Influence of photon reabsorption on temperature dependent quasi-steady-state photoluminescence lifetime measurements on crystalline silicon

Marc Rüdiger,[1,a] Thorsten Trupke,[2] Peter Würfel,[3] Thomas Roth,[1] and Stefan W. Glunz[1]

[1]*Fraunhofer Institute for Solar Energy Systems (ISE), Heidenhofstraße 2, 79110 Freiburg, Germany*
[2]*University of New South Wales, Sydney, 2052, New South Wales, Australia*
[3]*Institut für Angewandte Physik, Universität Karlsruhe, 76131 Karlsruhe, Germany*

Due to their robustness against various experimental artifacts and the high sensitivity at low minority carrier concentrations, quasi-steady-state photoluminescence lifetime measurements are well suited to provide the experimental data required for advanced defect spectroscopy methods. However, for a correct evaluation, photon reabsorption has to be considered. In this work it is evaluated quantitatively, to what extent and in which temperature range photon reabsorption in silicon wafers is significant. A method to correct the effect of photon reabsorption within silicon wafers on temperature dependent quasi-steady-state photoluminescence lifetime measurements is presented. © *2008 American Institute of Physics*. [DOI: 10.1063/1.2939586]

Quasi-steady-state photoluminescence (QSSPL) measurements[1] are used to determine the injection dependent effective minority carrier lifetime $\tau_{eff}(\Delta n)$ in silicon samples. Due to the method, these measurements are largely unaffected by experimental artifacts such as minority carrier trapping[2] or depletion region modulation,[3] as it can be found in photoconductance measurements.[4] The influence of photon reabsorption on QSSPL measurements at room temperature (300 K) can be neglected in many practical cases.[5] However, at elevated temperatures, the absorption coefficient increases, resulting in a larger influence of photon reabsorption and potentially leading to significant experimental errors. In order to get reliable data for the measured injection level dependent effective lifetime in silicon samples at various temperatures and to accurately fit defect parameters in advanced lifetime spectroscopy methods,[6] photon reabsorption must be accounted for quantitatively. In this work, photon reabsorption in the temperature range from 77 up to 600 K is theoretically analyzed.

To quantify the influence of photon reabsorption, the generalized Planck equation for the rate of spontaneous emission $dr_{emi,sp}(\lambda)$ per wavelength interval $d\lambda$ and volume element via indirect transitions[7] is used,

$$dr_{emi,sp}(\lambda) = \frac{C(\lambda)}{\lambda^4}\alpha_{BB}(\lambda,T)\exp\left(\frac{-hc}{\lambda kT}\right)\exp\left(\frac{\Delta\eta}{kT}\right)d\lambda \ ,$$

$$(1)$$

where $\alpha_{BB}(\lambda,T)$ is the absorption coefficient for band-to-band transitions and $\Delta\eta(z)$ describes the separation of the quasi-Fermi energies, which is set to zero in the following calculations. λ is the photon wavelength, hc/λ is the photon energy, k is Boltzmann's constant, and T is the sample temperature. C contains physical constants, and is set for simplicity to $C=1$ for all calculations presented here since only relative intensities are calculated.

For planar wafers, reabsorption effects can be taken into account by multiplying Eq. (1) by an exponential absorption term $\Theta_p = \exp(-\alpha z)$. z is the optical path length between the volume element in which spontaneous emission occurs and the surface from which the emission is detected. In many practical cases parasitic absorption processes such as free carrier absorption can be neglected and the total absorption coefficient α in the above reabsorption term can be replaced by the absorption coefficient for band-band transitions α_{BB}.

For a theoretical description of reabsorption effects in textured wafers, we assume Lambertian surfaces. To describe the spontaneous emission of such a wafer taking multiple total internal reflections at the surface into account, Eq. (1) has to be multiplied by

$$\Theta_t = [1 + (1 - 1/n^2)]\exp[-4\alpha(d-z)]$$

$$\times\exp(-2\alpha z)\sum_{i=0}^{\infty}(1-1/n^2)^{2i}\exp(-4i\alpha d),\qquad(2)$$

with d as the thickness of the wafer and $n=3.6$ as the refractive index of crystalline silicon.

