Quantum Electronics **41** (7) 626 – 630 (2011)

PACS numbers: 78.40.Fy; 72.80.Cw; 42.55.Rz
DOI: 10.1070/QE2011v041n07ABEH014515

Propagation of Nd-laser pulses through crystalline silicon wafers

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Abstract. **Propagation of pulses from an Nd:YAG laser (wavelength, 1.064 μm; pulse duration, 270 ns; pulse energy, 225 μJ) through crystalline silicon wafers is studied experimentally. Mathematical modelling of the process is performed: the heat conduction equation is solved numerically, the temperature dependences of the absorption and refraction of a substance, as well as generation of nonequilibrium carriers by radiation are taken into account. The constructed model satisfactorily explains the experimentally observed intensity oscillations of transmitted radiation.**

Keywords: *repetitively pulsed radiation, interaction of radiation with matter, semiconductors, nonequilibrium carriers, mathematical model.*

1. Introduction

Absorption of laser radiation propagating through a semiconductor is caused by different mechanisms. In the case of visible and near-IR radiation, absorption can be high due to generation of nonequilibrium carriers during the transfer of electrons from the valence band into the conduction band. In addition, the material is heated, thereby leading to a change in the equilibrium carrier concentration, corresponding to the current value of the temperature, and, consequently, to a change in the optical characteristics of the material. The change in the optical thickness of a material can, in particular, result in interference oscillations of the intensity of transmitted and reflected radiation.

Propagation of radiation through semiconductor wafers under different conditions has been investigated repeatedly. In some studies it was proposed to use interference oscillations of transmitted or reflected light for measuring low absorption coefficients and for controlling the thickness of thin films [1, 2]. In several papers reflection from a two-layer system was used, in particular, to study the epitaxial growth of a semiconductor layer on a substrate [3].

Of great interest are the studies of the combined effect of two radiations at different wavelengths. Short-wavelength radiation is selected so that it would be strongly absorbed by the semiconductor and change the concentration of free carriers. Long-wavelength radiation is weakly absorbed, and as a result, there appears some sort of interaction of radiations caused by changes in the properties of the medium [4].

The authors of paper [5] considered the combined problem: a thin (0.2 – 0.4 μm) film of amorphous silicon deposited on the surface of a dielectric (fused silica) is heated by radiation from a 0.248-μm KrF laser; its heating is measured with radiation from a 0.752-μm diode laser as a change in the refractive index and absorption.

However, propagation of near-IR radiation through $\sim$ 100-μm-thick wafers in the intensity range of $\sim 10^7$ W cm^{-2} is insufficiently studied. Interest in this area is due to the fact that such semiconductor materials as silicon and germanium are widely used in laser physics and technology, and for them the photon energy of, in particular, a 1.064-μm Nd:YAG laser turns to be of the order of the band gap. Therefore, absorption due to interband transitions is quite noticeable, but not prevalent. This fact is taken into account in paper [6] studying the effect of picosecond pulses (of duration $\sim$ 30 ps) from a garnet laser (photon energy $h\nu = 1.17$ eV) on 5 – 10-μm-thick $CdS_{1-z}Se_x$ semiconductor layers.

However, the results of all research executed so far cannot be directly transferred to the region of radiation and target parameters. In this regard, in this paper we investigated experimentally propagation of pulses from an Nd:YAG laser ($\lambda = 1.064$ μm; $\tau = 270$ ns; pulse energy, $E = 225$ μJ) through 350-μm-thick crystalline silicon wafers. We studied the time dependence of the radiation intensity $I_t(t)$ propagating through the wafer. In the experiments we observed the interference oscillations of $I_t(t)$.

