Transient heating of solids of finite size under bulk absorption of a light pulse

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The transient temperature associated with the bulk absorption of a rectangular laser pulse in a solid-state sample of finite size is calculated analytically and analyzed. Radiation is incident on the frontal surface with an arbitrary surface thermal conductivity. The opposite surface is thermostatically controlled and maintained at a constant equilibrium temperature. The general solution is obtained for pulses of arbitrary duration. The pulse duration is determined with respect to the relaxation time of the nonstationary thermal diffusion. This latter is the characteristic time of the problem.

Keywords: Transient temperature; Bulk absorption; Photothermal phenomena

1. Introduction

In order to determine the thermal diffusivity $\alpha$ and the thermal conductivity $\kappa$ of solids with the use of pulsed techniques [1-8], the sample is initially exposed to a laser pulse. Subsequent detection of the induced nonequilibrium temperature at the surface of the sample with the use of appropriate methods [9, 10] provides information on these parameters.

Theoretically, the key to solving this problem lies in the determination of the time- and coordinate-dependent temperature distributions of all the quasiparticles involved in the process of heat transfer (transient temperatures) [11-12]. In the majority of the works based on assumptions of the equality of the temperatures of all quasiparticles (the one-temperature model) [13], these distributions, as a rule, are determined using of formula given in [14], which, in many cases, leads to a reasonable agreement between theoretical and experimental data.

The basic problem of the above approach is that it is necessary to know the initial nonequilibrium temperature distribution in the sample. As a rule, this temperature distribution is postulated. In particular, Parker et al. [1] assumed that the radiation energy is instantly and uniformly absorbed at a small depth from the illuminated surface. Larson and Koyama [3] proposed an empirical formula with a fitting parameter. Tam and Sullivan [5] studied the bulk absorption of a light pulse and postulated the initial temperature distribution in semiconductors.

In our opinion, such method of finding of the temperature distributions in transient heat processes is not sufficiently acceptable for interpretation of experimental results obtained by means of modern techniques, and therefore more precise approach must be used. The main reason is that the transient temperature is formed under the influence of many factors, such as the amplitude and the duration of a laser pulse, the magnitudes of the coefficients of thermal conductivity and thermal diffusivity, the surface thermal parameters, the coefficients of light absorption and reflection. It is not possible to take logically and faithfully into account all these quantities within the limits of one empirical formula.

The most complex transient processes have been observed in semiconductors. In the general case, the process of heat transfer involves all quasiparticles, such as conduction electrons, holes, phonons, etc. The formation of temperature distributions of these quasiparticles depends on their thermal parameters, boundary conditions [15], magnitudes and mechanisms of energy exchange between these subsystems of quasiparticles [11,13], specific features of generation-recombination processes [16], and other factors. The numerical simulation performed for germanium by Andreas Othonos [10] revealed that, after irradiation with laser pulses (0.575 $\mu$m; power, 0.1 mJ/cm$^2$; duration, 4 ps), the temperatures of electrons and holes initially being in equilibrium at a temperature of 77 K increase to 5200 and 2400 K, respectively. However, the temperature of phonons increases to only 77.5 K. Hence, it is clear that any initial temperature, specified as a prior, cannot lead to results that will be adequate to the experimental situation, especially in the case where it is necessary to analyze the
experimental data and to interpret them from the standpoint of the observed physical processes.

In our earlier study [17], we attempted to obtain a rigorous analytical solution to the heat conduction equation in the case of excitation with rectangular laser pulses of arbitrary duration. The transient temperatures for short and long pulses were determined and analyzed in the framework of the simplest one-temperature model (under the assumption that the electron temperature is equal to the phonon temperature). Subsequently, the results of that work were generalized to the case of a two-temperature model (accounting electron-phonon interaction) in the nondegenerate semiconductors [11]. The non-zero approximation, which presumes the infinitely large phonon thermal conductivity with respect to the electron one, and the infinitely large electron thermal diffusivity with respect to the phonon one, has allowed to obtain the space-time dependencies of the electron temperature. The phonon temperature tends to the equilibrium one in this approximation. In [12] the transient temperatures of electrons and phonons were obtained in the limits of the rigorous two-temperature approximation, and there had been shown the complicated two-stage process of an electron temperature relaxation, and even the criteria of long and short pulses with respect to different subsystem quasiparticles was worked out. At this time, as well as in [17], the radiation absorption took place on the surface and the boundary conditions for electrons and phonons were assumed to be adiabatic. The two subsystems had isothermal contact with the environment at rear surface of the specimen.

