

Spectroscopic photothermal radiometry as a deep subsurface depth profilometric technique in semiconductors

D. Shaughnessy and A. Mandelis^{a)}

Photothermal and Optoelectronic Diagnostics Laboratories, Department of Mechanical and Industrial Engineering, University of Toronto, Toronto, Ontario M5S 3G8, Canada

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The theoretical and experimental aspects of spectroscopic photothermal radiometry (PTR) of semiconductors are presented and the potential of the technique for depth profilometry is established. A three-dimensional model of the PTR signal from a semiconductor excited by light of arbitrary optical penetration depth is presented. Numerical simulations of the PTR response to the electronic transport parameters and the optical penetration depth of the excitation source are presented. Intensity-modulated frequency scans and two-dimensional surface scans at fixed frequencies have been performed at several different absorption depths on a Si wafer with various degrees of mechanical damage introduced to either the front or the back surface. The electronic transport parameters obtained from fitting the frequency scans to the theoretical model and analysis of the experimental curves show that while the surface recombination velocities extracted from the fits do not vary significantly with excitation wavelength, the carrier recombination lifetime and the overall sensitivity of the photothermal radiometric signal to spatially localized damage is strongly influenced by the proximity of the injected excess carrier density centroid to the defect location. This correlation between the sensitivity of the PTR signal to a localized defect and the proximity of the injected carriers to the defect demonstrates the potential for spectroscopic PTR as a depth profilometric technique for semiconductors. © 2003 American Institute of Physics.
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I. INTRODUCTION

The correlation between carrier recombination lifetime and defect/impurity concentration in silicon has led to lifetime being used as a general measure of quality in the semiconductor industry. The numerous techniques that have been developed to monitor lifetime record the average recombination lifetime of the excited carriers. The high defect density near the surface generally results in a higher recombination rate at the surface compared to the bulk of the sample and has led to the use of the following expression to describe the measured effective lifetime:¹

$$\tau_{\text{eff}}^{-1} = \tau_{\text{bulk}}^{-1} + \tau_{\text{surface}}^{-1}. \quad (1)$$

In order to account for the spatial distribution of injected carriers it would be more accurate to introduce weighting factors to each mechanism. Exciting carriers well within the bulk of the material should decrease the influence of the surface recombination on the measured recombination lifetime and allow values more representative of the bulk lifetime to be obtained. Similarly, a strongly absorbed excitation source should produce a measured lifetime that is more strongly affected by surface conditions.

The aim of this study is to investigate the dependence of the sensitivity of the photothermal radiometric signal to spatially localized defects on the absorption coefficient of the

exciting radiation, and thus determine the potential for the application of spectroscopic photothermal radiometry (PTR) to depth profilometry of semiconductors.

II. THEORETICAL MODEL

The theoretical aspects for three-dimensional infrared PTR for a strongly absorbed incident radiation have been established previously² and are extended in this article to account for an arbitrary absorption coefficient $\beta(\lambda)$. The model is presented briefly in this article with a detailed description left for a future article.³

The transport of thermal energy and electronic carriers in an electronic material excited by a modulated source can be described by the temporal Fourier transforms of the heat conduction and Boltzmann transport equation, respectively. These coupled diffusion equations with the appropriate boundary conditions can be solved in Hankel space to determine the complete PTR signal. Assuming a Gaussian shaped excitation source and an isotropic material, despite the crystallographic structure of silicon, the solution can be integrated over the depth of the wafer, L , to yield the Hankel transform of the carrier-density-wave field, $N(r; \omega)$:

$$\tilde{N}(q; \omega) = E(q) \left(\frac{(1 - e^{-\xi_e L})}{\xi_e} [C_1(q) + C_2(q) e^{-\xi_e L}] - \frac{(1 - e^{-\beta L})}{\beta} \right), \quad (2)$$

^{a)}Electronic mail: mandelis@mie.utoronto.ca

where $\xi_e^2 = q^2 + (1 + i\omega\tau)/D\tau$, q is the variable in Hankel space resulting from the transformation, and the coefficients $E(q)$, $C_1(q)$, and $C_2(q)$ are functions of the absorption coefficient, β , the incident power, P , the reflectivity, R , the light frequency, ν , the beam radius, w , the carrier recombination lifetime, τ , the carrier diffusivity, D , and the front and back surface recombination velocities, S_1 and S_2 .

