TEMPERATURE DISTRIBUTION ON THE SURFACE OF A CRYSTAL INDUCED BY A LOCAL HEAT PULSE

G. A. Abduragimov, R. P. Meilanov,
and Ya. A. Ugai

UDC 536.2+548

We study the time evolution of the temperature field for small times in the presence of a local heat pulse on the surface of a solid.

In pulse laser processing of materials, heterogeneous chemical reactions, or oxidation of metals, a significant quantity of heat is released which can affect the kinetics of processes occurring at the surface or close to it. In particular, the formation of vacancies in a crystal lattice and the diffusion of impurities depend significantly on the change of temperature of the surface induced by the local heat pulse.

In the description of high intensity transport processes, where the potentials vary over a large range, it is necessary to determine accurately the time behavior of the temperature field during the initial instants of time. This can be done using models expressible as differential equations of the hyperbolic type [1-3].

We note that the local temperature field on the surface of a crystal subjected to an intense pulse source of heat and its effect on the formation of the liquid phase have been considered using the approximate (or even incorrect) equations of [4, 5], which were obtained in [5] from the solution of an equation of the parabolic type. This type of equation can only be used when the propagation velocity of heat is infinite.

The temperature field induced by a pulse source of heat on the surface of a crystal is described by the solution of the generalized heat equation. The finiteness of the propagation velocity of heat becomes significant if the time over which the temperature varies satisfies the inequality

$$\tau \lesssim \frac{L}{v}. \tag{1}$$

The temperature characterizes the equilibrium distribution of phonons, and this distribution is established after a time t_p. Therefore the characteristic time of variation of the temperature, using (1), must satisfy the condition

$$\tau_p \ll \tau \lesssim \frac{L}{v}. \tag{2}$$

In addition, the concept of a temperature changing in time makes sense if it changes sufficiently slowly: the equilibrium distribution of phonons is established over a length of order

$$l_p = v\tau_p. \tag{3}$$

Therefore the spatial scale of the variation in temperature must satisfy the condition

$$L \gg l_p. \tag{4}$$

Dagestan State Pedagogical Institute, Makhachkala. Translated from Inzhenerno-Fizicheskii Zhurnal, Vol. 50, No. 6, pp. 1013-1017, June, 1986. Original article submitted June 21, 1985.

0022-0841/86/5006-0730$12.50

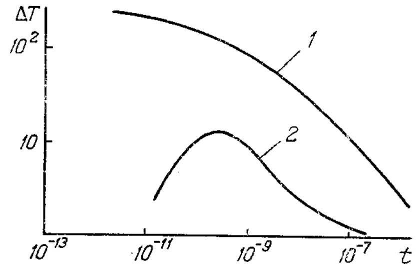

Fig. 1. Variation of local superheating temperature of germanium with time for different values of r: curve 1, $r = 10^{-6}$; curve 2, $r = 10^{-5}$ cm. T, °K; t, sec.

When the propagation velocity of heat is finite the heat equation has the form

$$\frac{\partial T(x, y, z, t)}{\partial t} + \frac{a}{v^2}\frac{\partial^2 T(x, y, z, t)}{\partial t^2} = a\nabla^2_{x,y,z} T(x, y, z, t). \tag{5}$$

Relations (2) and (4) define the ranges of characteristic times and distance scales where (5) is valid.

We consider a half-space $-\infty < x, y < \infty$, $z > 0$ with the boundary conditions

$$\begin{gathered} T(x, y, z, t)|_{t=0} = T_0;\ \lambda \frac{\partial T(x, y, z, t)}{\partial z}\bigg|_{z=0} = \\ = -q(x, y, t) - \tau_\text{p}\frac{\partial q(x, y, t)}{\partial t}; \\ \frac{\partial T(x, y, z, t)}{\partial t}\bigg|_{t=0} = 0;\ \frac{\partial T(x, y, z, t)}{\partial z}\bigg|_{z=\infty} = 0. \end{gathered} \tag{6}$$

Taking the Laplace transform with respect to t we have

$$\begin{gathered} T(x, y, z, s) = \frac{T_0}{s} + \frac{1}{\lambda}\int\limits_{-\infty}^{+\infty}\int\limits_{-\infty}^{+\infty} \frac{(1 + s\tau_\text{p})\, q(k_1, k_2, s) - \tau_\text{p} q(k_1, k_2, 0)}{\sqrt{k_1^2 + k_2^2 + \frac{s}{v^2}(s + \tau_\text{p}^{-1})}} \times \\ \times \exp\left[-z\sqrt{k_1^2 + k_2^2 + \frac{s}{v^2}(s + \tau_\text{p}^{-1})}\right] \exp\left[i(k_1 x + k_2 y)\right] dk_1 dk_2. \end{gathered} \tag{7}$$

