

Measurement of Surface Recombination Velocity and Bulk Lifetime in Si Wafers by the Kinetics of Excess Thermal Emission

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Abstract—A contactless nondestructive technique for measuring recombination parameters (surface recombination velocity and bulk and effective lifetime of free carriers) in Si wafers is proposed. The technique is based on the analysis of the relaxation kinetics of excess thermal emission in a wafer above the Si intrinsic absorption edge ($\lambda > 3 \mu\text{m}$) after excitation by a short laser pulse with a photon energy higher than the Si band gap. Experimental results for wafers 300 μm and 2 mm thick, excited by laser radiation with wavelengths of 0.96 and 1.06 μm at above-room temperatures are presented. The surface and bulk components of the effective lifetime are separated by extrapolating the final portion of the kinetics of excess thermal emission relaxation to the intersection with the y coordinate axis.

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1. INTRODUCTION

The effective carrier lifetime τ_{eff} is the most important parameter of Si wafers and devices based on them. Since Si electronics and optoelectronics have actively been developed in the last several years, measurement and control of this parameter have come to the fore. Many methods for measuring τ_{eff} were proposed. However, since τ_{eff} is controlled not only by bulk recombination properties (characterized by the bulk lifetime τ_b), but also by the surface state (characterized by the surface recombination velocity S), only separate measurements of bulk and surface parameters are much in demand.

To separate the surface and bulk components of the effective lifetime, stationary [1], phase-frequency [2], and kinetic [3, 4] techniques were used. All these techniques are based on the solution of the one-dimensional diffusion equation as applied to free carriers excited by laser radiation in a semi-infinite wafer. Analysis of the kinetics of photogenerated carrier density relaxation after turning off excitation makes it possible to separate τ_b and S using two independent measurements on a wafer excited by two lasers with different wavelengths [5]. Further consideration showed that separation is also possible by a single measurement (single laser wavelength) by comparing experimental and calculated curves [6, 7]. The relaxation kinetics of the spatially averaged density of photogenerated carriers, as a result of the solution of the diffusion equation, can be analytically described by an infinite sum of exponentially time-dependent quantities each dependent on τ_b and S [8]. However, as a detailed analysis of limiting properties of the solution showed, the value of S can be measured independently of τ_b

using linear extrapolation of the final portion of the relaxation kinetics.

Microwave reflection/absorption and infrared absorption are the most commonly used physical approaches for experimental control of the spatially averaged photogenerated carrier density. They are “pump-probe” approaches which require two radiation sources, i.e., for excess carrier generation and probing. As a result, continuous monitoring of the recombination properties of Si wafers during device fabrication is problematic.

In this paper, we present a measurement technique that does not require a probe radiation source. The operating principle of the method consists in the possibility of controlling the average photogenerated carrier density by measuring the thermal emission in the spectral region above the Si intrinsic absorption edge.

2. PHYSICAL GROUNDS OF THE METHOD

The physical bases of the method are as follows. Let us consider a Si wafer at a certain above-room temperature T . Free carrier photogeneration leads to an increase in the wafer emissivity $\Delta\varepsilon$ in the spectral region beyond the Si intrinsic absorption edge, where the main optical absorption mechanism is free-carrier absorption. In turn, this results in excess thermal emission in the indicated spectral region; its rate will be $\Delta P = \Delta\varepsilon P_{\text{bb}}$ (where P_{bb} is the blackbody radiation power at temperature T [9, 10]). If the condition $\alpha_{\text{fc}}d \ll 1$ is satisfied (where α_{fc} is the free-carrier absorbance

and d is the wafer thickness), the increase in the emissivity due to photogeneration is given by

$$\Delta\epsilon = \int_{-d/2}^{d/2} \Delta\alpha_{fc}(x)dx.$$

Taking into account that the free-carrier absorbance is related to the free-carrier density n in the wafer as $\alpha_{fc} = (\sigma_n + \sigma_p)n$, we obtain

$$\Delta\epsilon = (\sigma_n + \sigma_p) \int_{-d/2}^{d/2} \Delta n(x)dx = (\sigma_n + \sigma_p)d\Delta n_{av},$$

where $\sigma_{n,p}$ are the electron and hole absorption cross sections and Δn_{av} is the photogenerated carrier concentration averaged over the wafer thickness. Thus, the excess thermal emission power is directly proportional to the average photogenerated carrier concentration (Δn_{av}),

$$\Delta P = (\sigma_n + \sigma_p)d\Delta n_{av}P_{bb}.$$

From this it follows that measurements of the excess thermal emission power can allow control of modulation of photogenerated carrier concentration.