To explain the characteristics of the oscillations observed in experiments, we constructed a mathematical model that includes the heat conduction equation and takes into account the fact that radiation is absorbed by the material, thereby changing its optical characteristics, i.e., the refractive index and absorption. This change may result from both direct heating, accompanied by an increase in the concentration of equilibrium carriers, and from photogeneration of nonequilibrium carriers. Changes in the optical properties of the material lead to a change in the optical thickness of the wafer and, consequently, to the interference oscillations of the intensity of the transmitted radiation. The constructed model was studied numerically and allowed one to calculate the time dependence of the intensity of the transmitted radiation. The obtained results agree with experimental data.

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Received 6 December 2010; revision received 23 February 2011
Kvantovaya Elektronika **41** (7) 626 – 630 (2011)
Translated by I.A. Ulitkin

2. Experiment

In the experiments we used a setup shown schematically in Fig. 1. The radiation source was a repetitively pulsed Nd : YAG laser. The pulse duration was 270 ns, the pulse energy and repetition rate were 225 μJ and 4 kHz, respectively. The target was a 350-μm-thick plane-parallel single crystal silicon wafer with polished optical quality sides.

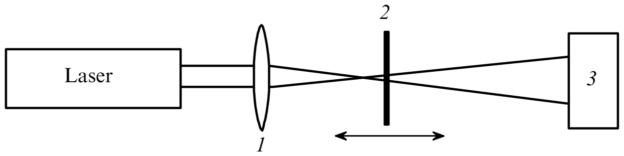

Figure 1. Scheme of the experimental setup: (*1*) focusing lens; (*2*) silicon wafer; (*3*) detector of transmitted radiation.

Laser radiation was focused onto a silicon wafer through a lens (the lens focus is in front of the wafer). To change the energy density at the surface, the target was moved along the laser radiation propagation direction with the help of micrometre adjustment screws. Silicon FD-24 photodiodes were used as detectors of transmitted and reflected radiation. We used an avalanche LFD-2A photodiode to study the structure of the transmitted laser pulse and a digital Tektronix TDS2022B oscilloscope to record the oscillograms. The error in measuring the intensity was approximately 1 %.

Figure 2 shows the measured time dependence of the intensity of radiation incident on the silicon wafer. The beam diameter was 500 μm. The typical time dependence of the intensity of radiation transmitted though the silicon wafer is presented in Fig. 3. In this case, transmitted light intensity oscillations with a period of ~ 0.04 μs are observed.

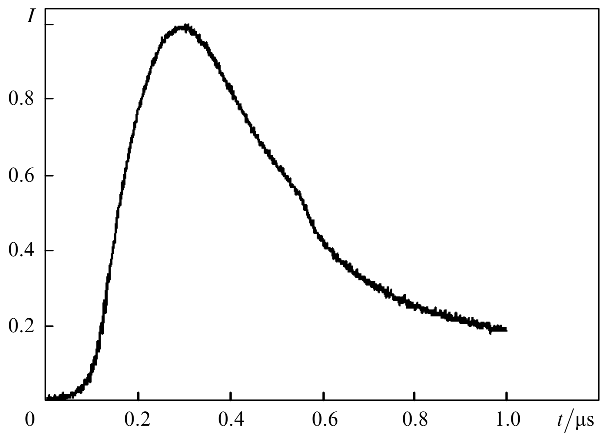

Figure 2. Normalised time dependence of the intensity of radiation incident on the wafer.

3. Mathematical model

The appearance of oscillations in the time dependence of the intensity of radiation transmitted through the semiconductor wafer is the result of a change in optical thickness of the target due to the absorption of light.

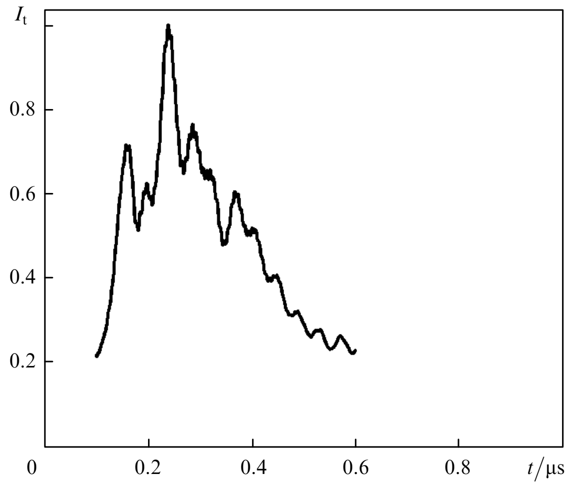

Figure 3. Normalised time dependence of the intensity of radiation transmitted through the wafer.

