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Photothermal analysis of heterogeneous semiconductor structures under a pulse laser irradiation

Roman Burbelo[1], Mykola Isaiev[2], Andrey Kuzmich[3]
Taras Shevchenko Kyiv National University, Physics Department,
64, Volodymyrska, 01601 Kyiv, Ukraine;
E-mail: rmb@univ.kiev.ua[1]; isaev@univ.kiev.ua[2]; kuzmich@univ.kiev.ua[2]

Abstract. The analysis of photothermal conversion in materials with modified properties of surface layer was made in this work. Influence of both physical and geometrical nonlinearities on the process of heat distribution was estimated.

Keywords: heterogeneous semiconductor structures, laser irradiation, photothermal effect.

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1. Introduction

Local heating by a laser beam is widely applied to materials processing. Use of modulated or pulse laser radiation is fundamental in researches of photoacoustic (PA) and photothermal (PT) phenomena. At the same time, the physical nature of energy conversion process, due to complexity of the phenomenon, is not clear. To do the full description it is necessary to consider that this effect bases on distribution of, at least, three types of fields (light, thermal, elastic) and energy conversion between them, often with attraction of an electronic subsystem of investigated materials. It is clear that there are serious problems in its description even for homogeneous continuous media. But these problems become even more complicated during the development of model of energy conversion process in inhomogeneous media.

In the present work peculiarities of process of photothermal conversion (PTC) are examined under a pulse laser irradiation of semiconductor materials with the modified properties of a surface layer (so-called layered structures), physical properties of which much differ from the properties of volume of a material.

It is necessary to note that when using pulse sources for excitation, the questions related with nonlinearity of the process of heat distribution are of special importance. This nonlinearity can have both physical and geometrical nature. The physical component connected with temperature dependence on thermal parameters, geometrical is related to structural heterogeneity of a material by values of thermal parameters. During the period of action of a light pulse (~10^{-8} s) the system has no time to renew a condition of thermodynamic balance, that is, there are processes that lead to growth of temperature in surface layer area of material [1, 2]. Thus, the processes of not integral but sharpen character start to dominate.

In this work, the case of temperature and spatial nonlinearity of thermal diffusivity of a material is examined. The equation of heat diffusivity can be written as follows:

$$c\rho\frac{\partial T}{\partial t}=\frac{\partial}{\partial z}\left(K(T,z)\frac{\partial T}{\partial z}\right)+I(1-R)\cdot\alpha\cdot g(t)\cdot e^{-\alpha z},$$

or

$$\frac{\partial T}{\partial t}=\frac{\partial}{\partial z}\left(D(T,z)\frac{\partial T}{\partial z}\right)+\frac{I(1-R)\cdot\alpha}{c\rho}\cdot g(t)\cdot e^{-\alpha z}. \qquad (1)$$

Where $D = K/c\rho$ is the coefficient of thermal diffusivity; function $g(t)$ describes the temporal distribution of the incident light intensity. In the case of single pulse, the result is:

$g(t)=H(t)+H(\tau-t)-1$, where $H(t)=\begin{cases}0, & t<0\\ 1, & t\geq 0\end{cases}$ is Heaviside function.

The task can be divided by two parts:

1. $D(T, z) = D(z)$ – the sample is structurally heterogeneous;

2. $D(T, z) = D(T)$ – the sample is structurally homogeneous, and coefficient of thermal diffusivity depends on temperature.

Case 1.

In the first case, the structure of the sample with separate layers is modeled, within the limits of each of them ($l_{i-1} < z < l_i$) the coefficient of thermal diffusivity is constant. To find temperature profiles, the method of finite elements is used. Having presented time and spatial coordinates in the form of $z = ih$, $t = j\tau$ and having used the implicit scheme, the following definition was obtained:

$T(z,t) \to T_{ij}$, $D(z) \to D_i$, $f(z,t) \to f_{ij}$,

$$\frac{\partial T}{\partial t} \to \frac{T_{ij} - T_{i-1j}}{\tau}, \quad \frac{\partial T}{\partial z} \to \frac{T_{i+1j} - T_{ij}}{h},$$

$$\frac{\partial D}{\partial z} \to \frac{D_{i+1} - D_i}{h}, \quad \frac{\partial^2 T}{\partial z^2} \to \frac{T_{i+1j} - 2T_{ij} - T_{i-1j}}{h^2}.$$

