

Numerical Simulations of Transient Photoconductance Decay

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ABSTRACT

Transient photoconductance decay (PCD) in ingots or wafers has been numerically simulated by a finite-element method (FEM). We examined two types of light sources for carrier injection in transient PCD measurements. Large discrepancies between the widely used asymptotic approximation and the FEM simulations of wafers were seen, and an empirical fitting of the FEM results suggests that the effect of surface recombination velocity on wafer lifetime may be much smaller, although the diffusion-limited surface lifetime remains the same. A single-exponential decay representing overall quality of a multicrystalline wafer is obtained even though the wafer comprises of grains with different lifetimes. If the grain sizes are much smaller than the carrier diffusion length, and if no surface or grain boundary recombination is present, then the inverse effective lifetime is found to be the volume-weighted sum of the inverse local lifetimes.

INTRODUCTION

Minority-carrier lifetime measurement by transient photoconductance decay [1] is one of the most extensively used characterization techniques for silicon photovoltaic (PV) materials. Unfortunately, to separate the effects of surface recombination from the bulk recombination property, one has to rely on the analytic solution based on the "virtual" one-dimensional treatment, uniform carrier-injection condition, and uniform minority-carrier lifetime [2].

The variety of Si PV materials requires that we have a quantitative understanding of the implications when such limitations are violated, especially on uniformity of excess carrier generation and material properties. With such knowledge, we may still be able to obtain the actual bulk lifetime in certain specimens or an effective lifetime reflecting the overall quality of a multicrystalline material. In our previous work [3], we have shown that the requirement of uniform carrier injection may be somewhat relaxed for lifetime measurements on ingots that have very high surface recombination (so that only the diffusion-limited surface term is needed for bulk-lifetime correction). For PCD measurements on wafers that have intermediate surface recombination velocities (10^2 - 10^4 cm/s), however, we found that the FEM lifetimes do not agree with the commonly employed formula [4] to account for the surface contribution. This paper extends the previous

work, including simulations of dynamic carrier distribution in ingots, single- and multicrystalline wafers, and examines the effect of light pulse on carrier injection and PCD signals.

MODELING

Two kinds of light sources are generally used in transient PCD measurements, with different implications on carrier generation. One is the δ -function type (such as a fast strobe light, or a Q-switched laser), in which the light duration is much shorter than the bulk lifetime, $\tau_p \ll \tau_b$. And the other is the step η -function type (such as a Quasi-cw diode-laser array driven by a square-wave current source), in which the illumination period is comparable or longer than the bulk lifetime, $\tau_p \approx \tau_b$. These light sources will be represented by a δ -function and a η -function in the generation term, G , in the carrier continuity equation. An absorption coefficient of 80 cm^{-1} is assumed for all simulations.

Electrons are assumed to be the minority carriers with diffusivity, D , of $30 \text{ cm}^2/\text{s}$. The bulk lifetime, $t_b(x,y)$, may have spatial variations as necessary. The two-dimensional continuity equation, is then numerically solved by a finite element method in

$$\frac{\partial \Delta n(x, y, t)}{\partial t} = \nabla \cdot \{D \cdot \text{grad} [\Delta n(x, y, t)]\} - \frac{\Delta n(x, y, t)}{t_b(x, y)} + G(x, y, t), \quad (1)$$

PDEase[®] [5] for dynamic distribution of excess electrons with fixed surface-recombination velocities S [3]. To find the PCD signal, the excess carrier concentration, Δn , was integrated over the cross-section (assuming the detection current is perpendicular to the cross-section) and plotted as a function of time to represent the photoconductance decay.

LIGHT SOURCE: δ - vs. η -FUNCTION

The main consequence of the two different light sources is that carrier distributions at the start of decay would be quite different, as seen in Fig.1 for carrier injection from the side of a round ingot (half of the ingot cross-section shown). The δ -source produces an exact profile of carrier distribution as the light absorption, whereas the η -source generates a deeper profile owing to the diffusion process (eventually balanced by the recombination process). As a result, the η -source can

sense deeper portions of the sample. If the material is uniform, both light sources will detect a similar effective lifetime after an initial fast decay in the case of a δ -light source as the carrier distribution eventually evens out in the sample (Fig.2).