There are several mechanisms of absorption. One of them is due to the thermal generation of equilibrium carriers. We estimate the temperature changes necessary for the emergence of at least one oscillation. The condition for the oscillation appearance is the fulfilment of relation $(4\pi/\lambda)\Delta nL \sim 2\pi$, where L is the thickness of the wafer; λ is the wavelength; Δn is the change in the refractive index caused by a change in the temperature. Consequently, $\Delta n \sim \lambda/2L$. The corresponding change in the temperature ΔT is $\sim \Delta n(\partial n/\partial T)^{-1}$. For the experimental parameters $\lambda = 1.064$ μm, $L = 350$ μm, $\partial n/\partial T \sim 0.0025$ K^{-1}, we obtain $\Delta T \sim$ 10 K. Thus, heating the wafer for a few dozens of degrees can lead to intensity oscillations of the transmitted wave.

To understand the real contribution of this mechanism to the overall picture, we estimate the temperature change produced by radiation in our experiments. Assuming that radiation penetrates into the wafer to a depth of $l \sim \alpha^{-1}$, where α is the absorption coefficient, and neglecting the thermal conductivity (due to the short duration of the pulse), we obtain $c\rho\alpha^{-1}\Delta T = I\tau$. Assuming that the density $\rho = 2.3$ g cm^{-3}, the specific heat $c = 0.7$ J g^{-1} K^{-1}, $\alpha \approx$ 50 cm^{-1}, $I \sim 10^6$ W cm^{-2} and $\tau \sim 300$ ns, we find $\Delta T = I\tau\alpha/(c\rho) \sim 10$ K. This means that as a result no more than two oscillations can emerge.

Thus, the emergence of many intensity oscillations of the transmitted radiation, observed in our experiments, cannot be explained by the thermal generation of carriers only.

Another mechanism for changing the optical thickness of the wafer consists in generation of nonequilibrium carriers due to interband transition of electrons under irradiation. Indeed, because at room temperature the band gap of silicon is $\Delta = 1.12$ eV and the photon energy is $h\nu = 1.16$ eV $> \Delta$, this mechanism can play a significant role at a sufficiently high radiation intensity.

Among other mechanisms of radiation absorption in semiconductors, we can specify a lattice and impurity absorption [7]. Evaluation of the contribution of these mechanisms has shown that their role is negligible in our experiment.

Finally, the oscillations could be due to the presence of an oxide film on the surface. However, in the present paper this fact can be ignored because the thickness of natural oxide layer on the surface of the samples did not exceed 0.1 μm and was much smaller than the wavelength of the radiation used.

In accordance with the above, the mathematical model includes the heat conduction equation with a volume source

$$\rho(T)c(T)\frac{\partial T}{\partial t}=\frac{\partial}{\partial x}\left(\chi(T)\frac{\partial T}{\partial x}\right)-\frac{\partial I}{\partial x},$$
$$\frac{\partial I}{\partial x}=-\alpha(T,\ N)I,\quad 0<x<L, \tag{1}$$

and with appropriate initial and boundary conditions that take into account the convective and radiative losses:

$$T(x,\ t)=T_0, \tag{2}$$

$$-\chi(T)\frac{\partial T}{\partial x}=-\eta(T-T_0),\ \ x=0, \tag{3}$$

$$\chi(T)\frac{\partial T}{\partial x}=-\eta(T-T_0),\ \ x=L. \tag{4}$$

Here, $\chi(T)$ is the thermal conductivity of silicon; η is the Newtonian heat exchange constant which is equal to 2×10^{-3} W cm^{-2} K^{-1}; $N=N(x,t)$ is the concentration of nonequilibrium carriers. Using the reference data [8–11] we constructed the interpolation formulas for temperature dependences of the specific heat, thermal conductivity, as well as absorption and refractive indices:

