Accurate determination of electronic transport properties of semiconductor wafers with spatially resolved photo-carrier techniques

Bincheng Li, Xianming Liu, Wei Li, Qiuping Huang, and Xiren Zhang

Institute of Optics and Electronics, Chinese Academy of Sciences,
P O Box 350, Shuangliu, Chengdu, Sichuan 610209, China

Corresponding author’s email address: bcli@ioe.ac.cn

Abstract. Spatially resolved photo-carrier techniques, in which a modulated and tightly focused laser beam with photon energy larger than the band gap of the semiconductor material under investigation is employed to generate free carriers, are applied to the simultaneous determination of the electronic transport properties of semiconductor wafers, that is, the carrier lifetime, the carrier diffusivity, and the front surface recombination velocity. The simultaneous determination is fulfilled by measuring and multi-parameter fitting the modulation-frequency-dependent three-dimensional distribution of photo-generated free carriers in a semiconductor wafer to a rigorous three-dimensional theoretical model. The uncertainties of the fitted parameter values are analyzed by investigating the dependence of a mean square variance including both amplitude and phase errors on the corresponding transport parameters and compared to that obtained by the conventional frequency-scan approach, in which only the frequency dependence of the amplitude and phase of the photo-carrier signals are recorded at the excitation spot. Both theoretical simulations and experimental results show that the accuracy of the simultaneous multi-parameter determination is greatly improved by the spatially resolved information of the photo-generated free-carrier diffusion in the semiconductor wafers.

1. Introduction

In order to control the quality, performance and reliability of silicon-based micro-electronic devices, the electronic transport properties, i.e., the carrier lifetime ($\tau$), the carrier diffusivity ($D$) and the front surface recombination velocity (FSRV) ($S_1$) of silicon wafers have to be determined accurately. In the past, various photo-excitation based methods, such as modulated free carrier absorption (MFCA) [1], photo-modulated thermoreflectance (PMR) [2], infrared photothermal radiometry (PTR) [3] and photo-carrier radiometry (PCR) [4] have been developed to determine the transport properties of silicon wafers. In these approaches, the transport properties of semiconductor wafers are determined simultaneously by multi-parameter fitting the modulation frequency dependence of the signal amplitude and phase measured at the excitation spot to a rigorous theoretical model. However, careful investigations have shown that only when the carrier diffusivity $D$ is known in prior with high precision, the carrier lifetime and FSRV values determined by the simultaneous multi-parameter fitting are acceptable [5, 6]. In practice, the carrier diffusivities of most wafers vary in a wide range, depending on the injection level and process parameters [7]. An inaccurate $D$ value could cause
considerable deviations of fitted $\tau$ and FSRV from the real values of measured wafers. It is therefore essential to develop sensitive and non-destructive approaches to determine accurately not only the carrier lifetime and FRSV, but also the carrier diffusivity simultaneously.

Recently, the laterally resolved MFCA technique (LR-MFCA) \[8\], in which the MFCA amplitude and phase are measured as functions of the pump-probe-beam separation at several modulation frequencies covering an appropriate range, has been employed to extract the transport properties of silicon wafers by multi-parameter fitting the LR-MFCA data to a rigorous three-dimensional model. In this paper, we report on the theoretical and experimental aspects of the laterally resolved photo-carrier techniques (either MFCA, or PCR, or their combination) for the simultaneous determination of the transport parameters of semiconductor wafers.

2. Theoretical models and simulations

Consider a homogeneous semiconductor wafer with a thickness $L$. The photo-carrier signal from a semiconductor wafer subject to photo-excitation from an intensity-modulated laser source (pump beam) with a photon energy larger than energy gap is directly proportional to the number of free carriers within the detection volume. For MFCA, the signal can be expressed as follows \[9\]

$$\Delta I(r, \omega) = \text{const} \int_0^\infty \Delta N(q, \omega) J_0(qr) dq,$$

while for PCR, the signal is \[4\]

$$S(\omega) = \text{const} \int_0^\infty \int_0^r \Delta N(q, \omega) J_0(qr) dq \cdot 2\pi rdr,$$

with

$$\Delta N(q, \omega) = E \frac{\left(1 - \exp(-\beta L)\right)}{\beta} \left(C_1 + C_2 \exp(-\beta L)\right) - \frac{\exp(-\alpha L)}{\alpha},$$

where

$$\beta^2 = q^2 + \frac{1 + j \omega \tau}{Dr},$$

$$C_1 = A_1 A_2 \frac{b_2 - b_1 \exp[-(\alpha - \beta)L]}{A_1 - A_2 \exp(-2\beta L)},$$

