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PHOTOTHERMAL TRANSFORMATION IN HETEROGENEOUS SEMICONDUCTORS STRUCTURES UNDER ITS PULSE LASER IRRADIATION: ROLE OF ELECTRON-HOLE DIFFUSION

TRANSFORMACJA FOTOTERMICZNA W HETEROGENICZNYCH STRUKTURACH PÓŁPRZEWODNIKOWYCH PRZY IMPULSOWYM POBUDZENIU LASEROWYM: ROLA DYFUZJI ELEKTRON-DZIURA

In this paper photothermal transformation in semiconductor structures with modified properties of subsurface layer under its irradiation by pulse laser (~10 ns) radiation was analyzed. It was show that the presence of this surface modified layer leads to increasing of surface temperature in comparison with homogeneous case. Moreover, this increasing could even compensate the temperature decreasing induced by thermal source redistribution caused by charge carrier diffusion.

Keywords: Photothermal transformation, heterogeneous structures, electron-hole diffusion, pulse laser irradiation

W pracy zaprezentowano wyniki badań konwersji fototermicznej w półprzewodnikowych strukturach ze zmodyfikowanymi własnościami warstwy wierzchniej, pod wpływem impulsów laserowych o długości 10 ns. Obecność takiej zmodyfikowanej warstwy prowadzi do zwiększenia powierzchniowej temperatury w porównaniu do temperatury jednorodnej struktury. W pracy pokazano, że wzrost temperatury może kompensować spadek temperatury indukowanej przez przepływ związany dyfuzją nośników ładunku.

1. Introduction

Investigation of interaction between laser irradiation with solid state is still important from applied point of view. Such powerful pulse laser irradiation is often used for rapid annealing [1], particularly in the processes of nanostructured materials fabrication [2]. Moreover, laser-based ultrasound techniques [3-6] are successfully applied for materials with different structures and dimensional investigation [7]. All these practical applications are often based on photothermal phenomena – conversion of absorbed optical energy into heat.

The overall description of such transformation "electromagnetic radiation – thermal energy" is challenging task, especially in inhomogeneous semiconductor structures, i.e. in this case the electron-hole plasma could lead to significant spatial redistribution of heat source [8, 9]. Based on perturbation approach [10], analytical solution that describe temperature field formation in homogeneous silicon under its irradiation by pulse laser irradiation was found. The results of modeling show that photoexcited charge carrier diffusion could lead to additional outflow of thermal source from irradiated surface of the sample and, as the result, for decreasing of surface temperature. From the other hand the results of numerical simulation [11] of temperature field formation in Si-based structure show that the presence of surface modified layer could lead to substantial transformation of thermal energy area localization (its decreasing) and to surface temperature increasing. Influence of photoexcited carrier diffusion was not considered there, therefore, role of diffusion on photothermal transformation in inhomogeneous semiconductors structure is not clear enough.

In this paper formation of temperature spatial distribution in Si-based structures with modified properties of subsurface layer (thickness of modification ~1 μm) under its irradiation by pulse laser irradiation was analyzed. The finite element method (FEM) was used for solution of coupled photoexcited carrier and thermal diffusivity equations.

2. Simulation of photothermal transformation

For definiteness sake in this paper was considered following Si-based structures: n and n^+ – type with major carrier density 10^{15} cm^{-3} and 10^{19} cm^{-3} respectively; n-n^+ layered structures with the same density as for n and n^+ (without comma). Under this doping level optical energy bandgap does not change greatly [12] and it is $E_g = 1.1$ eV. Hereinafter the case when this structures are illuminated by pulse (pulse duration $\tau = 20$ ns) laser irradiation with intensity $I_0 = 1$ MW/cm^2 and photons energy $E_{ph} = 2.3$ eV respectively will be considered. In this case (when $E_{ph}>E_g$) the main mechanism of photon energy absorption is presented by electron-hole pair creation, its next relaxation (Fig. 1) can be considered in two stages [13]:

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(i) fast (with characteristic time $\tau_{th} \sim 10^{-15} \div 10^{-12}$ s) charge carrier thermalization;
(ii) recombination (with characteristic time $\tau_r \sim 10^{-9} \div 10^{-3}$ s) of electron-hole pair.

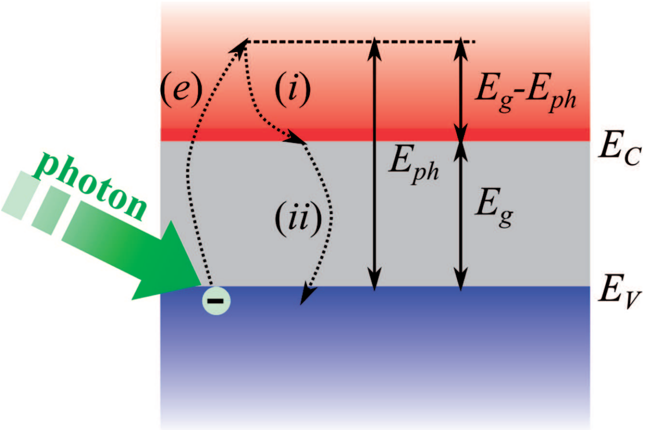

Fig. 1. Schematic sketch of considered approximation for electron excitation (*e*) by photon with energy $E_{ph}>E_g$ and its two stage relaxation: (i) fast thermalization; (ii) recombination of electron-hole pair