We consider the case $q(x, y, s) = \delta(x)\delta(y)q(s)$. Then $q(k_1, k_2, s) = q(s)$ and the integral in (7) can be evaluated exactly. Using the relations:

$$\int\limits_0^\infty \cos(ax) \exp\left[-\beta\sqrt{\gamma^2 + x^2}\right] \frac{1}{\sqrt{\gamma^2 + x^2}}\, dk = K_0\left[\gamma\sqrt{a^2 + \beta^2}\right],$$

$$\int\limits_0^\infty \cos(\gamma x) K_0\left[\alpha\sqrt{\beta^2 + x^2}\right] dx = \frac{\pi}{\sqrt{\alpha^2 + \gamma^2}} \exp\left[-\beta\sqrt{\alpha^2 + \gamma^2}\right],$$

we obtain

$$T(x, y, z, t) = \frac{T_0}{s} + \frac{(1 + s\tau_\text{p})\, q(s) - \tau_\text{p} q_0}{\lambda} \times \frac{2\pi}{r} \exp\left[-\frac{r}{v}\sqrt{s(s + \tau_\text{p}^{-1})}\right], \tag{8}$$

where $r = \sqrt{x^2 + y^2 + z^2}$.

Inverting the Laplace transform, we obtain for T(x, y, z, t)

$$T(x,\ y,\ z,\ t) = T_0 + \frac{2\pi q}{\lambda r}\Theta\left(t - \frac{r}{v}\right)\left\{\left(5 + \frac{1}{1 - \left(\frac{r}{vt}\right)^2}\right) \times\right.$$

$$\times \exp\left(-\frac{t}{2\tau_p}\right) I_0\left(\frac{t}{2\tau_p}\sqrt{1 - \left(\frac{r}{vt}\right)^2}\right) - \exp\left(-\frac{t}{2\tau_p}\right)\frac{I_1\left(\frac{t}{2\tau_p}\sqrt{1 - \left(\frac{r}{vt}\right)^2}\right)}{\sqrt{1 - \left(\frac{r}{vt}\right)^2}} - \tag{9}$$

$$-\frac{1}{2\tau_p}\int\limits_{\frac{2}{v}}^{t}\left[\left(4 + \frac{2\tau p}{t - \tau}\right) I_0\left(\frac{t - \tau}{2\tau_p}\right) - \left(4 + \frac{2\tau p}{t - \tau} +\right.\right.$$

$$\left.\left.+\frac{8\tau_p^2}{(t - \tau)^2}\right) I_1\left(\frac{t - \tau}{2\tau_p}\right) \exp\left(-\frac{t}{2\tau_p}\right) I_0\left(\frac{t}{2\tau_p}\sqrt{1 - \left(\frac{r}{vt}\right)^2}\right)\right] d\tau\right\},$$

where I_0 and I_1 are the Bessel functions of imaginary argument, r is the radius of a hemisphere surrounding the local heat source, and $\Theta(t)$ is the Heaviside unit step function. Equation (9) is obtained for the case $q(t) = q\delta(t)$.

As an example we consider the iodide method of growing homoepitaxial films of germanium. (The thermal conductivity of germanium is due to three different processes: phonon, bipolar, and electron. At 600°K the bipolar and electron parts are 2% and 0.1% [6] of the total thermal conductivity. Hence for the conditions considered here the thermal conductivity of germanium is determined mainly by phonons and therefore the application of the heat equation is completely justified.)

As is well known, in the iodide method the crystal grows via the reaction

$$2GeJ_2 \rightleftarrows Ge + GeJ_4 \tag{10}$$

at the surface of the crystal. The heat of the reaction at constant pressure is, according to the data of [7],

$$\Delta H_T = 32500 - 8T \text{ (cal/mole)} \tag{11}$$

We assume that on a pure germanium surface a single interaction event according to the reaction (10) occurs at the initial time t = 0. A quantity of heat $q = 2.07 \cdot 10^{-19}$ J is released, which leads to a local increase in the temperature of the surface. (The calculation shows that τ_{reac} and τ_p are $2 \cdot 10^{-16}$ sec and $2 \cdot 10^{-12}$ sec, respectively, so that $\tau_{reac} \ll \tau_p$ and therefore we can apply (9) to this problem).