The detected photon flux j_{det} is calculated by integrating Eq. (1) multiplied by $\Theta_{p,t}$ for planar or textured wafers, respectively, over the spectral wavelength range in which significant spontaneous emission occurs and over the thickness d of the wafer,

$$j_{det} = \int_0^\infty\int_0^d 1/n^2 \times dr_{emi,sp}(\lambda)\Theta_{p,t}\Phi_{det}d\lambda dz \ .\qquad(3)$$

In order to identify the significance of reabsorption for specific QSSPL experiments the spectral sensitivity of the detection system must be taken into account. In recent work on QSSPL, Si *pin* detectors or Si charge-coupled device cameras were used. In that case the effect of reabsorption becomes even more relevant due to the sensors sensitivity being limited to shorter wavelengths, which are most strongly affected by reabsorption. In QSSPL lifetime measurements an additional 1000 nm Schott Glass RG 1000 long pass (LP) filter was used to block any residual excitation light that was transmitted by the sample.

The spectral sensitivity of the detection system is accounted for in Eq. (3) by Φ_{det}. The spectral rate of spontaneous emission in Eq. (1) is determined by $\alpha_{BB}(\lambda,T)$ for a given separation of the quasi-Fermi levels. Reliable data for
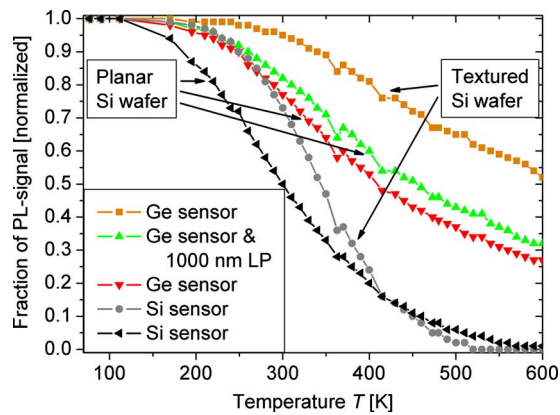
a)Electronic mail: marc.ruediger@ise.fraunhofer.de.

FIG. 1. (Color online) Fraction of photons spontaneously emitted by a planar or textured Si wafer, respectively, that are detected with and without being reabsorbed on an optical path $z=300$ μm. Calculations are shown for the total photon flux that would be measured with a Ge sensor and for the photon flux detected by a Si *pin* diode. The influence of a 1000 nm LP filter located between the sample and the sensor is also shown. Each curve is normalized to the corresponding photon flux that would be measured without reabsorption of photons.

FIG. 2. (Color online) Temperature dependent emitted photon flux versus effective bulk lifetime τ_{eff} of a planar 300 μm thick Si wafer. Realistic excess carrier distributions (by illumination from the front side) were taken into account, while the emitted photon flux was detected at the back side by using a Si *pin* sensor and a 1000 nm long pass filter. The detected signal is normalized to a detection under the same circumstances without reabsorption effect.

the temperature dependent absorption coefficient are thus required for a quantitative analysis of temperature dependent reabsorption effects. For wavelengths $\lambda \leqslant 1050$ nm ($hc/\lambda \geqslant 1.079$ eV), a theoretical model[8] for the absorption coefficient gives good agreement with experimental data over a wide temperature range. However, since the model only includes one-phonon processes for optical band-to-band transitions, the theory does not fit to the experimental data at longer wavelengths ($\lambda > 1050$ nm) where α is determined by multiphonon processes and where the spontaneous emission is still significant. Experimental data for the absorption coefficient were therefore used, where available. At temperatures $T=77$, 112, 170, 195, and 249 K absorption coefficient data determined from photoluminescence measurements were used.[9] For 195 and 249 K these data were extended for wavelength <990 nm by theory.[8] At room temperature the absorption coefficient data published by Keevers and Green[10] were used. For the calculations at elevated temperatures $T=363$, 415 and 473 K experimental data measured by Weakliem and Redfield[11] were used. In the spectral range $\lambda > 1200$ nm where no experimental data were available the room temperature data from Keevers and Green were extended to other temperatures by an extrapolation formula,[12]

$$\alpha_{\mathrm{ext}}(T) = \alpha_0(T_0)(T/T_0)^{T_0 c_\alpha(\lambda)}. \tag{4}$$

This relationship extrapolates the absorption coefficient α_{ext} from experimental absorption coefficient data[10] α_0 at temperature $T_0=300$ K to other temperatures and agrees well with experimental data in the temperature range of 200–500 K. In Eq. (4) $c_\alpha(\lambda)$ are normalized temperature coefficients.[12] Equation (4) was also used to calculate values for the absorption coefficient at temperatures for which no experimental data could be found in literature.