$$c(T)=844+0.118T-1.55\times10^{7}T^{-2}\ (\text{J kg}^{-1}\ \text{K}^{-1}),$$

$$\chi(T)=0.086678+8017.08/T^{1.5181}\ (\text{W cm}^{-1}\ \text{K}^{-1}),$$

$$\alpha(T)=0.514T-102.713\ (\text{cm}^{-1}),$$

$$n(T)=3.52463+0.00001834T^{1.38691}.$$

We assume that radiation is incident along the normal to the surface. Then, to calculate the temperature field in the wafer, use can be made of the known expressions for the field amplitude and radiation intensity in the plane-parallel wafer of thickness L:

$$\frac{I(x)}{I_0}=\left|\frac{A(x)}{A_0}\right|^2,\quad \frac{A(x)}{A_0}=d_{12}(0)$$
$$\times\frac{r_{12}(L)\exp[\mathrm{i}\Psi(L)]\exp[\mathrm{i}\Psi(L)-\mathrm{i}\Psi(x)]+\exp[\mathrm{i}\Psi(x)]}{1-r_{21}(0)r_{21}(L)\exp[2\mathrm{i}\Psi(L)]}. \tag{5}$$

Here A_0 and I_0 are the amplitude and intensity of radiation incident on the wafer; $A(x)$ and $I(x)$ are the field amplitude and intensity in the wafer; r_{12} is the amplitude reflection coefficient of the wave incident on the interface between media 1–2 (medium 1 is air, medium 2 is the wafer); r_{21} is the amplitude reflection coefficient of the wave incident on the interface between media 2–1; d_{12} and d_{21} are their corresponding amplitude coefficients of the wave propagation; for brevity, the time dependence in (5) is not specified;

$$\Psi(x)=\frac{2\pi}{\lambda}\int_0^x[n(x_1)+\mathrm{i}\kappa(x_1)]\mathrm{d}x_1\equiv\frac{2\pi}{\lambda}S(x)+\mathrm{i}G(x), \tag{6}$$

where $\kappa=\mathrm{Im}\sqrt{\varepsilon}$; ε is the dielectric constant of the wafer. The value of $G(x)$ is related to the absorption coefficient in the wafer by the equation

$$G(x)=\frac{1}{2}\int_0^x\alpha(x_1)\mathrm{d}x_1. \tag{7}$$

The argument at the coefficients r and d shows the surface from which radiation is reflected or through which it passes. The amplitude coefficients of reflection and transmission at wafer boundaries are expressed through the dielectric constant of the material by the equations

$$r_{21}=\frac{1-\sqrt{\varepsilon_2}}{1+\sqrt{\varepsilon_2}},\quad r_{12}=-r_{21},$$
$$d_{12}=\frac{2}{1+\sqrt{\varepsilon_2}},\quad d_{21}=\frac{2\sqrt{\varepsilon_2}}{1+\sqrt{\varepsilon_2}}, \tag{8}$$

where ε_2 is the dielectric constant of silicon on the appropriate boundary.

Finally, the wave transmission (of the intensity) through the wafer is given by the expression $D=|d_\mathrm{t}|^2$, where

$$d_\mathrm{t}=\frac{d_{12}(0)d_{21}(L)\exp[\mathrm{i}(2\pi/\lambda)S-G]}{1-r_{21}(0)r_{21}(L)\exp[\mathrm{i}(2\pi/\lambda)2S-2G]}. \tag{9}$$

In accordance with the foregoing, in the heat conduction equation we must substitute the expression for the intensity

$$I(x,t)=\left|\frac{A(x)}{A_0}\right|^2I_0(t), \tag{10}$$

where $I_0(t)$ is the intensity of radiation incident on the outer surface of the wafer.