Similarly, the Hankel transform of the thermal-wave field, $T(r; \omega)$, is found to have the form:

$$\begin{aligned} \bar{T}(q; \omega) = & B_1 \frac{(1 - e^{-\xi_t L})}{\xi_t} - B_2 \frac{(1 - e^{\xi_t L})}{\xi_t} \\ & + B_3 \frac{(1 - e^{-\xi_e L})}{\xi_e} + B_4 \frac{(1 - e^{-\xi_e L})}{\xi_e} e^{-\xi_e L} \\ & + B_5 \frac{(1 - e^{-\beta L})}{\beta}, \end{aligned} \quad (3)$$

where $\xi_t^2 = q^2 + i\omega/\alpha$ and the coefficients B_1 through B_5 are functions of the thermal diffusivity, α , the thermal conductivity, k , the band-gap energy E_g as well as the parameters present in the electronic coefficients. The complete PTR signal is found by taking the inverse Hankel transform of the above expressions and integrating over the effective detector area.

III. NUMERICAL SIMULATIONS

The theoretical model has been used to simulate the PTR signal over a range of frequencies suitable for the characterization of silicon (10 Hz–100 kHz) and for absorption depths of 0.68, 4.9, 10.7, and 33.4 μm , which correspond to excitation wavelengths of 514, 710, 810, and 950 nm, respectively. A sample thickness of 675 μm and a beam radius of 80 μm were used for all simulations and, unless otherwise noted, the transport parameters were taken as: $\tau = 1$ ms; $D = 25$ cm^2/s ; $S_1 = 300$ cm/s ; $S_2 = 600$ cm/s ; $C_p = 1 \times 10^{-20}$ a.u.; and $C_t = 150$ a.u. The ability of PTR to uniquely determine the transport parameters has been previously established⁴ and will not be discussed in this article. The purpose of the simulations presented in this article are to investigate the expected sensitivity of the PTR signal to each of the carrier transport parameters as the optical penetration depth of the exciting radiation is increased.

Simulations over a range of lifetimes from 10 μs to 10 ms show that there is no significant spectral dependence on the influence of lifetime on the PTR response. Neither the saturated amplitude at low frequencies (such that $\omega\tau < 1$) nor the position of the characteristic bend at $\omega\tau \sim 1$ is affected by a change in the optical penetration depth.

The influence of the carrier diffusivity on the PTR response is, however, affected by the optical absorption depth. While there is no spectral dependence of the PTR amplitude at high diffusivities, wavelengths with longer absorption depths exhibit higher amplitudes at lower diffusivities. Although decreasing diffusivity lowers the number of carriers leaving the field of view of the detector generally leads to an increase in the PTR amplitude, enhanced surface recombination resulting from lower diffusion away from the surface has the opposite effect and tends to decrease the PTR ampli-

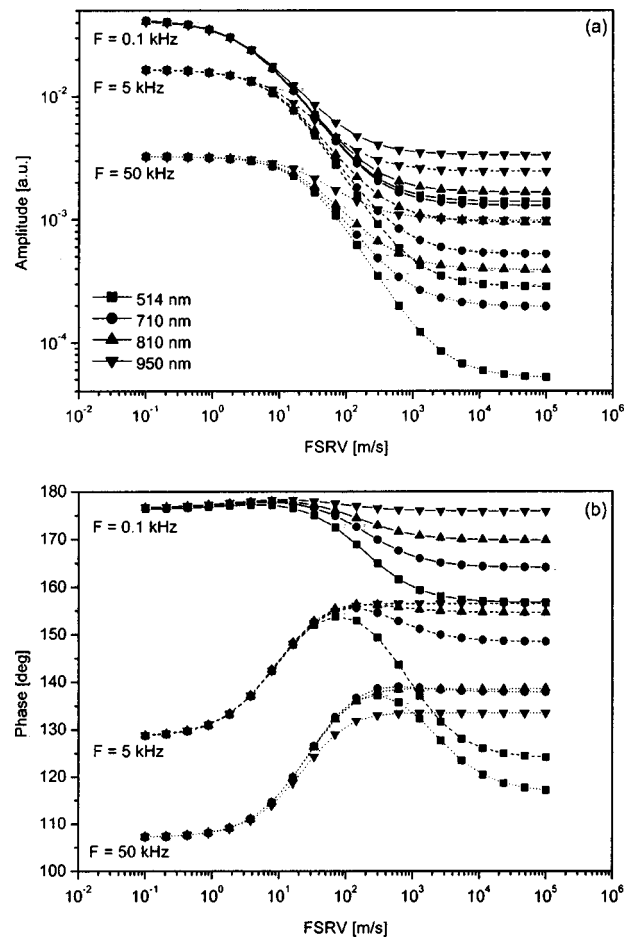


FIG. 1. Numerical simulations of the PTR amplitude (a) and phase (b) at 0.1, 5, and 50 kHz as a function of front surface recombination velocity for excitation wavelengths of 514, 710, 810, and 950 nm.