In [8], it was shown that the relaxation kinetics of the average concentration of carriers generated by a short (shaped as a δ function) laser pulse in a semi-infinite wafer is described by the dependence

$$\Delta n_{av}(t) = \sum_k B_k b_k \exp\left[-\left(\frac{1}{\tau_b} + a_k^2 D\right)t\right] \frac{\sin z_k}{z_k}, \quad (1)$$

where

$$z_k = \frac{a_k d}{2}, \quad b_k = -\frac{D a_k \cos z_k + S \sin z_k}{D a_k \sin z_k - S \cos z_k},$$

D is the diffusion coefficient and τ_b is the bulk carrier lifetime. The constants a_k are determined from the boundary conditions for the diffusion equation,

$$a_k d = 2 \arctan\left(\frac{S}{D a_k}\right) + k\pi. \quad (2)$$

In this case, it was assumed that recombination velocities S on both faces are identical. The coefficients B_k are determined from the initial condition and represent the initial ($\Delta n(x, t=0)$) spatial distribution of the photogenerated carrier density, taking into account multiple reflection of excitation radiation from the sample surface. The coefficients B_k depend on the excitation-radiation absorbance $\alpha(\lambda)$, reflectances from wafer faces, thickness d , constants a_k , and excitation radiation power. The expressions for coefficients B_k are given in [8].

As seen from (1), the time dependence Δn_{av} consists of an infinite number of terms each representing an exponentially decaying function. Analysis of

Eq. (2) shows that the value of constants a_k rapidly increases with the number k . This, in turn, means that the effect of terms with large numbers k will become negligible with time t . Thus, all the exponential terms contribute to the initial part of dependence (1); whereas, at $t \rightarrow \infty$, the dependence is represented by one exponential function with a time constant equal to the effective carrier lifetime (τ_{eff}),

$$\frac{1}{\tau_{eff}} = \frac{1}{\tau_b} + a_1^2 D. \quad (3)$$

Nonuniform absorption of excitation radiation results in the fact that the photogenerated carrier density near an exposed surface is initially higher than near an opposite surface. As a result, carriers begin to diffuse from the illuminated surface to the wafer depth. Simultaneously with this process, carrier recombination occurs. Therefore, the initial portion of the relaxation kinetics for the average photogenerated carrier density is caused not only by recombination processes, but also by carrier diffusion from the illuminated surface (each exponential term in (1) makes a contribution). This results in the semilog slope of the initial kinetics portion varying in time. Diffusion occurs until the spatial distribution of carriers over the wafer thickness takes its steady-state shape. From this time on, the photogenerated carrier density decreases with a time-independent slope defined by a time constant τ_{eff} over the entire wafer.

Let us consider the normalized relaxation kinetics of the average photogenerated carrier density: $\Delta n_{norm}(t) = \Delta n_{av}(t)/\Delta n_{av}(0)$. According to the above, the final portion of the dependence $\Delta n_{norm}(t)$ will be linear on the semilog scale. The straight line which extrapolates this linear portion intersects the vertical axis at the point y_i . In [7], it was shown that the section δ (Fig. 1) on the vertical axis between points $y=1$ and y_i is independent of the bulk lifetime in the wafer, but is a function of only the surface recombination velocity S . By means of the known Si wafer parameters, such as the diffusion coefficient D , thickness d , and absorbance $\alpha(\lambda)$, the function $S(\delta)$ can be numerically calculated from (1)–(3). This makes it possible to determine the surface recombination velocity from the relaxation kinetics of the excess thermal emission power above the Si intrinsic absorption edge and the numerically calculated dependence $S(\delta)$. We note that the function $S(\delta)$ is calculated using the normalized time dependence of the average photogenerated carrier concentration, which allows experimental measurements of the relaxation kinetics of the excess thermal emission power in relative units.

3. EXPERIMENTAL

The experiments were performed with single-crystal p -Si wafers with resistivity $\rho_p \approx 3200 \Omega \text{ cm}$; the initial bulk lifetime in ingots was $\tau_b \approx 500 \mu\text{s}$. Wafers were

cut from ingots as parallelepipeds, whose thickness after surface treatment (grinding and polishing) was $d_1 = 2 \text{ mm}$ and $d_2 = 300 \mu\text{m}$.