The bulk absorption of the rectangular light pulse was considered in [18] for the first time.

This study is a continuation of our systematic investigations. In the present work, the transient temperature associated with the bulk absorption of a rectangular light pulse of arbitrary duration was derived and analyzed in terms of the linear theory and the one-temperature approximation. In this case, it was assumed that the heat exchange can occur between the illuminated surface and the environment. The thermal conditions for the opposite surface were identical to those used in [11,12,17].

2. Mathematical Model

Let us assume that a rectangular light pulse with an intensity \( I_0 \) and a duration \( \tau \) is incident on the left surface \( x=0 \) of a homogeneous isotropic heat-conducting sample (see Fig. 1). The sample has the shape of a parallelepiped with a unit cross-sectional area. The lateral surfaces are adiabatically isolated. The frontal surface \( x=0 \) is characterized by a surface thermal conductivity \( \eta \) [19]. The opposite face of the sample \( x=l \) is maintained at a constant temperature equal to the environmental temperature \( T_0 \). It is assumed that the light intensity is sufficiently low, so that the kinetic coefficients do not depend on the local temperature.

The problem is divided into two parts corresponding to two time intervals: \( 0 \leq t \leq \tau \) and \( t > \tau \), where \( t \) is the current time. The first interval will be referred to as the active interval, because light is absorbed within this interval. The second interval will be termed the relaxation interval, because the laser pulse ends at the instant of time \( t = \tau \) and the system begins to relax into a thermodynamic equilibrium state.

The correct thermodynamic condition of introducing of the local temperature for the pulse processes can be written by means of the criterion \( \tau_m << \tau_h << \tau_e << \tau \), where \( \tau_m \), \( \tau_h \), \( \tau_e \) are the momentum relaxation time, the collision
time between the particles, and the energy relaxation time respectively. This criterion is the logical generalization of [20]. In the one-temperature approximation, which we consider here, just the phonons are reasonably considered to be the quasiparticles which realize the process of the thermal transport. The energy relaxation time for the phonons is $\tau_e = \tau_{fe}$ [20], where $\tau_{fe}$ is the rate of phonon-electron collisions. This means that the energy transport in the specimen can be considered in the limits of the hydrodynamical approximation right up to femtosecond pulses.

We introduce the nonequilibrium temperature with the use of the relationship $T(x, t) = T_0 + T_a(x, t)$. Under the assumption that the light absorption proceeds according to the Lambert law, the heat conduction equation can be written in the form [21]:

$$\frac{1}{a} \frac{\partial T_a(x, t)}{\partial t} - \frac{\partial^2 T_a(x, t)}{\partial x^2} = \frac{\beta_0}{\kappa} e^{-\beta x}$$

(1)

where $T_a(x, t)$ is the nonequilibrium addition to the transient temperature on the active interval; $a = \frac{\kappa}{\rho c}$ is the thermal diffusivity; $\kappa$, $\rho$, and $c$ are the thermal conductivity, the density, and the specific heat capacity, respectively; and $\beta$ is the light absorption coefficient.

The initial and boundary conditions for Eq. (1) have the following form:

$$T_a(x, t)|_{t=0} = 0$$

(2a)

$$T_a(x, t)|_{x=0} = 0$$

(2b)

$$\left( \kappa \frac{\partial T_a(x, t)}{\partial x} - \eta T_a(x, t) \right)|_{x=0} = 0$$

(2c)

The boundary condition (2c) determines the heat exchange between the frontal surface and the environment through the heat transfer. The heat exchange due to thermal radiation is ignored in our calculation.

On the relaxation interval $t \geq \tau$, heat sources are absent and the heat conduction equation takes the form

$$\frac{1}{a} \frac{\partial T_a(x, t)}{\partial t} - \frac{\partial^2 T_a(x, t)}{\partial x^2} = 0$$

(3)

where $T(x, t) = T_0 + T_a(x, t)$, $T_a(x, t)$ is the nonequilibrium addition to the nonequilibrium temperature on the relaxation interval.

The boundary conditions for this equation remain identical to those for the active interval, i.e., they are represented by equalities (2b) and (2c) with replacement of indices “$a$” by “$r$”. The initial condition is given by the equality

$$T_a(x, t+0) = T_r(x, t-0)$$

(4)

Equality (4) means that the temperature on the active interval at the instant of time $t = \tau$ is the initial temperature on the relaxation interval.

