Semi-infinite photocarrier radiometric model for the characterization of semiconductor wafer

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Abstract. The analytical expression is derived to describe the photocarrier radiometric (PCR) signal for a semi-infinite semiconductor wafer excited by a square-wave modulated laser. For comparative study, the PCR signals are calculated by the semi-infinite model and the finite thickness model with several thicknesses. The fitted errors of the electronic transport properties by semi-infinite model are analyzed. From these results it is evident that for thick samples or at high modulation frequency, the semiconductor can be considered as semi-infinite.

1. Introduction
In recent years the laser-induced infrared photocarrier radiometry (PCR) has been introduced as a pure carrier-density-wave diagnostic method for noncontact characterization of the electronic transport properties of semiconductors [1, 2]. PCR technology relies on the detection of the infrared emission from the semiconductor samples optically excited by an intensity-modulated laser beam with photon energy greater than the fundamental energy gap of the materials. The PCR signals can be calculated by integrating the carrier density over the detection volume. In former studies, the integrating range over the depth is from the front surface to the rear surface with finite thickness [3, 4]. However, for thick samples the excited free carriers cannot diffuse to the rear surface. The samples can be treated as semi-infinite and the PCR signal expression can be substantially simplified. In this article, a semi-infinite model for PCR is introduced and the scope of its application is discussed.

2. Theory of semi-infinite PCR model
When a semiconductor wafer is illuminated by a modulated laser with photon energy greater than the bandgap, free carriers are generated in the sample. Subsequently the photo-generated free carriers diffuse into the bulk of the sample until they recombine. The range the free carriers can cover is the ac carrier diffusion length, which is determined by

$$L_{ac} (\omega) = \frac{D \tau}{\sqrt{1 + \omega^2 \tau^2}}.$$  (1)

Here $\tau$ is the lifetime of the free carrier and $D$ is the ambipolar diffusion coefficient, and $\omega$ is the modulation angular frequency of the exciting laser. For single-crystalline silicon which is mostly used as substrate in industry, the carrier diffusion length are 122.5$\mu$m and 21.8$\mu$m at modulation frequency
of 100Hz and 500kHz respectively, with $\tau = 10\mu s$ and $D = 15cm^2/s$. The typical thicknesses of silicon wafers are approximately 525µm, 675µm and 750µm for 4, 8 and 12 inches wafers [5, 6]. The ac carrier diffusion length is a quarter or less of the wafer thickness in this case. Therefore, only few photo-generated free carriers can diffuse to the rear surface of the sample, and the sample can be considered as semi-infinite.

The ambipolar diffusion equation in frequency domain governing the carrier distribution in the semiconductor is:

$$\nabla^2 N(\vec{r}, \omega) - \sigma^2(\omega)N(\vec{r}, \omega) = \frac{g(\vec{r}, \omega)}{D},$$

where $\sigma(\omega)$ is the carrier wave number

$$\sigma(\omega) = \sqrt{\frac{1 + i\omega\tau}{D\tau}}.$$

The partial differential equation can be transformed into a one dimensional ordinary differential equation through the application of Hankel transformation. The corresponding boundary conditions for carrier transport can be described by the surface recombination equations

$$D \left. \frac{\partial \tilde{N}(\xi, z; \omega)}{\partial z} \right|_{z=0} = S_i \tilde{N}(\xi, 0, \omega)$$

$$D \left. \frac{\partial \tilde{N}(\xi, z; \omega)}{\partial z} \right|_{z=\infty} = 0$$

The solution to the carrier diffusion equation is

$$\tilde{N}(\xi, z; w) = E(\xi) \left( \frac{D\alpha + s_i}{Dk + s_i} e^{-\omega} - e^{-\omega} \right),$$

with

$$E(\xi) = \frac{A e^{\xi^2/4}}{\alpha^2 - \kappa^2}, \alpha = \frac{\alpha P\eta(1-R)}{4\pi Dh}, \kappa^2 = \xi^2 + \sigma^2.$$

Where $s_i$ is the front surface recombination velocity, $\alpha$ is the absorption coefficient, $P$ is the incident power, $\eta$ is the optical-to-electronic quantum efficiency, $R$ is the reflectivity at the excitation wavelength, $r_b$ is the beam radius, $h\nu$ is the photon energy of the incident radiation, and $\xi$ is the Hankel integration variable.

