EVOLUTION OF TEMPERATURE DISTRIBUTION IN IMPLANTED Si-BASED STRUCTURES: PULSE MODE OF LASER IRRADIATION

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We present the results explaining the general tendency in peculiarities of the process of heat distribution in semiconductor structures with modified properties of the surface layer under a pulse laser irradiation. It is shown that the presence of a structural inhomogeneity (modified layer) and the influence of a nonlinear dependence of the thermal diffusivity coefficient result in both a substantial transformation of the area of localization (its decrease) of thermal energy and an increase of the surface temperature.

1. Introduction

Photoacoustic (PA) diagnostics has lately been a rapidly developing field of investigation of material properties. This method is grounded on the photothermal transformation (PTT) under no stationary heating of the medium by electromagnetic radiation (e.g., by laser radiation).

The recent growth of the interest in the PA diagnostics is mainly related to the development of new PA methods and a successful application in materials science and particularly in micro- and optoelectronics [1]. It should be mentioned that the number of realized applications of the PA effect is relatively large, while the physical nature of the phenomenon is not well understood because of its complexity. It is mainly due to the fact that the overall description of the effect involves a propagation of fields of at least three types (light, thermal, and elastic ones), the energy exchange between them, and even the consideration of the electron-hole subsystem in semiconductor materials. It is clear that there are significant unanswered questions in the description of the effect even for homogeneous continuous media. While developing a model of the PA effect for inhomogeneous media (e.g., layered structures), this problem becomes even more complicated. There are a lot of similar unresolved problems ranging from the description of a light absorption mechanism in inhomogeneous media to the influence of interfaces on the propagation of thermal waves induced by nonstationary light absorption, and so on.

Today, the problem of calculating the time evolution of a spatial distribution of temperature fields in a material is very actual for various areas of materials science (for example, for the determination of thermal parameters; the calculation of a PA signal, which allows one to find elastic constants of a material; the laser processing, *etc.*).

In [2], the analytical solution of the heat equation was analyzed, by taking the outflow of heat from the surface into account. The results testify that the temperature curve maximum moves in the depth of a sample. In that work, only structural homogeneous materials were analyzed; the results obtained are not suitable for calculating the thermal fields in inhomogeneous structures. This problem was partially solved in [3], where the thermal structure of a specimen was modeled with separate layers, so that the coefficient of thermal diffusivity was constant within the limits of each layer. In other words, a homogeneous heat equation can be written for each layer. By applying the Laplace transformation and introducing the resistivity matrix that describes the boundary thermal resistance between adjacent layers, the transfer matrices were deduced. Thus, the description of the diffusion of heat in inhomogeneous structures was given, by introducing the *effective thermal conductivity* (generalized to the entire structure). But the nonlinear processes of heat diffusion cannot be considered within such a method.

The purpose of the given work is to analyze the formation of temperature profiles, as a result of the action of short laser impulses ($\sim 10^{-8}$ s) on semiconductor silicon-based structures (Si is one of the basic materials of modern microelectronics), in which the near-surface layer properties have been essentially modified according to technological requirements. These changes (e.g., see [2], where the influence of the implantation of monocrystalline silicon on the coefficient of thermal diffusivity of a material with modified structure was investigated) can be as large as several orders of magnitude for the quantities that define thermal properties of materials. Since the action of high-energy laser radiation on media represents a great interest, we will also analyze the nonlinear dependence of the coefficient of thermal diffusivity on the temperature.

2. Mathematical Model

Let us consider the following nonlinear equation of thermodiffusion dependent on time:

$$\frac{\partial T}{\partial t} = \frac{\partial}{\partial z}\left(D(T,z)\frac{\partial T}{\partial z}\right) + f(z)g(t), \tag{1}$$

where D is the coefficient of thermal diffusivity which depends in the general case on a spatial coordinate (in inhomogeneous samples) and on the temperature; $f(z)$ is the function which characterizes a spatial distribution of heat sources in the sample. In a case which is considered with regard for the Bouguer–Lambert law (the heat source is a laser radiation absorbed by a material), we have

$$f(z) = \frac{I(1-R)\alpha\exp(-\alpha z)}{c\rho}.$$

The function $g(t)$ describes the temporal distribution of the incident light intensity. In the case of a single impulse, $g(t) = H(t) - H(t-\tau)$, where $H(t)$ is the Heaviside function.