Then the equation (1) becomes:

$$D_{i+1j}T_{i+1j} - \left(D_{ij} + D_{i+1j} + \frac{h^2}{\tau}\right)T_{ij} + D_{ij}T_{i-1j} = \\ = -\frac{h^2}{\tau}T_{ij-1} - f_{ij}h^2 . \qquad (2)$$

The given system of equations, together with the boundary conditions, can be written as follows

$$c\rho D \left.\frac{\partial T}{\partial z}\right|_{z=0-0} = 0 \Rightarrow c\rho D_{0j}\frac{T_{1j} - T_{0j}}{h} = \\ = 0 \Rightarrow T_{1j} - T_{0j} = 0,$$

$$T\big|_{z=z_{\max}} = 0 \Rightarrow T_{i_{\max}j} = 0,$$

and it determines temperature profiles.

For definiteness, the case when the thickness of a layer l lies within the limits of 0.1 to 1 μm, the thickness of the sample $z_{\max} = 300$ μm is considered. The value of thermal diffusivity for the top layer is $D_1 = 0.09$ cm^2/s and for crystal-substrate material is $D_2 = 0.94$ cm^2/s. The values correspond to a real situation, for example, when surface of the monocrystalline Si plate is processed (i.e., is under modification).

In Fig. 1, simulations that correspond to the considered situation are presented. Bold lines illustrate spatial distributions for a homogeneous sample with D_1 and D_2:

– change of the thermal diffusivity value for material by one order (the case when the material thermal parameters of a surface layer are changed as a result of technological processing D_2–D_1) results in significant increase of temperature (approximately three-fold) and decrease of the heat localization area within the near surface layer of material;

– results of calculations show that the smaller is the thickness of the modified layer (practically the thickness changes may occur within the range from one to ten micrometers down to fractions of micrometer), the quicker is the process of temperature decrease when approaching to that of the homogeneous sample. In this case, the solution is identical to the solution for the single-layered sample with the value D characteristic for material crystal-substrate. On the other hand, when increasing the thickness of the modified layer the curve that corresponds to temperature distribution approaches to a curve for the monolayer sample with the coefficient of thermal diffusivity close to that in the top layer of the structure.

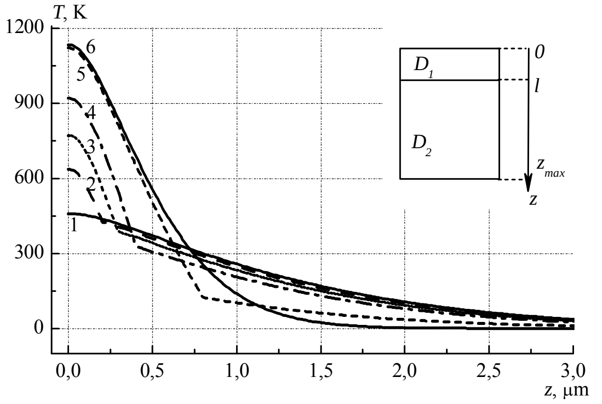

Fig. 1. Temperature depth profiles in samples as a result of laser irradiation ($\tau = 20$ ns) for homogeneous samples: curves *1* – $D = 0.94$ cm^2/s, *6* – $D = 0.09$ cm^2/s; for a double-layer structure with the different thickness of the modified layer: curves *2* – $l = 0.2$ μm, *3* – 0.3, *4* – 0.4, *5* – 0.8 ($D_1 = 0.09$ cm^2/s, $D_2 = 0.94$ cm^2/s).

Case 2.

It is necessary to note that the detailed description of dynamics for the heat distribution process can be made only by means of numerical methods. Thus, the urgency of search and development of methods for the analysis of the nonlinear problem is obvious.

So in [1], at the analysis of the nonlinear equation for thermal conductivity, in case of representation $K(T,z) = K(T) \sim T^{\sigma}$, the partial solution has been obtained. This solution testifies that the front of a thermal wave is motionless, and half-width of the heated area is constant. Taking into account the fact that the coefficient of thermal conductivity depends on temperature localization of heat in the media, the so-called effect of heat inertia takes place.

In the work [2], the approximate “method of parametrized perturbation technique in Green’s function formulation” is examined to describe the nonlinear dynamic heat process in silicon irradiated by a pulsed laser beam. The analysis of solutions obtained using this method at different parameters of laser irradiation shows that with account of nonlinearity $D(T)$ the process of lattice temperature growth occurs, and spatial temperature distributions change in comparison with those in linear case.