$$A_1 = \frac{D/\beta - S_1}{D/\beta + S_1},$$

$$b_1 = \frac{D/\alpha + S_1}{D/\beta + S_1},$$

$$C_2 = \frac{b_1 A_1 - b_2 A_2 \exp[-(\alpha - \beta)L]}{A_1 - A_2 \exp(-2\beta L)},$$

$$A_2 = \frac{D/\beta + S_2}{D/\beta - S_2},$$

$$b_2 = \frac{D/\alpha - S_2}{D/\beta + S_2},$$

Here $\alpha$ and $R$ are the absorption coefficient and surface reflectivity of the semiconductor wafer at the excitation wavelength, respectively. $w$, $P$ and $hv$ are the radius, power and photon energy of the pump beam. $\eta$ is the quantum yield. $S_2$ is the rear surface recombination velocity (RSRV). $r_d$ is the radius of the detector in PCR, and $f$ the modulation frequency.

Figure 1 shows the photo-generated free carrier density distributions in a Si wafer calculated at modulation frequency 1kHz, 10kHz, 100kHz, and 1MHz, respectively. In the calculations, the following parameters are used: $D=20$ cm$^2$/s, $r=10$ $\mu$m, $S_1=10^4$ cm/s, $S_2=10^4$ cm/s and $w=50$ $\mu$m. The carrier density is a function of both position $r$ and modulation frequency $f$. At frequency below 10kHz, the carrier density distribution is approximately independent of the modulation frequency. As the frequency further increases, the carriers confine to the photo-generation volume. Due to surface recombination, the maximum carrier density appears approximately 13 $\mu$m below the surface at low frequency region. As expected, the carrier density also decreases as the radial position increases. The carrier distribution is further affected by the transport properties of the semiconductor wafer, and the influences are different at different positions and modulation frequencies. Therefore, by measuring and
multi-parameter fitting the modulation-frequency-dependent carrier distributions to the rigorous theoretical model, the transport properties can be simultaneously determined.

Figure 1. Photo-generated free carrier density distributions calculated at modulation frequency 1kHz, 10kHz, 100kHz, and 1MHz, respectively.

Figure 2. Calculated modulation frequency dependence of the MFCA signal amplitude (a) and phase (b) at different two-beam separations.

Experimentally, the direct measurement of the three-dimensional photo-generated free-carrier distribution is difficult. However, the three-dimensional carrier distribution can be indirectly reconstructed by detecting (1) the detection position (that is, the two-beam separation in FCA technique) dependence of the amplitude and phase of the PCR or FCA signals at different modulation frequencies covering a wide range, (2) the modulation frequency dependence of the amplitude and phase measured at different detection positions relative to the excitation spot, or (3) the frequency dependence of the amplitude and phase measured with different detection volumes (that is, the detection areas). As an example, Fig. 2 shows the frequency dependence of the MFCA amplitude and phase obtained at two-beam separation of 0, 30, 60, 90, and 120μm, respectively. The pump beam radius is assumed to be 30μm. As the theory predicts, at each modulation frequency, the MFCA amplitude decreases and the phase lag increases as the two-beam separation increases, following the trend of the carrier distribution. In principle, the dependence can be used to determine simultaneously the electronic transport properties of the semiconductor wafer via fitting the experimental data to the theoretical model by minimizing a mean square variance defined as
Here $A_T(f_j, r_i)$, $\phi_T(f_j, r_i)$ and $A_E(f_j, r_i)$, $\phi_E(f_j, r_i)$ are the theoretical and experimental amplitude and phase at modulation frequency $f_j$ and two-beam separation $r_i$, respectively. $N_j$ is the total number of data points at modulation frequency $f_j$ and $m$ is the number of different modulation frequencies covering an appropriate range. Normally, three transport parameters, i.e., the carrier lifetime, the carrier diffusivity and FSRV are simultaneously determined by multi-parameter fitting. The RSRV is fixed to a typical value during the fitting procedure.

Figure 3. Simulated sensitivities of the square variance to the transport parameters for (a) combined MFCA and PCR data, and (b) MFCA data measured at 3 two-beam separations of 30, 60, 90\(\mu\)m.