The carrier density can be integrated over the depth to obtain

$$\tilde{N}(\xi, w) = \int_0^\infty \tilde{N}(\xi, z; \omega) dz = E(\xi) \left( \frac{D\alpha + s_i}{Dk + s_i} \frac{1}{\alpha} \right).$$

The PCR signal can be expressed in final form by performing an inverse Hankel transform and integrating over the detector area with radius $r_d$

$$S_{PCR} = C \int_0^{r_d} 2\pi r \int_0^{\infty} \tilde{N}(\xi; \omega) \xi J_0(\xi r) d\xi dr = C \int_0^{\infty} \tilde{N}(\xi; \omega) J_1(\xi r_d) d\xi.$$

Where $J_1$ is a first order Bessel function of the first kind and coefficient $C$ is used to normalize the theoretically calculated PCR response.

### 3. Comparative study of the semi-infinite and finite thickness model

Simulations of the PCR signal are performed using the finite thickness model with different sample thicknesses and the semi-infinite model, with the results shown in Fig. 1. The inset in Fig. 1(a) zooms in the low-frequency range for a better observation. Experimental parameter values assumed in the calculations include: exciting laser wavelength $\lambda=830nm$, the laser beam radius is 25µm, and the effective radius of detector is 55µm. Characteristic parameters of single-crystalline silicon are used in the simulation, with the typical values $\tau = 10\mu s$, $D = 15cm^2/s$ and $s_i = 10m/s$ [7].
In order to have the accurate results concerning the differences of the two models, we define the percentage deviation $\Delta S = (S_{\text{semi}} - S_{\text{fini}}) / S_{\text{semi}}$, where $S_{\text{semi}}$ and $S_{\text{fini}}$ are signals calculated by semi-infinite model and finite thickness model. The percentage deviations of amplitude ($\Delta S_{\text{amp}}$) and phase ($\Delta S_{\text{pha}}$) are presented in Fig. 2. We can see clearly that for sample thickness greater than 500$\mu$m the semi-infinite model is in good conformity with the finite thickness model, with $\Delta S_{\text{amp}} < 1\%$ and $\Delta S_{\text{pha}} < 3\%$ in the whole modulation frequency domain. The values of $\Delta S_{\text{pha}}$ are much higher than $\Delta S_{\text{amp}}$ at low modulation frequency. Because the phase values are approach to zero and small change will bring in large relative deviation. If the acceptable $\Delta S$ is set to 2\% for amplitude and 5\% for phase, the semi-infinite model can work well at modulation frequency higher than 10kHz, 27kHz and 65kHz for samples with thicknesses of 400$\mu$m, 300$\mu$m and 200$\mu$m respectively. However, the semi-infinite is not suitable for the thin sample (100$\mu$m) even at high modulation frequency of 300kHz, when the sample cannot be considered to be semi-infinite.

Fig. 1. PCR signals (amplitude and phase) simulated by semi-infinite model and finite thickness model with different wafer thicknesses.

Fig. 2. Percentage deviations between the semi-infinite model and finite thickness model for different wafer thicknesses.

To determine the electronic transport properties of the samples via a multi-parameter fit to a semi-infinite model, the theoretical results of the finite thickness model should be compared first. In simulations, we first create several sets of PCR data by the finite thickness model with different
sample thicknesses. Then we perform multi-parameter fits of the simulated data to the semi-infinite model via a least-squares process to extract the effective transport properties of $\tau$, $D$, and $s_1$. In the multi-parameter fitting process, the square variance defined in Ref.4 is minimized. Errors are defined as $(P_f - P_i)/P_i$, where $P_f$ and $P_i$ are the fitted and initial parameters ($\tau$, $D$ or $s_1$). Figure 3 shows the fitting variances and the errors between the fitted electronic parameters and the given initial values. We can see the front surface recombination velocity has the largest errors because the effects of the surface property may be more obvious for thinner samples. When the sample thickness is four times of the DC diffusion length, the errors for $\tau$, $D$ and $s_1$ are -8.8%, 3.5% and -17.8% respectively. The values decrease to -2.7%, 1.1% and -5.3% for sample with thickness five times of the DC diffusion length.

![Fig. 3. Fitting errors and variances by semi-infinite model with PCR data generated from the finite thickness model with different thicknesses. Initial electronic transport parameters are $\tau = 10\mu$s, $D = 15\text{cm}^2/\text{s}$ and $s_1 = 10\text{m/s}$. DC diffusion length is calculated as 122$\mu$m.](image)

**4. Conclusions**

To summarize, a semi-infinite model has been derived to describe the PCR signal. Comparative results show that the semiconductor of finite thickness can be considered as semi-infinite for thick samples or the PCR experiment are performed at high modulation frequency.

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