Under (i) processes the part of photon energy (E_{ph}-E_g) transferred to lattice thermal energy. This processes are important under ultrafast (pico-, femtoseconds) processes analysis[14], but in considered case the assumption that they are instantaneous could be made. Under (ii) processes the rest part of photon energy (E_g) transferred to the lattice thermal energy. These processes are slower compared to (i) and it could lead throw the charge carrier diffusion to significant thermal source spatial redistribution. This redistribution strongly depends on electronic transport properties of investigated structures [15].

3. Charge carrier and thermal diffusivity equations

For simulation of photothermal transformation the cylindrical system coordinates as shown at the Fig. 2 was chosen. The case of the excitation radiation intensity by Gaussian law in cross-section distributed was considered. When the irradiation incident normally to the samples surface the charge carrier diffusion equation can be presented in the following form:

$$\frac{\partial \delta n}{\partial t} = \vec{\nabla}\left(D\vec{\nabla}\delta n\right) - \frac{\delta n}{\tau_r} + \frac{2\pi P_0 (1-R)}{E_{ph} b^2}\alpha \exp\left(-\int\limits_0^z \alpha dz\right) \exp\left(-\frac{2r^2}{b^2}\right) g(t), \qquad (1)$$

here P_0 – power of incident radiation, α – optical absorption coefficient, R – reflective coefficient, b – radius of the beam cross-section, $g(t)$ – function that describe temporal intensity distribution,D – coefficient of non-equilibrium charge carrier diffusion, δn – density of photoexcited charge carrier distribution. Let us note that symbol n traditionally denote to the electron density, in the case of hole distribution the symbol p often used, but hole diffusion equation has the same kind with difference only in diffusion coefficient and life-time, so it was skipped and it will be explained in details below.

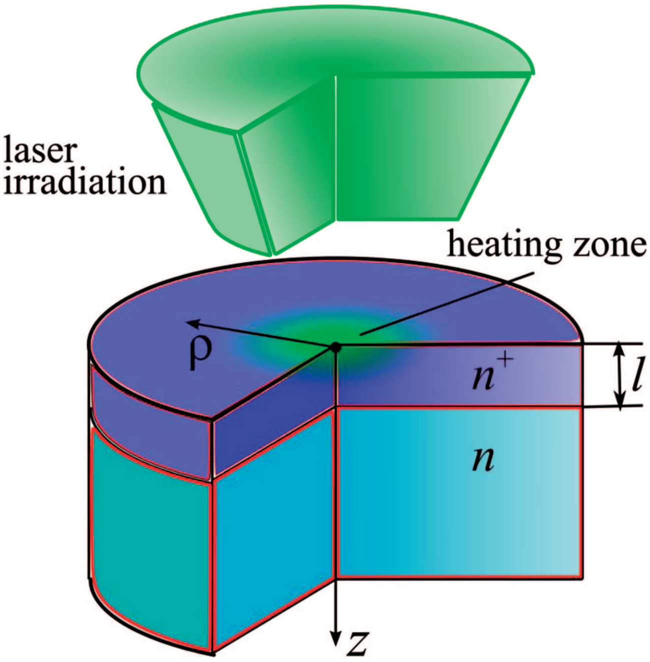

Fig. 2. Schematic sketch of studied structures geometry: surface of heterogeneous Si-based structure (n-n^+) is illuminated by pulse laser irradiation

The absence of non-equilibrium charge carriers before beginning of laser pulse action ($\delta n(\boldsymbol{r},0) = 0$) was chosen as initial condition for Eq. (1). In this paper also influence of surface recombination on photothermal transformation was considered, thus boundary conditions for (1)

$$\begin{cases} D\left.\dfrac{\partial \delta n}{\partial z}\right|_{z=0} = s\delta n \\ \delta n|_{z\to\infty} = 0 \end{cases},$$

here s – surface recombination velocity.

The corresponding heat diffusivity equations for temperature (T) is

$$c\rho\frac{\partial T}{\partial t} = \vec{\nabla}\left(K\vec{\nabla}T\right) + E_g\frac{\delta n}{\tau_r} + \frac{2\pi P_0 (1-R)}{b^2}\frac{E_{ph}-E_g}{E_{ph}}\alpha \exp\left(-\int\limits_0^z \alpha dz\right) \exp\left(-\frac{2r^2}{b^2}\right) g(t), \qquad (2)$$

here c and ρ – specific heat capacity and density of investigation structure, K its thermal conductivity. The third term of this equation right hand side corresponds to (i) processes and the second to the (ii) processes. The equilibrium with external environment ($T(\boldsymbol{r},\ 0) = T_{ext} = 300$ K) before beginning of heating was chosen as initial condition for Eq. (2). The boundary conditions for this equation

$$\begin{cases} K\left.\dfrac{\partial T}{\partial z}\right|_{z=0} = -sE_g\delta n \\ T|_{z\to\infty} = T_{ext} \end{cases}.$$

It should be mentioned that the second term in right hand side of Eq. (2) and these boundary conditions couple charge diffusivity and photothermal processes.