SINGLE-CRYSTAL WAFERS

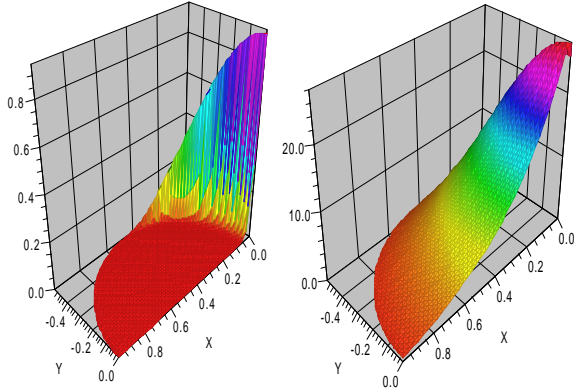


Fig.1 Left: Δn after a δ -light source is turned off; Right: Δn after an η -light source is turned off.

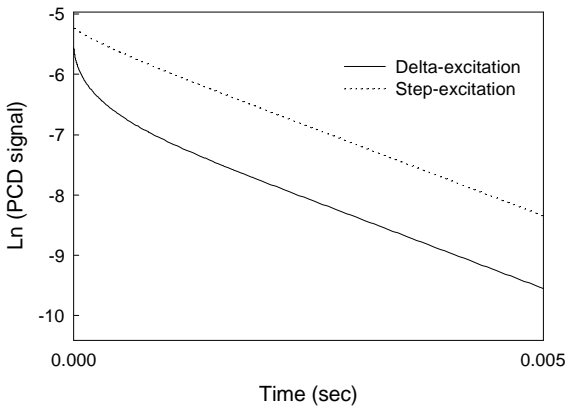


Fig.2 PCD decay curves from a δ -light source and an η -light source.

Monitoring lifetime on processed wafers is a very important application of PCD. For wafers with partially passivated surfaces, it is customary to use the asymptotic approximation [2,3] to separate the surface effects from τ_b ,

$$\frac{1}{t} = \frac{1}{t_b} + \left(\frac{d}{2S} + \frac{d^2}{p^2 D} \right)^{-1}, \quad (2)$$

where d is the wafer thickness. The two terms within the brackets are the surface recombination and diffusion-limited sub-surface contribution, respectively, assuming a uniform carrier injection in the entire wafer. However, the simulation results in Fig. 3, for intermediate S between 10^2 and 10^5 cm/s and thin wafers (<0.1 cm), do not agree with equation (2).

After an extensive fitting search, an excellent empirical formula was obtained (see Fig. 4) as,

$$\frac{1}{t} = \frac{1}{t_b} + \left(a \frac{d}{2S} + \frac{d^2}{p^2 D} \right)^{-1}, \quad (3)$$

where the fitting parameter $a \approx 29$ for the given bulk lifetime $\tau_b = 10^{-4}$ s.

In other words, the simulation suggests that

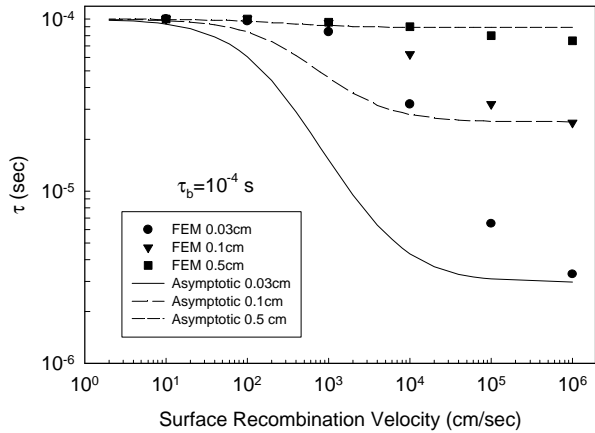


Fig.3 Simulated lifetime (dots) vs. Eq.(2) (curves) as a function of surface recombination velocity and wafer thickness.