In all calculations, we will take $I = 10$ MW/cm^2, $\tau = 20$ ns, $R = 0.37$, $\alpha = 5\times10^4$ cm^{-1}, $c = 0.8$ J/(g·K), $\rho = 2.3$ g/cm^3 as constant and will trace a change of the coefficient of thermal diffusivity only.

The following boundary conditions are more often realized in practice:
– $(\partial T/\partial z)|_{z=0} = 0$ – absence of heat outflow from the sample's surface in an external environment;
– $T|_{z=z_{\max}} = 0$ – contact of the sample's bottom surface with the thermostat ($z_{\max} = 300$ μm – thickness of a sample);
The initial conditions are as follows:
– $T|_{t=0}$ – the uniform distribution of the temperature in the sample before the irradiation (we will accept that the initial temperature is zero without any loss of generality: we will consider only a rising over the initial temperature).

According to our purpose, we will consider the cases of irradiation of a homogeneous sample and a sample with modified properties of a subsurface layer (two-layer structure) by short laser impulses. For definiteness, we will consider monocrystalline silicon (p-type, $D_0 = 0.94$ cm^2/s, $N_p \sim 10^{12}$ cm^{-3}) and two-layer structure "implanted layer + crystal substrate Si" – Si_{p+p^+} ($N_p \sim 10^{20}$ cm^{-3}, $D_{p^+} = 0.25$ cm^2/s). We set the modified layer thickness $d_{p^+} = 0.6$ μm and assume that, in the case of strong light absorption ($\alpha^{-1} = 0.2$ μm), practically all radiation is absorbed in the first layer. In the first and second cases, we will estimate also a role of the temperature dependence of the coefficient of thermal diffusivity ($D(T)$).

3. Thermal Diffusivity does not Depend on Temperature

3.1. *Homogeneous sample (D = const)*

Let us analyze the temperature distribution at the irradiation of a structurally homogeneous sample. We will consider that the coefficient of thermal diffusivity does not depend on the temperature (D = const). In this case, a solution of Eq. (1) can be obtained analytically in the form

$$T_1(z,t) = \begin{cases} \sum\limits_{n=0}^{\infty} f_n(t)\cos(a_n z), & t \le \tau, \\ \sum\limits_{n=0}^{\infty} f_n(\tau)\frac{\exp(-a_n Dt)}{\exp(-a_n D\tau)}\cos(a_n z), & t \ge \tau, \end{cases}$$

$$f_n(t) = A_n(1-\exp(-a_n^2 Dt)),$$

$$A_n = \frac{2}{z_{\max}}\frac{I(1-R)\alpha}{c\rho D a_n^3}\frac{(-1)^n\exp(-\alpha z_{\max}) + \alpha/a_n}{1+(\alpha/a_n)^2},$$

$$a_n = \left(\frac{\pi}{2}+\pi n\right)\frac{1}{z_{\max}}.$$

In Fig. 1, we present the calculated temperature profiles at the irradiation of a Si sample by a laser impulse with the duration $\tau = 20$ ns at various moments of the temporal cycle "heating — the heating end — cooling". Such temporal intervals are chosen to show the general tendency of process of distribution of heat to show that such a tendency holds during the whole cycle with heating and cooling.

3.2. *Structurally inhomogeneous sample (D = D(z))*

We now analyze the temperature distribution at the irradiation of an ion-implanted monocrystalline Si sample (two-layer structure Si_{p+p^+}, the thickness $d_{p^+} = 0.6$ μm). We will model the given structure by a system

