, \quad t > 0; \quad (18.1)$$

$$v_1(\mathbf{r}, t = 0) = T_0 - w(\mathbf{r}, t = 0), \quad \mathbf{r} \in V; \quad (18.2)$$

$$\lambda_n\frac{\partial v_1}{\partial n}\bigg|_S - \alpha v_1|_S = 0, \quad \mathbf{r} \in S, \quad t > 0, \quad (18.3)$$

and inhomogeneous partial differential equation with homogeneous initial and boundary conditions for function $v_2(\mathbf{r}, t)$:

$$\frac{\partial v_2}{\partial t} = a_1\frac{\partial^2 v_2}{\partial x_1^2} + a_2\frac{\partial^2 v_2}{\partial x_2^2} + a_3\frac{\partial^2 v_2}{\partial x_3^2}$$
$$+\frac{F(\mathbf{r}, t)}{c\rho} - \frac{\partial w}{\partial t}, \quad \mathbf{r} \in V, \quad t > 0; \quad (19.1)$$

$$v_2(\mathbf{r}, t = 0) = 0, \quad \mathbf{r} \in V; \quad (19.2)$$

$$\lambda_n\frac{\partial v_2}{\partial n}\bigg|_S - \alpha v_2|_S = 0, \quad \mathbf{r} \in S, \quad t > 0. \quad (19.3)$$

In order to solve (18) we use the method of separation of variables $v_1(\mathbf{r}, t) = R(\mathbf{r})Q(t)$:

$$\frac{1}{Q}\frac{\partial Q}{\partial t} = \frac{1}{R}\left[a_1\frac{\partial^2 R}{\partial x_1^2} + a_2\frac{\partial^2 R}{\partial x_2^2} + a_3\frac{\partial^2 R}{\partial x_3^2}\right] = -\lambda^2 \quad (20.1)$$

$$\Rightarrow \begin{cases} \frac{dQ}{dt} + \lambda^2 Q = 0 \\ a_1\frac{\partial^2 R}{\partial x_1^2} + a_2\frac{\partial^2 R}{\partial x_2^2} + a_3\frac{\partial^2 R}{\partial x_3^2} + \lambda^2 R = 0, \end{cases} \quad (20.2)$$

$$\lambda_n\frac{\partial R}{\partial n}\bigg|_S Q - \alpha R|_S Q = 0$$

$$\Rightarrow \lambda_n\frac{\partial R}{\partial n}\bigg|_S - \alpha R|_S = 0 \quad \text{at} \quad Q \neq 0. \quad (20.3)$$

Equation (20.2) with the homogeneous boundary condition of the third kind (20.3) is the problem on eigenvalues λ^2 and eigenfunctions $R(x_1, x_2, x_3)$, whose solving is performed by the method of separation of variables $R(x_1, x_2, x_3) = X(x_1)Y(x_2)Z(x_3)$

$$a_1 X'' + \beta_1^2 X = 0,$$
$$\lambda_1 X'|_{x_1=0} - \alpha X|_{x_1=0} = 0,$$
$$\lambda_1 X'|_{x_1=l_1} + \alpha X|_{x_1=l_1} = 0; \quad (21.1)$$
$$a_2 Y'' + \beta_2^2 Y = 0,$$
$$\lambda_2 Y'|_{x_2=0} - \alpha Y|_{x_2=0} = 0,$$
$$\lambda_2 Y'|_{x_2=l_2} + \alpha Y|_{x_2=l_2} = 0; \quad (21.2)$$
$$a_3 Z'' + \beta_3^2 Z = 0,$$
$$\lambda_3 Z'|_{x_3=0} - \alpha Z|_{x_3=0} = 0,$$
$$\lambda_3 Z'|_{x_3=l_3} + \alpha Z|_{x_3=l_3} = 0; \quad (21.3)$$
$$\beta_1^2 + \beta_2^2 + \beta_3^2 = \lambda^2. \quad (21.4)$$

The derived problems (21) are completely similar to problems (11) and their solution is determined by expression (13).