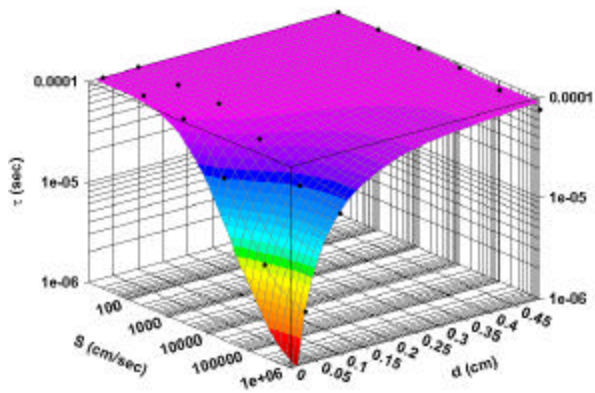


Fig.4 Best fit of lifetime data vs. surface recombination velocity and wafer thickness.

when doing PCD measurements on wafers, one is only seeing the effect of a small fraction of the actual surface recombination velocity. The diffusion-limited term remains valid. This means that if one tries to derive surface recombination velocity from the PCD lifetime measurement, the S value could be well underestimated.

The reason for such a big discrepancy between the asymptotic approximation [3] and the FEM simulation is unclear. A comparative simulation between uniform and non-uniform injection conditions indicates a slightly higher lifetime for the non-uniform injection case due to diffusion limiting the front-surface recombination activity, but it is not nearly enough to account for the difference.

MULTICRYSTALLINE WAFERS

Two common misconceptions about lifetime measurements on non-uniform materials (e.g., multicrystalline wafers) pervade. One is that the measured effective lifetime is the inverse of the inverse sum of lifetimes of different regions (e.g., [6]), borrowed from the concept of different recombination mechanisms at the same physical location,

$$\frac{1}{\bar{t}} = \sum \frac{1}{t_i}, \quad (4)$$

which means the lowest lifetime will dominate the effective lifetime. Another is that a single-valued effective lifetime is non-existent.

Simulation provides a way to examine the misconceptions. Fig. 5 is a simplified cross-section of a model multicrystalline wafer with three grains having bulk lifetimes of 100, 35, and 200 μs , and volume fractions of 1/6, 1/2, and 1/3, respectively. The two grain boundaries are assumed to have a recombination velocity of $S_b = 1,000 \text{ cm/s}$. All the free surfaces have a recombination velocity of $S = 10,000 \text{ cm/s}$. The wafer is 10 mm x 0.5 mm in cross-section.

Fig. 6 depicts the distribution of carriers at the turn-off of an η -light source and at 40 μs after that. It is seen that higher concentrations of carriers generated in the higher-lifetime grains diffuse to the lower-lifetime grain in the middle, as well as being drawn to the surfaces and grain boundaries. The PCD signal shown in Fig. 7 as the dotted line displays a single-exponential decay, and an effective lifetime of 51 μs is obtained. Of course, if a δ -light source were used, the initial decay would be faster and a similar effective lifetime may be attained after a few initial decades of decay.

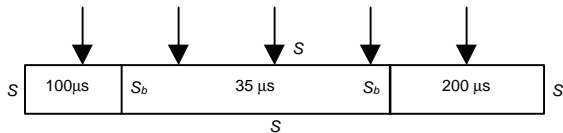


Fig.5 A model multicrystalline wafer.