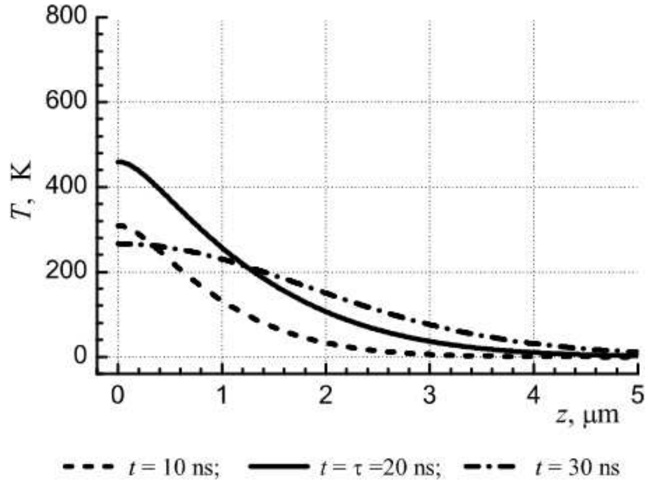

Fig. 1. Temperature distributions for a homogeneous sample at various moments of the temporal cycle

which consists of two layers. It is possible to write the coefficient of thermal diffusivity as

$$D(z) = \begin{cases} D_1 = D_{p^+}, & z < d_{p^+}, \\ D_2 = D_0, & z \geq d_{p^+}, \end{cases} \tag{2}$$

where D_1 and D_2 are the coefficients of thermal diffusivity of the top and bottom (crystal substrate Si) layers, respectively. In Fig. 2, we present the relevant temperature profiles calculated by the finite-element method. As seen from Fig. 2,*a*, it is possible to describe the temperature profiles in the sample by the function $T_2(z,t) = F(z,t,D_1,D_2,d_{p^+})$. The given function at a point $z = d_{p^+}$ has the simple discontinuity of the first derivative. It is a result of the "sharp border" model 2 and physically arises from the continuity of a heat flux through the boundary between the first and second layers $(D_1(\partial T/\partial z)|_{z=p^+ +0} = D_2(\partial T/\partial z)|_{z=p^+ -0})$. Under the condition $D_1 = D_2$, the shape of the given curve passes in that of a curve which corresponds to a homogeneous sample (Section 3.1). The presence of such a break has unforeseen consequences in the case where one needs to conduct the subsequent calculations (e.g., the use of the Laplace transformation in calculations of a PA signal leads to the appearance of "boundary frequencies"). This break can be removed, if we replace the "sharp border" model by the "transient layer" model, in which the coefficient of thermal diffusivity changes not by jump, but, for example, according to a linear law $D(z) = a + bz$ (see Fig. 2,*b*, insertion). Here, a and b are constants which can be found from the condition of