tude. The wavelengths with shorter absorption depths are more strongly affected by this enhanced surface recombination leading to a divergence of the PTR amplitude curves from the various absorption depths as the diffusivity decreases. The separation in the PTR phase is relatively slight compared to that of the amplitude.

The front surface recombination velocity (FSRV) affects the amplitude and phase of the PTR signal across the entire frequency range of interest (Fig. 1) and the variation of the signal with increasing FSRV is strongly dependent on the absorption depth of the excitation source. Lower carrier densities due to higher FSRVs result in lower amplitudes at all frequencies and the decrease in amplitude is clearly much greater for shorter optical absorption depths. The PTR phase at very low FSRV is dominated by the electronic signal and has essentially no spectral dependence. As the FSRV increases the phase lag decreases as near-surface carrier recombination increases and shifts the carrier centroid nearer to the surface. While the phase saturates for the longer wavelengths, the lag of the more strongly absorbed wavelengths then begins to increase due to the increasing prevalence of the thermal contribution from the surface recombination. The PTR signal is clearly expected to become less sensitive to the quality of the front surface as the absorption depth increases.

Although the results of the FSRV simulations would sug-

gest that changes in the back surface recombination velocity (BSRV) would have a stronger affect when using deeper penetrating wavelengths, the increase in the absorption depth for the chosen wavelengths is relatively small compared to the thickness of the wafer, and the PTR signal sensitivity to the BSRV exhibited no spectral dependence.

IV. EXPERIMENTAL RESULTS

The experimental setup for PTR measurements has already been reported.⁵ In order to perform spectroscopic measurements, the excitation source must be a tunable laser (e.g., an Ar⁺ pumped TiSa laser) capable of producing wavelengths that range from strong surface absorption to deep bulk penetration in Si. The IR emissions from the sample are focused onto a liquid nitrogen cooled HgCdTe detector and the signal is demodulated using a lock-in amplifier.

The sample used for this investigation was a thermally oxidized, boron doped *p*-type Si wafer with a resistivity of 20 Ω cm ≤ ρ ≤ 40 Ω cm, a thickness of 675 μm, and one polished surface. Mechanical damage (5 mm × 5 mm) of different severity was introduced in two spatially distinct regions, referred to as the high-level damage and low-level damage regions, on the bare surface using silicon carbide paper (No. 800).

Surface maps (15 mm × 15 mm) were performed over both damaged regions at several frequencies for each of the wavelengths mentioned in Sec. III. Frequency scans and two-dimensional transverse scans were performed at each wavelength using excitation/detection from the polished surface and from the bare/damaged surface in order to separately investigate the effect of defects near the front surface and the back surface.

Fits of the frequency scans with excitation/detection on the polished surface show that the introduction of mechanical damage on the back surface affects not only the BSRV but also the lifetime and that the effect on the lifetime is more pronounced at the larger optical absorption depths. The PTR monitored lifetime on the intact wafer is ~ 1 ms at each wavelength considered. Introduction of the low-level damage affected only the lifetime from the 950 nm scan, which was reduced to 0.4 ms. Introduction of high-level damage significantly decreased the lifetime at all four wavelengths, from 500 μs for 514 nm excitation to 150 μs for 950 nm excitation, and again shows a correlation between penetration depth and the influence of the deep subsurface defect on the lifetime. Whether the defects are considered as surface defects, which is not supported by the simulations that show no spectral dependence on the BSRV for the wavelength range of interest, or the defects are severe enough to be considered as bulk defects, it is clear that the measured lifetime is dependent on the vicinity of the injected carrier centroid to the defect location and can indeed be represented by a weighted function similar to Eq. (1).