3. Analytical Solution

3.1. The Active Interval $0 \leq t \leq \tau$

The general solution of Eq. (1) can be represented as the sum of two functions,

$$T_a(x, t) = T_{a1}(x) + T_{a2}(x, t)$$

(5)

One function, $T_{a1}(x)$, does not depend on the time and is the solution of the stationary heat conduction equation

$$\frac{d^2 T_{a1}(x)}{dx^2} + \frac{\beta_0}{\kappa} e^{-\beta x} = 0$$

(6)

with the boundary conditions (2b) and (2c).

The solution to Eq. (6) is trivial and has the form

$$T_{a1}(x) = \frac{I_0}{\kappa \beta} \left( 1 + \frac{\xi}{\eta} e^{-\beta x} - e^{-\beta x} \right)$$

(7)

where $\xi = \frac{\kappa}{\eta}$ is the parameter determining the thermal properties of the frontal surface [19]. The conditions $\xi \to \infty$ and $\xi \to 0$ correspond to an ideal adiabatic isolation and an ideal isothermal contact, respectively.

It is easy to see that the temperature $T_{a2}(x, t)$ satisfies Eq. (3) with the replacement $T_a(x, t) \to T_{a1}(x, t)$ and the initial condition

$$T_{a2}(x, t)|_{t=0} = -T_{a1}(x)$$

(8)

where $T_{a1}(x)$ is defined by relationship (7).

The boundary conditions are given by expressions (2b) and (2c) with the replacement $T_a(x, t) \to T_{a2}(x, t)$.

By representing the function $T_{a2}(x, t)$ as the product

$$T_{a2}(x, t) = X(x) Y(t)$$

of two unknown functions of the variables $x$ and $t$ and using the conventional method by separating the variables, we obtain

$$X(x) = a_1 \cos \left( \frac{\mu x}{T} \right) + a_2 \sin \left( \frac{\mu x}{T} \right)$$

(9a)

$$Y(t) = e^{-\frac{\beta t}{T}}$$

(9b)
where $a_1$ and $a_2$ are unknown constants, which can be found from the boundary conditions (2b) and (2c). The solvability condition for the system of equations with respect to the unknowns $a_1$ and $a_2$ leads to the transcendental equation for determining the spectrum of eigenvalues $\mu$; that is,

$$
\text{tg } \mu = -\xi \mu 
$$

(10)

Equation (10) is invariant with respect to the replacement $\mu \to -\mu$. Therefore, it will be sufficient to consider only positive values of $\mu$.

After the appropriate manipulations, we have

$$
T_{x_2}(x,t) = \sum_{n=1}^{\infty} a_n \left( \sin \left( \frac{\mu_n x}{T} \right) + \xi \mu_n \cos \left( \frac{\mu_n x}{T} \right) \right) e^{-\mu_n^2 \tau} 
$$

(11)

Here, $a_n$ are unknown coefficients, $\mu_n$ is the eigenvalue of the parameter $\mu$ with the number $n$, and $\tau = \frac{t}{\alpha}$, the time of nonstationary thermal diffusion (the characteristic time of the problem) [12].

In order to determine the coefficients $a_n$, we substitute relationship (11) into the boundary condition (8) and use the orthogonality condition

$$
\int_0^1 \Phi_n(x) \Phi_k(x) \, dx = \delta_{nk} \left\| \Phi_n \right\| 
$$

(12)

Where

$$
\Phi_n(x) = \sin \left( \frac{\mu_n x}{T} \right) + \xi \mu_n \cos \left( \frac{\mu_n x}{T} \right), \delta_{nk} = \begin{cases} 1, & n = k, \\ 0, & n \neq k; \end{cases}
$$

$$
\left\| \Phi_n \right\| = \frac{1}{2} \left( 1 + \xi + \xi^2 \mu_n^2 \right).
$$

As a result, the transient temperature on the active interval takes the following form:

$$
\tau_{x_2}(x,t) = \frac{4}{\pi^2} \int_0^\infty \frac{1 + \beta e^{-\beta} - e^{-\beta} + \xi e^{-\beta} - e^{-\beta} \xi}{1 + \xi + \xi^2 \mu_n^2} \sum_{n=1}^{\infty} a_n \left( \sin \left( \frac{\mu_n x}{T} \right) + \xi \mu_n \cos \left( \frac{\mu_n x}{T} \right) \right) e^{-\mu_n^2 \tau} 
$$

(13)

where

$$
a_n = \frac{-2 \mu_n \beta c}{\kappa} \frac{1 + \beta \mu_n^2 + \mu_n^2 + \beta \mu_n^2}{1 + \xi + \xi^2 \mu_n^2} \left( 1 + \xi + \xi^2 \mu_n^2 \right) 
$$