In this work, the case of approximation of thermal diffusivity coefficient in the form of $D(T,z) = D(T) = \frac{D_0}{1 + a \cdot T}$ is examined. This representation corresponds to real experimental data for Si [3].

Since the system (2) in this case becomes nonlinear, the iterative method of Newton-Raphson is used in order to find solutions [4]. To do this, in zero approach the calculated temperature diffusivity coefficient is taken from the previous time interval, that is $D_{ij}^{0} = D(T_{ij-1})$, then (2) will have the following form:

$$-T_{0j}^{(0)} + T_{1j}^{(0)} = 0$$

::

$$D_{i+1j}^{(0)} T_{i+1j}^{(0)} - \left(D_{ij}^{(0)} + D_{i+1j}^{(0)} + \frac{h^2}{\tau} \right) T_{ij}^{(0)} + D_{ij}^{(0)} T_{i-1j}^{(0)} =$$

$$= -\frac{h^2}{\tau} T_{ij-1} - f_{ij} h^2$$

::

$$T_{i_{\max} j}^{(0)} = 0$$

Having solved this system of equations, a set $T_{ij}^{(0)}$ has been obtained, whence it is possible to find $D_{ij}^{(1)} = D\left(T_{ij}^{(0)}\right)$ and again substitute it in (2). Hence, on a step k a set of values $D_{ij}^{(k)} = D\left(T_{ij}^{(k-1)}\right)$ was obtained. Then:

$$-T_{0j}^{(k)} + T_{1j}^{(k)} = 0$$

::

$$D_{i+1j}^{(k)} T_{i+1j}^{(k)} - \left(D_{ij}^{(k)} + D_{i+1j}^{(k)} + \frac{h^2}{\tau} \right) T_{ij}^{(k)} + D_{ij}^{(k)} T_{i-1j}^{(k)} =$$

$$= -\frac{h^2}{\tau} T_{ij-1} - f_{ij} h^2$$

::

$$T_{i_{\max} j}^{(k)} = 0$$

So $T_{ij}^{(k)}$ is found.

This procedure is being continued till $\left| T_{ij}^{(k+1)} - T_{ij}^{(k)} \right| < \varepsilon$, where ε is the accuracy set in advance. If this condition is fulfilled, $T_{ij} = T_{ij}^{(k+1)}$. In Fig. 2, the results of numerical calculation in case of dependence of temperature diffusivity coefficient on temperature are presented.

This graphic shows that the presence of physical and geometrical nonlinearity leads to localization of heat in surface layer area of a material. It must be taken into account when investigating PA and PT phenomena.

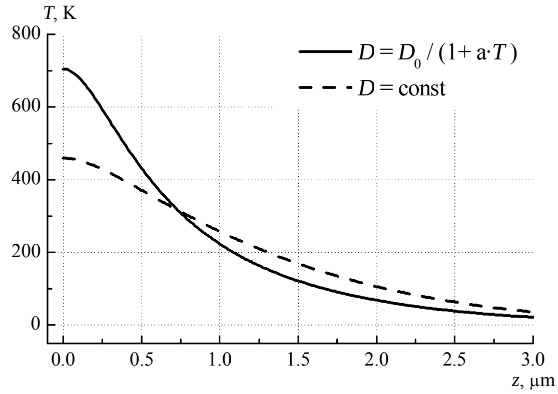

Fig. 2. Temperature depth profile in homogeneous samples for the case of thermal diffusivity dependence on temperature (solid curve) and for the case D = const (dash curve).

Finally, it is necessary to note that for the full description of a nonlinear problem of thermal conductivity it is necessary to consider the role of electron-hole plasma generated by light as well as the dependence of optical absorption from T. Such analysis will be done in future.

References

1. A.A. Samarsky, N.V. Zmytrenko, S.P. Kurdyumov, A.P. Mykhaylov, Thermal structures and fundamental length in an environment with nonlinear heat conductivity and by volume sources of heat // *Dokl. Akademii Nauk SSSR* **227**, No. 2, p. 321 (1976) (in Russian).
2. Dae M. Kim, D.L. Kwong, Rajiv R. Stah et al., Laser heating of semiconductors – effect of carrier diffusion in nonlinear dynamic heat transport process// *J. Appl. Phys.* **52**, No. 8, (1981).
3. A.S. Okhotina (Ed.), *Thermal Conduction of Solids*. Energoatomizdat Publ., Moscow, 1984 (in Russian).
4. E.A. Volkov, *Numerical Methods*. Fizmatlit Publ., Moscow, 2003 (in Russian).