In turn, eigenfunctions of problem (20.2), which are determined by expression

$$R_{mnk}(x_1, x_2, x_3) = D_{mnk}$$
$$\times\left[\frac{\lambda_1}{\sqrt{a_1}}\frac{\beta_{1,m}}{\alpha}\cos\left(\frac{\beta_{1,m}}{\sqrt{a_1}}x_1\right) + \sin\left(\frac{\beta_{1,m}}{\sqrt{a_1}}x_1\right)\right]$$
$$\times\left[\frac{\lambda_2}{\sqrt{a_2}}\frac{\beta_{2,n}}{\alpha}\cos\left(\frac{\beta_{2,n}}{\sqrt{a_2}}x_2\right) + \sin\left(\frac{\beta_{2,n}}{\sqrt{a_2}}x_2\right)\right]$$
$$\times\left[\frac{\lambda_3}{\sqrt{a_3}}\frac{\beta_{3,k}}{\alpha}\cos\left(\frac{\beta_{3,k}}{\sqrt{a_3}}x_3\right) + \sin\left(\frac{\beta_{3,k}}{\sqrt{a_3}}x_3\right)\right], \quad (22)$$

are orthogonal in the parallelepiped $(0 < x_1 < l_1) \times (0 < x_2 < l_2) \times (0 < x_3 < l_3)$, and their squared norm is:

$$||P_{mnk}(x_1, x_2, x_3)||^2$$

$$= ||X_{1,m}(x_1)||^2 ||X_{2,n}(x_2)||^2 ||X_{3,k}(x_3)||^2.$$

The function $Q(t) = \exp\{-\lambda^2 t\}$ will be a solution to equation, and the series over all eigenfunctions

$$v_1(x_1, x_2, x_3, t)$$

$$= \sum_{m,n,k=1}^{\infty} C_{mnk} \exp\left\{-\left(\beta_{1,m}^2 + \beta_{2,n}^2 + \beta_{3,k}^2\right)t\right\}$$

$$\times R_{mnk}(x_1, x_2, x_3)$$

will be a solution $v_1(\mathbf{r}, t)$ of problem (18).

In this case, the coefficients should satisfy initial condition (18.3), whereas boundary condition (18.3) has already been used to determine eigenfunctions R_{mnk}, i.e., coefficients C_{mnk} will have the form:

$$C_{mnk} = \frac{1}{||R_{mnk}||^2} \int\!\!\!\int\!\!\!\int_0^{l_1,l_2,l_3} [T_0 - w(\xi_1, \xi_2, \xi_3)]$$

$$\times R_{mnk}(\xi_1, \xi_2, \xi_3) d\xi_1 d\xi_2 d\xi_3.$$

Inhomogeneous partial differential equation with homogeneous initial and boundary conditions (19) will be solved by expansion of the function $v_2(\mathbf{r}, t)$ in series over eigenfunctions $\check{R}_{mnk}(x_1, x_2, x_3)$, assuming that boundary condition (19.3), i.e., $\check{R}_{mnk}(x_1, x_2, x_3) \equiv R_{mnk}(x_1, x_2, x_3)$, where R_{mnk} is determined by (22), was used to determine the eigenfunctions. We also expand function $f(\mathbf{r}, t) = \frac{F(\mathbf{r},t)}{c\rho} - \frac{\partial w}{\partial t}$ in a similar series:

$$v_2(x_1, x_2, x_3, t)$$

$$= \sum_{m,n,k=1}^{\infty} v_{2,mnk}(t) R_{mnk}(x_1, x_2, x_3), \quad (23.1)$$

$$f(x_1, x_2, x_3, t)$$

$$= \sum_{m,n,k=1}^{\infty} f_{mnk}(t) R_{mnk}(x_1, x_2, x_3), \quad (23.2)$$

and $f_{mnk}(t)$ are Fourier coefficients in expansion $f(\mathbf{r}, t)$ over eigenfunctions:

$$f_{mnk}(t) = \frac{1}{||R_{mnk}||^2} \int\!\!\!\int\!\!\!\int_0^{l_1,l_2,l_3} f(\xi_1, \xi_2, \xi_3)$$

$$\times R_{mnk}(\xi_1, \xi_2, \xi_3) d\xi_1 d\xi_2 d\xi_3. \quad (24)$$

To determine $v_{2,mnk}(t)$, we substitute (23) into (19.1), (19.2) and taking

$$a_1 \frac{\partial^2 v_2}{\partial x^2} + a_2 \frac{\partial^2 v_2}{\partial y^2} + a_3 \frac{\partial^2 v_2}{\partial z^2}$$

$$= \sum_{m,n,k=1}^{\infty} v_{2,mnk}(t)[-(\beta_{1,m}^2 + \beta_{2,n}^2 + \beta_{3,k}^2)$$

$$\times R_{mnk}(x_1, x_2, x_3)]$$

into account, we transform (19.1), (19.2) to the form (dot denotes derivative over time):

$$\frac{\partial v_2}{\partial t} - \left[a_1 \frac{\partial^2 v_2}{\partial x^2} + a_2 \frac{\partial^2 v_2}{\partial y^2} + a_3 \frac{\partial^2 v_2}{\partial z^2} + f\right]$$

$$= \sum_{m,n,k=1}^{\infty} [\dot{v}_{2,mnk}(t) + (\beta_{1,m}^2 + \beta_{2,n}^2 + \beta_{3,k}^2)v_{2,mnk}(t)$$

$$- f_{mnk}(t)] R_{mnk}(x_1, x_2, x_3),$$

$$\sum_{m,n,k=1}^{\infty} v_{2,mnk}(t=0) R_{mnk}(x_1, x_2, x_3) = 0.$$

In view of the orthogonality of eigenfunctions R_{mnk}, we derived the Cauchy problem for an inhomogeneous differential equation of the first order with a homogeneous initial condition:

$$\dot{v}_{2,mnk}(t) + (\beta_{1,m}^2 + \beta_{2,n}^2 + \beta_{3,k}^2)v_{2,mnk}(t)$$

$$- f_{mnk}(t) = 0,$$

$$v_{2,mnk}(t=0) = 0.$$

The solution to this problem will be the function

$$v_{2,mnk}(t) = \int_0^t f_{mnk}(t)$$

$$\times \exp\{-(\beta_{1,m}^2 + \beta_{2,n}^2 + \beta_{3,k}^2)(t-\tau)\} d\tau, \quad (25)$$

and we obtain a final solution to problem (19), substituting (24) into (25), and (25) into (23.1):

$$v_2(x_1, x_2, x_3, t) = \sum_{m,n,k=1}^{\infty} \frac{1}{||R_{mnk}||^2}$$

$$\times \int_0^{l_1,l_2,l_3,t} \left[f(\xi_1, \xi_2, \xi_3, \tau) R_{mnk}(\xi_1, \xi_2, \xi_3) d\xi_1 d\xi_2 d\xi_3 \right.$$

$$\left. \times \exp\{-(\beta_{1,m}^2 + \beta_{2,n}^2 + \beta_{3,k}^2)(t-\tau)\} d\tau \right]$$

$$\times R_{mnk}(x_1, x_2, x_3).$$

CONCLUSIONS

It has been shown in this paper that synchrotron X-ray heating of crystals that have anisotropic thermal properties and experience heat exchange with the environment are described by a heat conductivity equation with sources and boundary conditions of the third kind. The analytical solution to this equation

was found based on the example of a crystal that has the shape of a rectangular parallelepiped.

In fact, these results are an analytical solution to the heat conductivity equation with a source and boundary conditions of the third kind in an orthotropic rectangular parallelepiped and have both fundamental importance and broad applications in heat conductivity problems of anisotropic media, such as the heat conductivity of space and aircraft construction materials.

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