The used experimental setup for measuring the time dependence of the excess thermal emission power is schematically shown in the inset of Fig. 1a (the setup was assembled at the Lashkarev Institute of Semiconductor Physics, National Academy of Sciences of Ukraine, Kyiv). Laser diodes at wavelengths of $\lambda_1 = 0.96$ and $\lambda_2 = 1.06 \mu\text{m}$ were used as excitation sources. Excitation radiation was directed to the surface of the sample placed in a heater maintaining a constant above-room temperature. Since the problem of free carrier diffusion–recombination was considered in a one-dimensional formulation, the transverse size of the laser spot on the illuminated face was several times larger than the wafer thickness. The excess thermal emission from the rear wafer surface was measured in a wide spectral range (3 – $12 \mu\text{m}$) using a cooled CdHgTe photodetector. The photodetector signal was fed to an analog-to-digital converter, where it was digitized and stored for further processing. The excitation laser-radiation power was chosen from the condition of low photoionization to provide the inequality $\alpha_{\text{fc}}d \ll 1$. To implement the above technique for measuring S and τ_b , the excitation-pulse duration should be rather short (much shorter than the effective carrier lifetime). In the experiments presented here, it was $\sim 100 \text{ ns}$.

4. RESULTS AND DISCUSSION

Figure 1a shows the relaxation kinetics of excess thermal emission of the p -Si wafer 2 -mm thick at $T = 373 \text{ K}$. We can see that the section δ decreases as the laser radiation wavelength increases (the absorbance $\alpha(\lambda)$ decreases): $\delta_1 = 0.136$ for $\lambda_1 = 0.96 \mu\text{m}$ and $\delta_2 = 0.44$ for $\lambda_2 = 1.06 \mu\text{m}$. At $\alpha(\lambda) \rightarrow 0$, uniform absorption will occur in the wafer, hence, carrier diffusion from the illuminated face is excluded. In this case, the carrier relaxation kinetics will be described only by the effective lifetime, and the section $\delta \rightarrow 0$. In the opposite case, as $\alpha(\lambda)$ increases, the number of injected carriers near the illuminated surface significantly increases. Therefore, along with recombination, the relaxation kinetics of the average photogenerated carrier density (hence, the excess thermal emission) will be affected by diffusion from the surface, which does cause an increase in the semilog slope of the initial kinetics portion and an increase in the section δ . Diffusion from the illuminated surface discontinues with time (as seen in Fig. 1a, this occurs at $t > 100 \mu\text{s}$ in the case at hand), and the relaxation process at all $\alpha(\lambda)$ can be represented by a single exponential function with a time constant equal to the effective carrier lifetime. The experimental values of the effective carrier lifetime, determined by the slope of the final portion of the relaxation kinetics of the excess thermal emission, are $154 \mu\text{s}$ for $\lambda_1 = 0.96 \mu\text{m}$ and $162 \mu\text{s}$ for $\lambda_2 = 1.06 \mu\text{m}$.