It was noted above that in our case intrinsic absorption of the wafer material is essential. To take it into account, we consider generation of nonequilibrium carriers and the resulting change in the optical thickness of the sample.

Let $N(x,t)$ be the concentration of nonequilibrium carriers, and ω_p be the plasma frequency corresponding to this concentration. The dielectric constant of the wafer is

$$\varepsilon(\omega)=\varepsilon_0(\omega)+\varepsilon_\mathrm{e}(\omega), \tag{11}$$

where $\omega_\mathrm{p}^2=4\pi e^2N(x,t)/m$; $m=0.3m_\mathrm{e}$ is the reduced mass of the electron; m_e is the electron mass [8]; $\varepsilon_\mathrm{e}(\omega)=\omega_\mathrm{p}^2/(\omega^2-\ \mathrm{i}\omega\gamma)$ is the contribution of nonequilibrium carriers to the dielectric constant. The absorption coefficient

$$\alpha=\frac{4\pi}{\lambda}\mathrm{Im}\sqrt{\varepsilon(\lambda)}. \tag{12}$$

The distribution of $N(x,t)$ over the wafer thickness is determined from the equation

$$\frac{\partial N(x,t)}{\partial t}=g(x,t), \tag{13}$$

where $g(x,t) = \zeta\alpha_i I(x,t)/(h\nu)$ is the function of the bulk carrier generation; α_i is the intrinsic absorption; ζ is the quantum yield of generation (20 % – 30 % for silicon); $I(x,t)$ is the intensity distribution in the wafer. Strictly speaking, in addition to generation of carriers, equation (13) should have taken into account recombination processes, among which radiative and nonradiative recombinations (including Auger recombination) as well as recombination of the defects are possible. However, the recombination time at the achieved carrier concentrations is generally large compared to the pulse duration and is equal to $10^{-5} - 10^{-6}$ s. The time of the Auger recombination is 10^{-5} s [12], and the recombination at defects is $10^{-3} - 10^{-4}$ s [7]. For this reason, the recombination processes in the equation are ignored.

To find the dependence of $N(x,t)$ it is necessary to solve equation (13) numerically, taking into account (12), together with the equation for the intensity

$$\frac{\partial I(x,t)}{\partial x} = -\alpha I(x,t). \qquad (14)$$

Knowing the concentration of nonequilibrium carriers, we can calculate the correction to the absorption coefficient $\alpha(T)$:

$$\alpha = \frac{4\pi}{\lambda}\operatorname{Im}\sqrt{\varepsilon_0 + \varepsilon_e} = \frac{4\pi}{\lambda}\operatorname{Im}\left(\sqrt{\varepsilon_0} + \frac{\varepsilon_e}{2\sqrt{\varepsilon_0}}\right)$$

$$= \alpha_0 + \frac{2\pi}{\lambda}\operatorname{Im}\frac{\varepsilon_e}{n_0}, \qquad (15)$$

where $\alpha_0 = \alpha_0(T)$ is the absorption caused only by the equilibrium carriers whose concentration corresponds to the temperature T.

Similarly, we find the refined expression for the refractive index

$$n = \operatorname{Re}\sqrt{\varepsilon} = \operatorname{Re}\sqrt{\varepsilon_0 + \varepsilon_e} = \operatorname{Re}\left(\sqrt{\varepsilon_0} + \frac{\varepsilon_e}{2\sqrt{\varepsilon_0}}\right)$$

$$= n_0 + \operatorname{Re}\frac{\varepsilon_e}{2n_0}, \qquad (16)$$

where $n_0 = \operatorname{Re}\sqrt{\varepsilon_0} = n_0(T)$ is the refractive index defined only by equilibrium carriers.