(14)

3.2. The Relaxation Interval $t \geq \tau$

Equation (3) on the relaxation's time interval is solved by the same method. The general solution is represented in the form of expression (5) with the same boundary conditions (2b) and (2c). The initial condition has the form

$$
T(x,t) \big|_{t=0} = T_{a_1}(x) + T_{a_2}(x,t = \tau) 
$$

(15)

By omitting the intermediate manipulations similar to those performed for the active interval, the final relationship for the temperature at $t \geq \tau$ can be written as follows:

$$
T(x,t) = \sum_{n=1}^{\infty} a_n \left( \sin \left( \frac{\mu_n x}{T} \right) + \xi \mu_n \cos \left( \frac{\mu_n x}{T} \right) \right) e^{-\mu_n^2 \tau} 
$$

(16)

where the quantities $a_n$ are defined by expressions (14).

From Eq. (16) we see that just the term of the Fourier series with the smallest time exponent, $\mu_n \tau$, defines the characteristic relaxation time of the temperature till its equilibrium. That is, the characteristic relaxation time of the temperature,

$$
\tau_r = -\frac{\tau_0}{\mu_{\text{min}}},
$$

(17)

where the figure, $-\frac{\tau_0}{\mu_{\text{min}}} < \tau_r < \frac{4 \tau_0}{\pi^2}$. The exact value of $\mu_{\text{min}}$ depends on the magnitude of the parameter $\xi$ which defines the relation between properties of bulk heat conduction and surface heat conduction. Hence, the characteristic relaxation time of the temperature, $\tau_r$, is as follows,

$$
\frac{\tau_0}{\pi^2} \leq \tau_r < \frac{4 \tau_0}{\pi^2}
$$

Relationships (13) and (16) completely describe the transient temperature caused by the excitation of the sample with the laser pulse. The behavior of temperature relaxation is governed by the surface thermal conductivity (entering into the parameter $\xi$) and the ratio between the pulse duration $\tau$ and the time of nonstationary thermal diffusion $\tau_0$. Since the time of nonstationary thermal diffusion, $\tau_0$, depends on the thermal diffusivity, the analysis of the relaxation portion of the temperature distribution enables one to determine this important parameter.

From (13) and (16) follows that the transient temperature is generally presented as the Fourier series which contains both sines and cosines. Let us note that the eigenvalues $\mu_n$ depend on the condition of the heat contact which is defined by the parameter $\xi$ (see (11)). Equation (10) reduces to the equation $\sin \mu = 0$ in the limiting case of isothermal contact ($\xi \to 0$), whereas expressions (13) and (16) will represent the Fourier sine-series. In the case of adiabatic contact ($\xi \to \infty$) Eq. (10) reduces to the equation $\cos \mu = 0$ whereas the series (13) and (16) will contain only sines. The reason of this is the fact that the boundary conditions of the first gender must be utilized in the role of boundary conditions at isothermal conditions, i.e., just nonequilibrium function must be equal to zero. At adiabatic contact, we handle the boundary conditions of the second
gender, i.e., the derivative of the temperature must be equal to zero.

4. Conclusions

The evolution in time of the temperature distribution is obtained in a solid in one-dimensional case under bulk absorption of the light pulse of the rectangular form of an arbitrary duration. It is established that the temperature distribution depends on the characteristic time of the thermal diffusion, \( \tau_0 = \frac{l^2}{\alpha} \), where \( l \) is the specimen length, and \( \alpha \) is the thermal diffusivity of the sample. Moreover, the temperature distribution depends on the bulk thermal conductivity, the surface thermal conductivity of the front surface, and the light absorption coefficient. It is established that the characteristic relaxation time of the temperature is of order of the characteristic time of the thermodiffusion, \( \tau_c \sim \tau_0 \) (see expression (17)). That is why, the value of the temperature decreases according to the exponential law, \( \exp(-t/\tau_0) \) in the period of the temperature decrease. Hence, if in the experiment we measure the time period, \( \tau_{1/2} \), during of which the temperature of the front surface decreases twice then we can obtain the characteristic time \( \tau_0 \), because \( \tau_0 \sim \tau_{1/2} \ln 2 \). Since \( \tau_c = \frac{l^2}{\alpha} \) then, knowing the specimen length, \( l \) (the thermal diffusivity, \( \alpha \)), we can find the thermal diffusivity, \( \alpha \) (the specimen length, \( l \)).

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