4. Results of simulation and discussions

In Fig. 3 the spatial distribution of non-equilibrium charge carrier density (a) and thermal profile (b) for the homogeneous n-Si for different surface recombination velocities (s =0, 10, 10^6 cm/s) at the end of pulse laser action in the epicenter of laser heating are presented. This data was obtained by solving of Eq. (1) and Eq. (2) by FEM. The processes of charge carrier generation and its further diffusion were considered in approximation of bipolar generation ($\delta n = \delta p$). The respective thermal and electron-hole transport parameters were taken from [16]. Fig. 3a shows that for different values of surface recombination velocities the charge carrier density profile changes significantly. Nevertheless, as one can see from the Fig. 3b, the temperature distribution does not depend noticeably on this parameter. So below only the case of s =0 was considered.

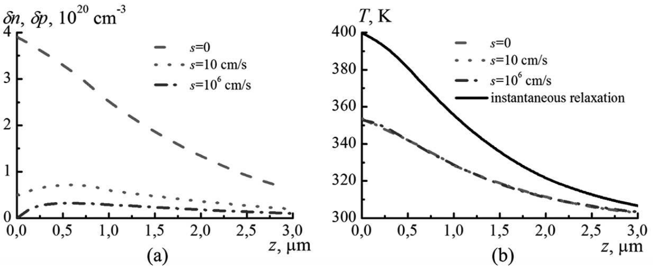

Fig. 3. Spatial distributions of electron-hole plasma density (a) and temperature (b) in homogeneous n-Si at the end of laser pulse action ($t = \tau$ =20 ns) for different values of charge carriers surface recombination velocity

Let us notice that in this case temperature rise ($\Delta T = T - T_{ext}$) in $(E_{ph}-E_g)/E_{ph}$ times less than for the case of instantaneous charge carrier relaxation [11] (solid black line at the Fig. 3b). This is due to the fact that charge carrier life-time is much bigger than pulse duration and electron-hole pairs do not have time to recombine.

At Fig. 4 the results of numerical simulation of temperature profile in the epicenter of laser heating for n-n^+ structure are presented (the thickness of modified layer l =1 μm). The life-time and diffusion length for n^+-layer were taken from [17], thermal parameters from [18] respectively. In this case the tendency that was mention above also observed – the absolute value of temperature rise in $(E_{ph}-E_g)/E_{ph}$ times less than for the case of instantaneous charge carrier relaxation (red dash line at the Fig. 4).

As one can see from the Fig. 4 the presence of surface modified layer leads to increasing of surface temperature ($T(0,t)$) in comparison with homogeneous case (n-Si). Moreover, this increasing could even compensate the temperature decreasing caused by electro-hole diffusion. For demonstration of this at the Fig. 4 the temperature profile for the case of instantaneous charge carrier relaxation approximation for n-Si also presented.

Let us notice that under higher power densities of laser irradiation the temperature dependence of thermal and electro-hole parameters on temperature as well as on charge carrier concentration have been accounted.

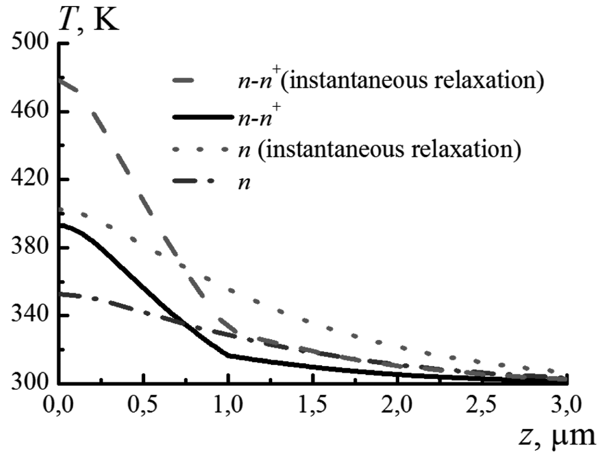

Fig. 4. Temperature profiles in Si-based structures under its irradiation by pulse laser irradiation ($t = \tau$ =20 ns): solid black and red dash lines for n-n^+ structures for the case of influence charge carriers diffusion and instantaneous electron-hole relaxation respectively; blue dash-dot and green dot lines for homogeneous n-Si for the case of influence charge carriers diffusion and instantaneous electron-hole relaxation respectively

5. Conclusions

In this paper the results of photothermal transformation investigation in heterogeneous semiconductors structures under its pulse laser irradiation are presented. The finite elements method was used for solution of coupled photoexcited carrier and thermal diffusivity equations. The results of simulation show that the presence of surface modified layer leads to surface temperature increasing to counterbalance of electron-hole diffusion action.

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