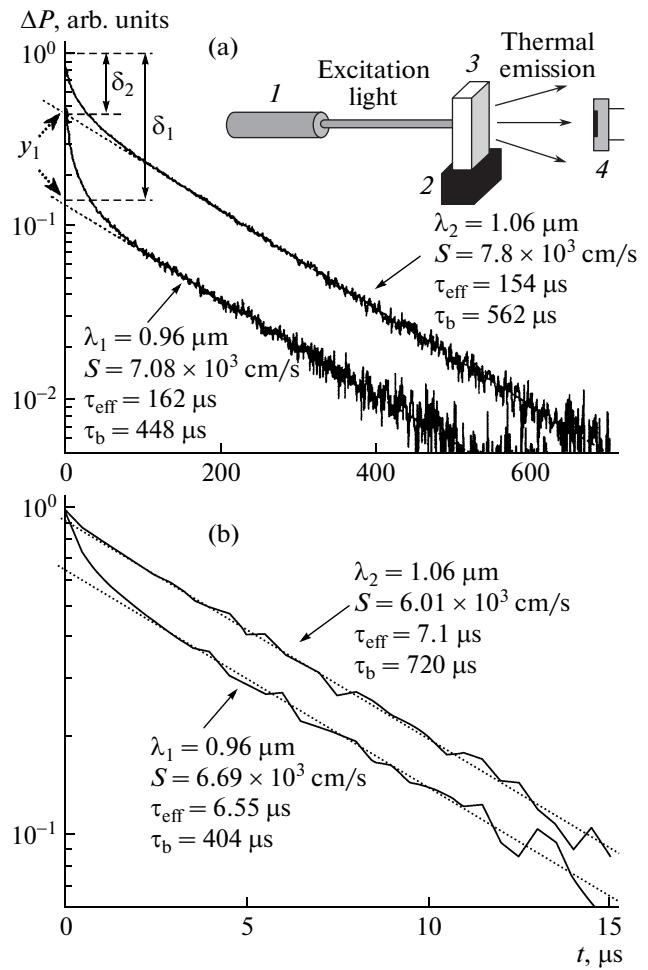


Fig. 1. Relaxation kinetics of excess thermal emission of Si wafers (a) 2 mm and (b) $300 \mu\text{m}$ thick upon excitation by laser radiation with wavelengths of 0.96 and $1.06 \mu\text{m}$ at $T = 373 \text{ K}$. The inset shows the experimental scheme: (1) excitation source, (2) heater, (3) sample, and (4) photodetector.

To determine the surface recombination velocity, it is necessary to know the absorbances at exciting laser radiation wavelengths ($\alpha(\lambda_1)$ and $\alpha(\lambda_2)$) and the carrier diffusion coefficient D . We used the spectral dependences $\alpha(\lambda)$ presented in [11]. The (bipolar) diffusion coefficient was recalculated from the available electron and hole mobilities [12]. Since the section δ is independent of the bulk lifetime, the surface recombination velocity is uniquely determined from the numerically calculated dependence $S(\delta)$ at corresponding wafer parameters and temperature ($T = 373 \text{ K}$ in the case at hand). Figure 2 shows such dependences for wafers of thickness $d_1 = 2 \text{ mm}$ and $d_2 = 300 \mu\text{m}$. In this case, the values of the absorbance and diffusion coefficient were taken as $\alpha(\lambda_1) = 299 \text{ cm}^{-1}$, $\alpha(\lambda_2) = 43.5 \text{ cm}^{-1}$, and $D = 18 \text{ cm}^2/\text{s}$. $S = 7.08 \times 10^3$ and $7.8 \times 10^3 \text{ cm/s}$ for $\lambda_1 = 0.96 \mu\text{m}$ and $\lambda_2 = 1.06 \mu\text{m}$, respectively, correspond to the experimentally determined δ_1 and δ_2 . The available surface recombination

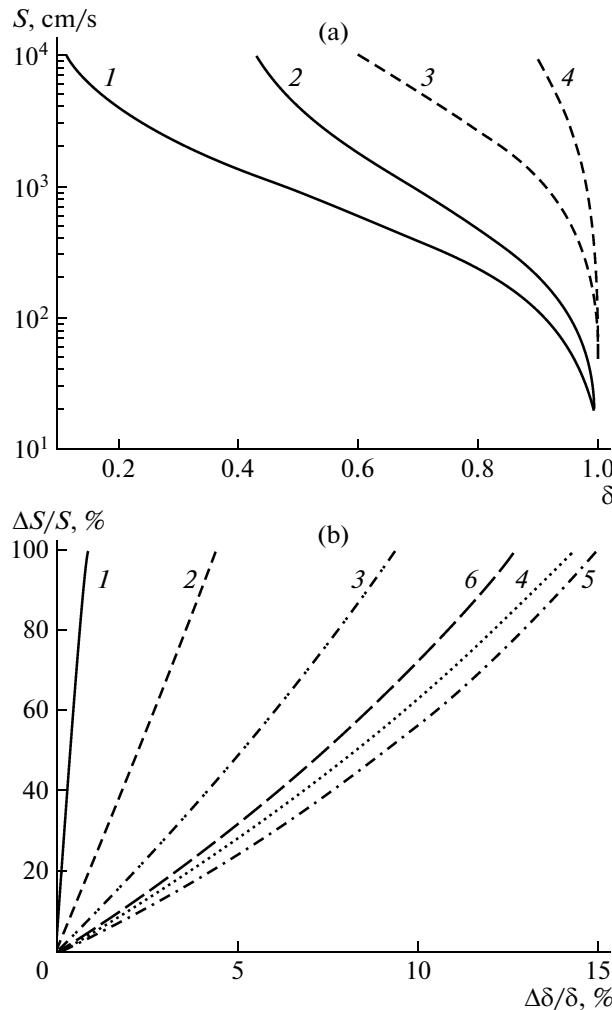


Fig. 2. (a) Calculated dependences $S(\delta)$ for Si wafers of various thicknesses d , excited by radiation with various wavelengths λ at $T = 373$ K: $d = (1)$ 2 mm, $\lambda = 0.96$ μm ; (2) $d = 2$ mm, $\lambda = 1.06$ μm ; (3) $d = 300$ μm , $\lambda = 0.96$ μm ; and (4) $d = 300$ μm , $\lambda = 1.06$ μm . (b) Dependences of the relative error of the surface recombination velocity determination on the relative error of S measurements at $T = 373$ K, $d = 300$ μm , $\lambda = 0.96$ μm , and $S = (1) 10^2$, $(2) 5 \times 10^2$, $(3) 10^3$, $(4) 2 \times 10^3$, $(5) 5 \times 10^3$, and $(6) 10^4$ cm/s .