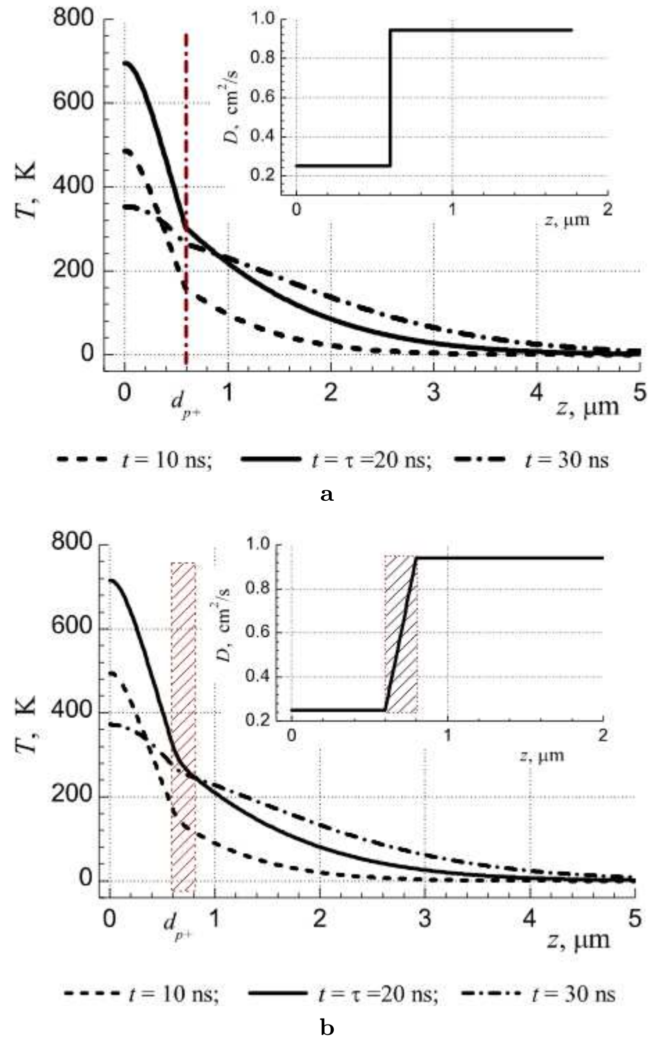

Fig. 2. Temperature distributions for a two-layer structure Si_{p+p^+} at various moments of the temporal cycle; the insert shows a model dependence $D(z)$ (*a*). Temperature distributions for a two-layer structure Si_{p+p^+} in the "transient layer" model at various moments of the temporal cycle; the insert insert shows a model dependence $D(z)$ (*b*)

continuity of the function $D(z)$:

$$D|_{z=p^+ +0} = D_{p^+},$$
$$D|_{z=p^+ +l-0} = D_0,$$

where l is the transient layer thickness. In Fig. 2,*b*, we give the temperature distributions for the "transient layer" model. Evidently, the break is removed in this case.

On the whole, by comparing the results of Sections 3.1 and 3.2, it is clear that the presence of a modified

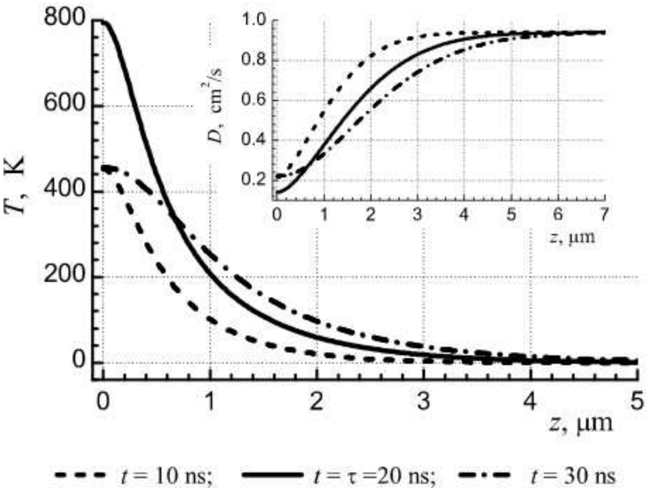

Fig. 3. Temperature distributions in homogeneous Si for $D(T)$ (physical nonlinearity); the insert shows the model dependence $D(T(z,t))$ at various moments of the temporal cycle

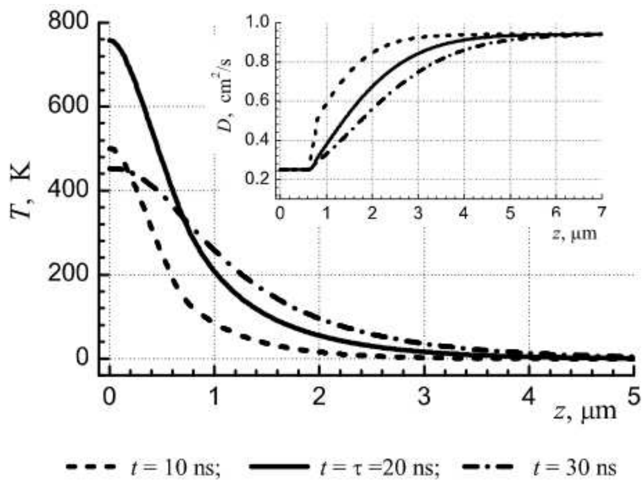

Fig. 4. Temperature distributions for a two-layer structure Si_{p+p^+}; the insert shows the dependence $D(z,T(z,t))$ at various moments of the temporal cycle

layer (structural heterogeneity) leads to a reduction of the area of thermal energy localization.

4. Thermal Diffusivity Depends on Temperature

4.1. Homogeneous sample ($D = D(T)$)

In this case, the situation becomes essentially more complicated, as the coefficient of thermal diffusivity becomes temperature-dependent. To find the temperature profiles, we use a modified finite-element method as in [7].