The frequency scans on the region with low-level front surface damage also show trends based on the excitation wavelength (Fig. 2.) The PTR signals resulting from the shorter wavelengths exhibit an essentially thermal response as manifested by the strong slope throughout the low fre-

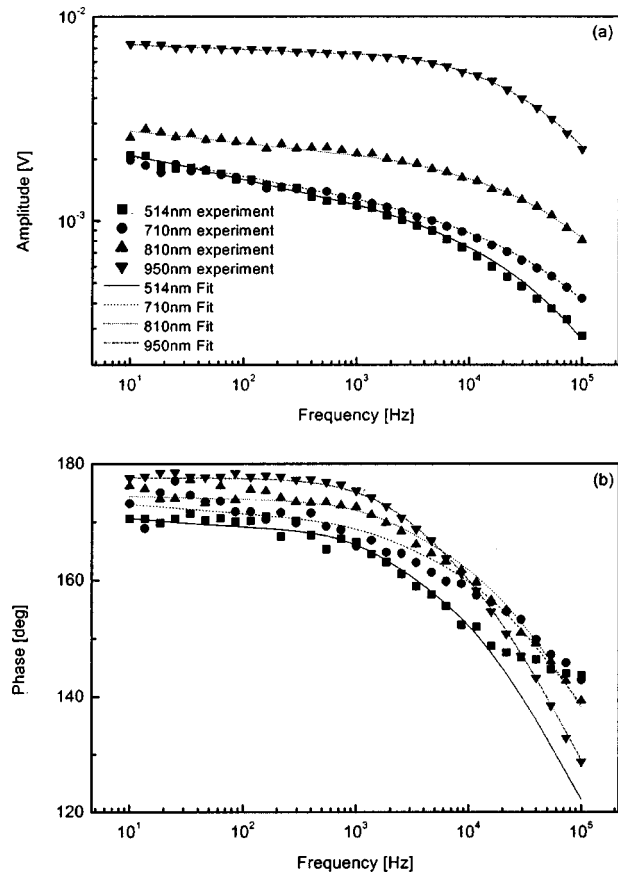


FIG. 2. PTR amplitude (a) and phase (b) of experimental frequency scans and theoretical fits with excitation incident on low-level damaged surface.

quency range. As the optical penetration depth increases the slope begins to decrease and the amplitude “knee” at $\omega\tau \sim 1$ characteristic of the PTR signal from an electronic material becomes more prevalent. Fitting results are not presented for these frequency scans because the tail at high frequencies of the more strongly absorbed wavelengths, which is most likely a result of the high degree of damage to the crystallographic structure near the surface, prevents the experimental curves from being fit to the present theory. This

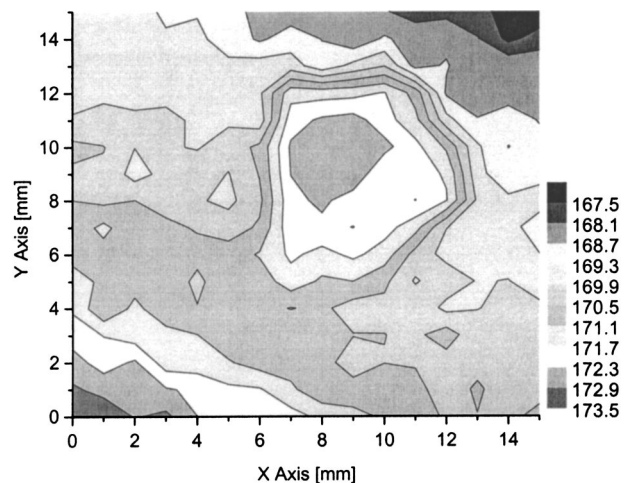


FIG. 3. Surface map of region containing 5 mm × 5 mm high-level damage on back surface at 1 kHz modulation frequency using 810 nm excitation.

strong evidence of the correlation between the location of a defect to the centroid of the injected carrier density and the defect's influence on the PTR signal suggests that lifetimes more representative of the true bulk lifetime can be obtained by utilizing a deep penetrating excitation source.

The results of the two-dimensional surface maps of the defects on the back surface are consistent with the simulations; only the intermediate frequencies are able to image the defect when using the PTR phase (Fig. 3). A change in phase at intermediate frequencies with no change at high and low frequencies is a characteristic unique to the back surface recombination velocity and the results demonstrate the ability of PTR to map BSRV by looking for phase variations in only the midfrequency range while scanning the sample.

These results suggest that continuous spectroscopic measurements or a combination of two-dimensional transverse

maps at the appropriate frequencies along with frequency scans at the appropriate wavelengths can potentially be used to develop depth profiles over the entire wafer that could be used to characterize the material in all three dimensions, identify the location of subsurface defects and impurities, and monitor the thickness of doping layers.

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