velocities and effective lifetimes also make it possible to estimate the bulk lifetime in samples from (3) as $\tau_b = 448$ and 562 μs for measurements using lasers with $\lambda_1 = 0.96$ and $\lambda_2 = 1.06$ μm , respectively.

Figure 1b shows the relaxation kinetics of excess thermal emission from polished Si wafers 300 μm thick. For this thickness and wavelength $\lambda_2 = 1.06$ μm , the calculated dependences $S(\delta)$ show that δ changes merely from 1 to 0.91 as S changes from 10 to 10^4 cm/s . Therefore, the measurements of the surface recombination velocity, performed using the laser with $\lambda_2 = 1.06$ μm seem problematic. For the wavelength $\lambda_1 = 0.96$ μm , the corresponding change in δ is from 1 to 0.6. The thinner the wafer, the shorter the wave-

length of the laser that should be used as an exciting source. Measurements performed using the laser with $\lambda_1 = 0.96$ μm yield the following recombination parameters of the wafer: $\tau_{\text{eff}} = 6.55$ μs , $S = 6.69 \times 10^3$ cm/s , and $\tau_b = 404$ μs .

Figure 2b shows the dependence of the relative error of the determination of the surface recombination velocity on the relative error of δ measurements in wafers 300 μm thick for excitation by radiation with a wavelength of 0.96 μm . A minimum error is achieved in the S range from 10^3 to 10^4 cm/s . This makes the proposed technique promising for control of the surface recombination velocity in Si solar elements. As is known, the surface recombination velocity on the front surface of a solar cell results in a significant decrease in the energy conversion efficiency at $S > 10^3$ cm/s , whereas the efficiency very weakly depends on S at $S < 10^3$ cm/s [13]. Therefore, correct measurements of the surface recombination velocity $S > 10^3$ cm/s are much in demand for solar cells. At $10^3 \text{ cm/s} < S < 10^4 \text{ cm/s}$ and the relative error of the measured value $\Delta\delta/\delta < 5\%$, $\Delta S/S$ does not exceed 50%. Estimations show that the measurement error of the surface recombination velocity decreases with increasing wafer thicknesses and excitation radiation absorbance. For example, for wafers 2 mm thick under conditions that $\lambda = 0.96$ μm , 5×10^2 $\text{cm/s} < S < 10^4$ cm/s , and $\Delta\delta/\delta < 5\%$, the relative error $\Delta S/S$ does not exceed 12%. The determination error of the bulk lifetime τ_b is larger than the determination error of S . It depends on the extent of the difference between τ_{eff} and $(a_1^2 D)^{-1}$.

In addition to the random error arising directly during measurements of the excess thermal emission power, the systematic error should also be taken into account, which is caused by inaccurate choice of initial parameters (the wafer thickness, diffusion coefficient, and absorbance) and violation of method application conditions. For example, violation of the $\alpha_{fc}d \ll 1$ inequality leads to overestimated recombination velocities. In addition, the longer the exciting radiation wavelength, the larger the systematic error.

5. CONCLUSIONS

Thus, we presented a technique for measuring recombination parameters in Si wafers by analyzing the relaxation kinetics of excess thermal emission of a wafer above the Si intrinsic absorption edge upon excitation by a short laser pulse with a photon energy larger than the Si band gap. This method does not require an additional radiation source for probing photogenerated free carriers; hence, it is more appropriate for continuous control of recombination parameters at various production stages of Si devices (in particular, solar cells). One more important advantage of the method is the possibility of determining the surface

recombination velocity and the effective and bulk lifetimes from a single measurement. The method is applicable to both thick (with thickness larger than the diffusion length) and thin wafers. The possibility is also noteworthy of determining the surface recombination velocities on both wafer faces from two measurements of the kinetics of excess thermal emission during sequential irradiations of the front and rear wafer surfaces.

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