In the calculation of the temperature field induced by local heating of the germanium surface we used the following data at a temperature of 623°K, where crystallization of the homoepitaxial film is induced: $\rho = 5.324 \cdot 10^3$ kg/m^3 [8], $\lambda = 4.026 \cdot 10^1$ W/m•°K [9]. $v = 4.8 \cdot 10^3$ m/sec [9], $c = 3.645 \cdot 10^2$ J/kg•°K [10], $a = 2.074\ 10^{-5}$ m^2/sec. The speed of sound in germanium was determined from the formula $v \simeq (E/\rho)^{1/2}$ [11]. The Young's modulus E was calculated with the help of the relation [12] $E = (c_{11} - c_{12})(c_{11} + 2c_{12})/(c_{11} + c_{12})$. The values of c_{ij} were taken from [9].

Figure 1 shows the results for the case where all of the heat released on the surface of the crystal completely penetrates inward along the normal to the surface. In this case heat losses due to thermal exchange with the gas flux and due to radiation can be neglected in the first approximation because the thermal conductivity of a semiconductor is large compared to that of a gas and the radiation rate. The maximum deviation of the local temperature from 623°K was $5 \cdot 10^2$ and was observed when $\tau = 10^{-11}$-10^{-12} sec; $r = 10^{-6}$ cm. At a distance of $\sim 10^{-4}$ cm ($t \simeq 10^{-7}$ sec) the temperature reduces to its equilibrium value.

NOTATION

x, y, z, Cartesian coordinates; L, characteristic spatial scale of temperature variations; v, mean propagation velocity of thermal phonons; τ_p, l_p, relaxation time and mean free path of a thermal phonon; τ, characteristic time of temperature variations; a, thermal diffusivity; λ, thermal conductivity; q, heat flux power; T_0, initial temperature of the surface of the crystal; K_0, MacDonald function; T, absolute temperature; ΔH, reaction heat; ρ, density of the material; C, heat capacity; c_{ij}, elastic coefficients.

LITERATURE CITED

1. A. V. Lykov, Theory of Thermal Conduction [in Russian], Vysshaya Shkola, Moscow (1967).
2. A. A. Baranov and V. L. Kolpashchikov, Relativisitic Thermomechanics of Continuous Media [in Russian], Nauka i Tekhnika, Minsk (1979).
3. Ya. S. Podstrigach and Yu. M. Kolyano, Generalized Thermomechanics [in Russian], Naukova Dumka, Kiev (1976).
4. P. Baeri, S. U. Compisano, G. Foti, and E. Rimini, "Arsenic diffusion in silicon melted by high-power nanosecond laser pulsing," Appl. Phys. Lett., 33, No. 2, 137-139 (1978).
5. V. A. Arslambekov, "On the mechanism of formation of oxide films in metals," in: Interaction Mechanisms of Metals with Gases [in Russian], Nauka, Moscow (1964).
6. R. Berman, Thermal Conduction of Solids [Russian translation], Mir, Moscow (1979).
7. R. F. Rolsten, Iodide Metals and Iodides of Metals [Russian translation], Mir, Moscow (1968).
8. Handbook of Crystallochemical, Physicochemical, and Physical Properties of Semiconductors [in Russian], Standartov, Moscow (1973).
9. G. V. Somsonova (ed.), Properties of Elements (Handbook) [in Russian], Part 1, Metallurgiya, Moscow (1976).
10. V. P. Glushko (ed.), Thermodynamic Properties of Materials [in Russian], Vol. 2, Nauka, Moscow (1979).
11. K. P. Yakovleva (ed.), Short Physicotechnical Handbook [in Russian], Part 1, Fiz.-Mat. Lit., Moscow (1960).
12. Modern Crystallography [in Russian], Vol. 4, Nauka, Moscow (1981).

SOME PROPERTIES OF THE HEAT-TRANSFER PROCESS IN A MOTIONLESS MEDIUM, TAKING ACCOUNT OF HEAT-FLUX RELAXATION

E. I. Levanov and E. N. Sotskii

UDC 536.24.02

The solution of a hyperbolic system of heat-transfer equations in which account is taken of the temperature dependence of the thermal conductivity and relaxation time of the heat flux is investigated.

1°. A wide range of physical problems leads to the need for detailed study of heat transfer. The Fourier law is most often used to describe this process

$$\mathbf{W} = \mathbf{W}_F = -\varkappa \operatorname{grad} T. \tag{1}$$

However, the limits of applicability of the Fourier law are prescribed by the requirement of smallness of the free-path length and time of the particles in comparison with the characteristic space–time scales of temperature variation and are often overstepped in the case of intense heat transfer. Note also that the heat flux cannot exceed the maximum value determined by the conventional situation in which all the particles suddenly change their direction of motion and move in the same direction.

M. V. Keldysh Institute of Applied Mathematics, Academy of Sciences of the USSR, Moscow. Translated from Inzhenerno-Fizicheskii Zhurnal, Vol. 50, No. 6, pp. 1017-1024, June, 1986. Original article submitted February 1, 1985.