The uniqueness and uncertainty range of the multi-parameter fitted results are determined by the sensitivities of the square variance to individual transport parameter. The sensitivities can be investigated by calculating the dependence of the square variance on each transport parameter. In the calculations, the simulated MFCA or PCR data are fitted by changing one transport parameter and keeping the other two as free parameters to minimize the square variance in a multi-parameter fitting procedure. Figure 3 shows the variance versus the deviations of the transport parameters for fitting the frequency dependence of (a) combined MFCA and PCR signals and (b) MFCA signals measured at 3 two-beam separations. In (a), both MFCA and PCR signals are measured at the excitation spot. The MFCA signals are detected with a probe beam with 25\(\mu\)m-diameter and the PCR signals are detected with a detector with 1mm-diameter, while the pump beam radius is assumed to be 15\(\mu\)m. In (b), the pump beam radius is assumed to be 30\(\mu\)m and the frequency dependence are measured with two-beam separation of 30, 60, and 90\(\mu\)m, respectively. If we assume the acceptable variance levels are $1 \times 10^{-4}$ and $2 \times 10^{-4}$, respectively, taking into consideration the fact that the signal amplitude decreases with increasing two-beam separation, the uncertainty ranges are $D$: $\pm 7.9\%$, $r$: $\pm 6.2\%$, and $S_1$: $\pm 11.9\%$ for case (a) and $D$: $\pm 2.9\%$, $r$: $\pm 25.3\%$, and $S_1$: $\pm 42.7\%$ for case (b), respectively. These uncertainty ranges are significantly better than that obtained with a single frequency scan in conventional photo-carrier techniques, which normally are in the ranges of $\pm 30\%$ for $D$ and $r$ and over $\pm 50\%$ for $S_1$, respectively. In addition, the accurate determination of the carrier diffusivity could significantly improve the uncertainty ranges of the lifetime and FSRV, which are sensitive to the error of the diffusivity value due to the inter-correlations among the three transport parameters in the conventional photo-carrier techniques.
3. Experimental results and discussions

A MFCA experiment was performed to extract simultaneously the electronic transport properties of a silicon wafer. The experimental arrangement is schematically shown in Fig. 4, which is a combined setup for simultaneous MFCA and PCR measurements. Briefly, free carriers are generated within a Si wafer by an intensity-modulated laser beam (830nm). The photo-generated free carriers are detected by measuring the intensity modulation of the transmitted beam of a continuous-wave probe laser beam (1570nm) with an InGaAs detector in MFCA, as well as by collecting and detecting the infrared photo-carrier emissions with a pair of paraboloidal mirrors and another InGaAs detector in PCR. A function generator is used to control the modulation frequency of the excitation beam for frequency scans and a motorized translation stage is employed to move the focused excitation spot on the surface of the wafer for position scans. The sample used in the experiment is a (100)-oriented n-type silicon wafer, with 7-10 $\Omega$ cm resistivity and 525 $\mu$m thickness.

Figure 4. Experimental arrangement for combined MFCA and PCR measurements.

Figure 5. Experimental frequency dependence of MFCA amplitude (a) and phase (b) measured at 11 two-beam separations of 0 to 100 $\mu$m, with a step of 10 $\mu$m.

To extract simultaneously the transport properties, the MFCA and/or PCR signals should be recorded relating to the three-dimensional photo-carrier distributions, as mentioned in section 2. As an example, Fig. 5 shows the modulation frequency dependence of MFCA amplitude and phase measured at 11 two-beam separations of 0 to 100 $\mu$m, with a step of 10 $\mu$m. These frequency dependence are used to determine simultaneously the three transport parameters, $D$, $\tau$, $S_l$ via multi-parameter fitting. At first, the frequency dependence at each two-beam separation are used to determined $D$, $\tau$, and $S_l$ independently, as does in conventional photo-carrier techniques. The determined $D$ and $\tau$ values
change in a wide range, from 7.1 to 18.2 cm$^2$/s for $D$ and 15.3 to 26.1$\mu$s for $\tau$, respectively. The statistical results are 12.6$\pm$3.2 cm$^2$/s and 20.9$\pm$3.7$\mu$s. To improve the determination accuracy of the carrier diffusivity and lifetime, the frequency dependence of the MFCA amplitude and phase measured at 4 two-beam separations of 10, 30, 60, and 90$\mu$m are used simultaneously to determine $D$, $\tau$, and $S_1$. The experimental frequency dependence and the corresponding theoretical best-fits are presented in Fig. 6. Obviously, good agreements in both MFCA amplitude and phase are obtained. The best-fit results are $D = 14.6$ cm$^2$/s, $\tau = 18.5\mu$s and $S_1 = 29000$ cm/s, with a square variance of 3.17$\times$10$^{-3}$. A careful investigation on the uncertainty of the fitted values shows a much better determination accuracy for the carrier diffusivity and a more reliable value for carrier lifetime.

Figure 6. Experimental frequency dependence (symbols) and corresponding theoretical best-fits (lines) of MFCA amplitude (a) and phase (b) measured at 4 two-beam separations of 10, 30, 60, and 90$\mu$m, respectively.

4. Conclusions
Theoretical simulations and experimental results have shown that the laterally resolved photo-carrier techniques together with multi-parameter fitting are capable of determining simultaneously the multiple transport parameters of semiconductor wafers with a high accuracy, as compared to the conventional photo-carrier techniques. The determination accuracy could be further improved by increasing the signal-to-noise ratios of the experimental photo-carrier signals.

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