With regard for the fact that the thermal conductivity in hyperpure silicon has the phonon character and using experimental data [5], we get the explicit dependence of the coefficient of thermal diffusivity on the temperature: $D(T) = D_0/(1 + aT)$.

In Fig. 3, we give the results of calculations of the temperature profiles in a homogeneous sample in the case where the coefficient of thermal diffusivity depends on the temperature.

Comparing results of Sections 3.1 and 4.1, it is clear that the presence of the physical nonlinearity (dependence D on T) also leads to a reduction of the localization area of thermal energy.

4.2. Structurally inhomogeneous sample ($D((T, z))$

Let us consider a two-layer structure Si_{p+p^+} (the thickness $d_{p^+} = 0.6$ μm). We consider that the top (modified) layer has a constant coefficient of thermal diffusivity, because the scattering of phonons by crystal defects (in the presence of impurities in the concentration indicated in Section 2) prevails over the phonon-phonon scattering. For the bottom layer (substrate Si), we take the coefficient of thermal diffusivity in the form $D(T) = D_0/(1 + aT)$.

The scheme for calculations of temperature profiles does not differ essentially at this point from that used in Section 4.1. We note that, in this case (as in Section 3.2), the temperature profile curve has a discontinuity of the first derivative, resulting from a difference in values of the coefficients of thermal diffusivity of the first and second layers. But it is smoothed out as a result of the descending dependence of the coefficient of thermal diffusivity on the temperature. In some cases (e.g., at $t \ll \tau$ and $t \gg \tau$), this break can become substantial. That is why, for its diminution, we will use the "transient layer" model with a linear law $D(T, z) = a(T) + b(T)z$, as it was made in Section 3.2. Here, $a(T)$ and $b(T)$ are functions of the temperature, which can be found from the conditions of continuity of the function $D(z)$:

$$D|_{z=p^++0} = D_{p^+},$$
$$D|_{z=p^++l-0} = D(T).$$

In Fig. 4, we present the temperature distributions within the "transient layer" model.

Comparing the results given in Section 4, we will pay attention to the presence of layers in a sample (structural heterogeneity $D = D(z)$) in the case where the coefficient of thermal diffusivity depends on a temperature (physical non-linearity $D = D(T)$) and does not lead to substantial differences in the curves of temperature distributions as distinct from the results in Section 3, where the dependence $D = D(z)$ leads to a reduction of the localization area of thermal energy.

We note that, in all cases, the amount of the absorbed energy of a laser impulse is the same. Therefore, by the law of energy conservation, a reduction of the area of heat localization in the process of energy conversion "light-heat" and the further diffusion of heat in a material lead to an increase of the temperature in the surface layer of the sample.

5. Conclusions

Here, we have considered the process of formation of temperature profiles in spatially inhomogeneous silicon-based structures at their irradiation by a short ($\tau = 20$ ns) laser impulse. A modified finite-element method was applied to the analysis of solutions of the nonlinear equation of thermodiffusion. This has given an opportunity to find an approximate solution for systems that have a layered structure with arbitrary ratios between the thermal parameters of layers and values of their thicknesses.

We have demonstrated the difference of the processes of formation of temperature distributions in cases where the coefficients of thermal diffusivity depend or do not depend on the temperature in homogeneous and inhomogeneous doped Si-based structures.

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ФОРМУВАННЯ ТЕМПЕРАТУРНИХ ПОЛІВ В ЛЕГОВАНИХ СТРУКТУРАХ НА ОСНОВІ Si ПРИ ЛАЗЕРНОМУ ОПРОМІНЕННІ: ІМПУЛЬСНИЙ РЕЖИМ

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Р е з ю м е

У роботі представлено результати аналізу, які пояснюють загальну тенденцію в особливостях процесу поширення тепла в напівпровідникових структурах на основі Si з модифікованими властивостями приповерхневого шару при опроміненні їх коротким лазерним імпульсом. Показано, що наявність структурної неоднорідності (модифікованого шару) та врахування впливу нелінійної залежності коефіцієнта температуропровідності приводить до суттєвої трансформації області (її зменшення), локалізації теплової енергії та збільшення температури в приповерхневому шарі матеріалу.