To calculate the fraction of photons that escape from the surface of a planar silicon wafer without being reabsorbed, the ratio of the photon flux emitted by a volume element within the wafer that is located at a distance $z \neq 0$ from the surface and at $z=0$ (i.e., no reabsorption) was determined. In Fig. 1 that fraction is shown for different detector/filter combinations as a function of the sample temperature for a typical sample thickness of $d=300$ μm. Reabsorption is thus
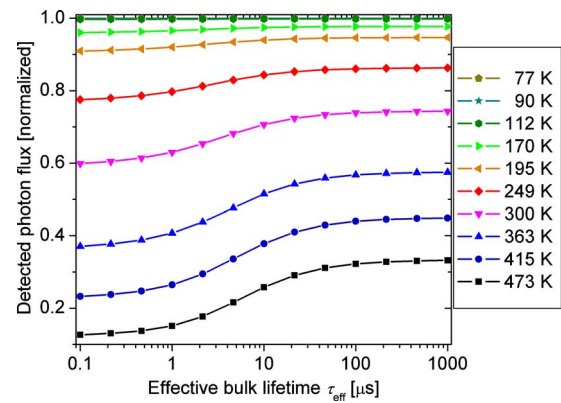
negligible at low temperatures, whereas the significance of reabsorption effects increases by temperature and becomes significant at temperatures between 200 and 300 K, depending on the measurement setup, respectively.

The small kinks in the curves shown in Fig. 1 are caused by a small mismatch between experimental and extrapolated data for the absorption coefficient. At elevated temperatures of $T=473$ K, reabsorption effects become quite substantial reaching 90% for detection with a Si *pin* detector. Figure 1 also shows that a significant reduction in reabsorption effects can be expected at elevated temperatures by measuring the total emitted photon flux, i.e., by using a Ge sensor instead of a Si sensor. In any combination of wafer and sensor, the effect of reabsorption can be reduced by using a 1000 nm long pass filter (shown in Fig. 1 for detection with Ge sensor). The 1000 nm long pass filter blocks the highly affected short wavelength photons from the detected signal. Using an even longer wavelength cutoff filter would further reduce reabsorption effects at the cost of a lower total luminescence signal.

For more realistic calculations, excess carrier profiles at different temperatures ranging from 77 to 473 K were calculated using PC1D simulations[13] for a 300 μm thick *p*-type silicon wafer with a base doping of 10^{16} cm^{-3} (cf., Ref. 5). At each temperature the effective bulk lifetime τ_{eff} was varied in a range between 0.1 and 1000 μs, while the recombination velocities of the front and rear surfaces and the reflectivity of all surfaces were set to zero. Monochromatic quasi-steady-state illumination under low injection conditions (light intensity 0.001 W/cm^2) with a wavelength of $\lambda =810$ nm from the front side of the wafer was used. The above assumption of a negligible separation of the quasi-Fermi levels is then no longer appropriate. The actual minority carrier distribution is used to calculate $\Delta\eta(z)$, according to $\Delta\eta(z) \propto \Delta n(z)$, where low injection conditions are assumed.

Figure 2 shows the normalized detected photon flux for various temperatures and effective lifetimes for detection with a Si *pin* sensor and a 1000 nm LP filter located behind the rear surface of the wafer. Each data point is normalized to the photon flux that would be measured under the same conditions but without reabsorption. The data show that the ef-

TABLE I. Maximal relative variations of the detected PL signal at certain temperatures by varying the bulk lifetime from 0.1–1000 μs (cf., Fig. 2). Results are shown for detection of the signal from the rear surface via a Ge sensor, a combination of Si pin sensor plus 1000 nm LP, and a combination of Si pin sensor plus a 1 mm thick Si filter held at the sample temperature, respectively.