4. Results of modelling

The formulated mathematical model was studied numerically. Figure 4 shows the calculated time dependence of the concentration N of nonequilibrium carriers on the surface ($x = 0$) of the wafer. The fact that during the passage of the laser pulse through the wafer we have high values of N ($\sim 10^{19}$ cm^{-3}), confirms the need to take into account nonequilibrium carriers in calculations of the effect of radiation on the target under these conditions.

Figure 5 presents the time dependence of the transmitted light intensity obtained in the numerical solution of equations (1)–(4) with the account for generation of nonequilibrium carriers [see (15) and (16)]. It is seen that the model can explain the existence of many oscillations observed in experiments. It follows from the comparison of theoretical calculations and experimental results shown in Fig. 6 that the model satisfactorily describes the characteristic period and amplitude of the oscillations observed in experiments.

Thus, without using fitting parameters it is possible to explain the observed features of Nd:YAG-laser radiation

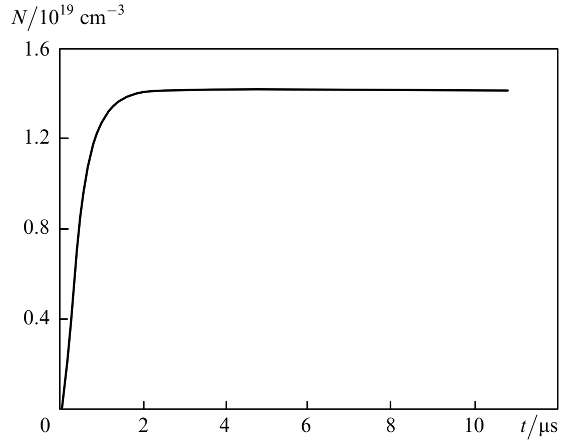

Figure 4. Time dependence of the nonequilibrium carrier concentration N on the front surface of silicon.

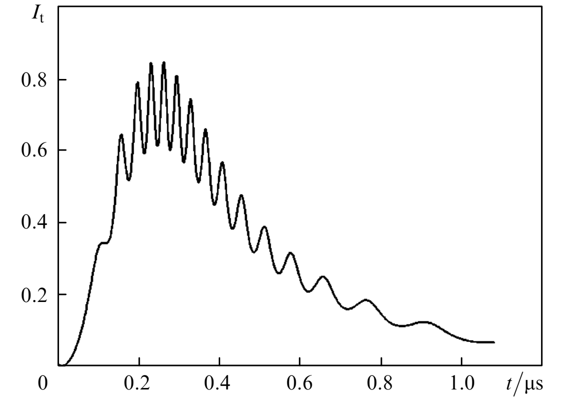

Figure 5. Normalised time dependence of the intensity of radiation transmitted through the wafer, obtained by numerical solution of equations that take into account generation of nonequilibrium carriers.

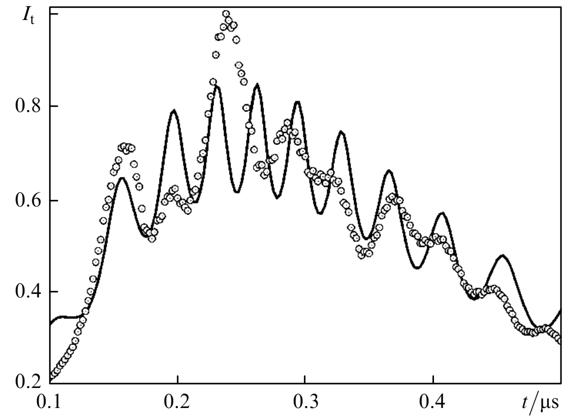

Figure 6. Normalised time dependence of the intensity of radiation transmitted through the wafer (points – experimental results, curve – results of numerical modelling).

propagation through silicon wafers. This allows one to use the developed methods for calculating the heating dynamics of the wafers made of the indirect-band semiconductors in the near-IR spectrum, where both equilibrium and non-equilibrium carriers play simultaneously a significant role in the absorption.

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