Now let us assume that all the surfaces and grain boundaries are perfectly passivated, and the carrier diffusivity is infinitely large (which is equivalent to grain sizes \ll diffusion length). The solid curve in Fig. 7 is the corresponding PCD signal. An average (among the different grains) lifetime of 60 μs is observed. That is just the inverse of the volume-weighted sum of inverse local lifetimes. This effective lifetime represents overall quality

$$\frac{1}{\bar{t}} = \sum_i \frac{v_i}{t_i}, \quad (5)$$

of the entire wafer,

where v_i is the ratio of the volume having a lifetime of t_i ,

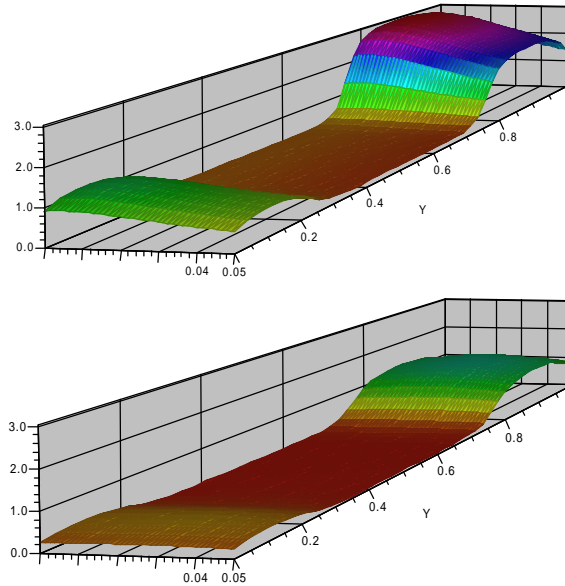


Fig.6 Top: Initial carrier distribution after η -light is off. Bottom: At $t = 40 \mu\text{s}$ after decay.

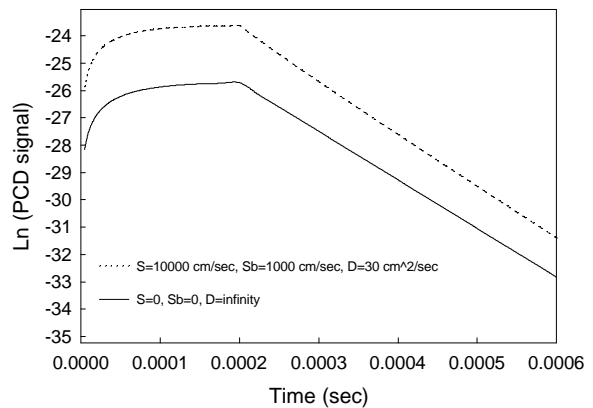


Fig. 7 PCD signals of the multicrystalline wafer shown in Fig.5, using an η -light source.

whereas the value given by Eq.(4) would be only 23 μs .

The physical explanation is that although the low-lifetime regions act as carrier sinks, the carriers have to move fast, and the low- τ regions must have enough capacity to make all of the grains seem to be in the same physical location.

CONCLUSIONS

We have examined two types of light sources for carrier injection in transient PCD measurements. The η -type is better for sensing the interior of a sample because of the diffusion-enhanced profile of excess carriers. The δ -type produces an initial fast decay due to pronounced surface contribution, but will yield similar lifetime values to those from an η -type source in a later part of the decay.

Large discrepancies between the uniform-injection, one-dimensional asymptotic approximation and the FEM simulations for thin wafers (<0.1 cm) and intermediate surface-recombination velocities (between 10^2 - 10^5 cm/s) could not be explained by non-uniform carrier distribution alone. An empirical fitting suggests that if the asymptotic formula, Eq. (2), is to be used to derive the surface recombination velocity, the S value could be well underestimated.

A single-exponential decay representing overall quality of a multicrystalline wafer is obtained even though the wafer comprises grains with different lifetimes. When grain sizes are much less than the effective carrier diffusion length, carrier distribution remains uniform, and no surface or grain boundary recombination is present, the inverse effective lifetime of a multicrystalline wafer is found to be the volume-weighted sum of inverse local lifetimes.

ACKNOWLEDGEMENTS

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