Temperature T (K)	Ge sensor	Si sensor and LP	Si sensor and 1 mm Si filter
195	2%	4%	2%
249	5%	11%	5%
300	10%	24%	7%
363	23%	55%	14%
415	31%	93%	20%
473	40%	162%	32%

fect of reabsorption strongly varies with the temperature and that even at a defined temperature the reabsorption probability changes as a function of τ_{eff}, especially in the range of 1–50 μs.[5] Table I summarizes the relative variation of the fraction of detected photons between very small (0.1 μs) and very large effective lifetimes (1 ms), respectively, for specific temperatures and three different detector configurations. In addition to the detection by a Ge sensor and the combination of a Si sensor and a 1000 nm long pass filter, the combination of a Si sensor and a 1 mm thick Si filter was simulated. Internal reflectivity at the front and back side of the filter were set to 10%, taking multiple internal reflections into account. Photon recycling within the filter and the luminescence from the filter itself was assumed to be negligible. The filter was assumed to be held at the sample temperature. In that case the Si filter acts dynamically, i.e., its absorption properties change in such a way that those photons that are strongly absorbed within the sample will also strongly be absorbed in the filter. This arrangement leads to a further reduction of reabsorption effects, but at the cost of a reduced total PL signal by two to three orders of magnitude.

As discussed in Ref. 1, the measured relative PL signal is calibrated using a scaling factor A_i. The determination of A_i is normally done at only one given temperature and at a relatively large injection level, the latter equivalent to a specific τ_{eff}. Using this calibration factor without accounting for reabsorption effects, the measured minority carrier lifetime determined from QSSPL measurements at other temperatures and/or other minority carrier densities will be inaccurate in proportion to the fractions of detected light presented in

Fig. 2. These artifacts can be eliminated by introducing a calibration correction matrix $\zeta_i(T, \tau_{\text{eff}})$ so that

$$A_{i,\text{corr}} = \zeta_i(T, \tau_{\text{eff}})A_i \, , \tag{5}$$

where A_i is the absolute scaling factor determined at temperature T and at minority carrier lifetime τ_{eff}. $A_{i,\text{corr}}$ is the new calibration factor to be used. The calibration correction matrix has to be normalized to the value, at which the PL intensity is initially calibrated. The corresponding $A_{i,\text{corr}}$ can be used at all other temperatures and lifetime values. While in principle an iterative process would be necessary to get the most accurate results, one iteration of this procedure is sufficient in practice, due to the generally small corrections being made.

In summary, photon reabsorption on QSSPL measurements in crystalline silicon is theoretically quantified and a method is presented, how to correct this influence by introducing a calibration correction factor ζ_i. Using this approach allows more accurate experimental values for the injection and temperature dependent minority carrier lifetime to be determined, which in turn allows more accurate fitting of defect parameters in advanced lifetime spectroscopy methods.[6]

[1]T. Trupke and R. A. Bardos, Proceedings of the 31st IEEE Photovoltaic Specialists Conference, Orlando, Florida, USA, 2005 (unpublished).

[2]D. Macdonald and A. Cuevas, Appl. Phys. Lett. **74**, 1710 (1999).

[3]P. J. Cousins, D. H. Neuhaus, and J. E. Cotter, J. Appl. Phys. **95**, 1854 (2004); M. Bail, M. Schulz, and R. Brendel, Appl. Phys. Lett. **82**, 757 (2003).

[4]R. A. Sinton and A. Cuevas, Appl. Phys. Lett. **69**, 2510 (1996).

[5]T. Trupke, J. Appl. Phys. **100**, 063531 (2006).

[6]S. Rein, T. Rehrl W. Warta, and S. W. Glunz, J. Appl. Phys. **91**, 2059 (2002).

[7]P. Würfel, S. Finkbeiner, and E. Daub, Appl. Phys. A: Mater. Sci. Process. **60**, 67 (1995).

[8]R. A. Smith, *Semiconductors* (Cambridge University Press, New York, 1978).

[9]T. Trupke, M. A. Green, P. Würfel, and P. P. Altermatt, J. Appl. Phys. **94**, 4930 (2003).

[10]M. J. Keevers and M. A. Green, Appl. Phys. Lett. **66**, 174 (1995).

[11]H. A. Weakliem and D. Redfield, J. Appl. Phys. **50**, 1491 (1978).

[12]M. Green (private communication).

[13]D. A. Clugston and P. A. Basore, Proceedings of the 26th IEEE Photovoltaic Specialists Conference, Anaheim, California, USA, 1997 (unpublished).