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Injection dependence of spontaneous radiative recombination in c-Si: experiment, theoretical analysis, and simulation

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***Abstract* - The radiative recombination coefficient *B* in crystalline bulk silicon is enhanced by the Coulomb attraction between electrons and holes. This effect – and hence *B* – is reduced at high carrier densities due to screening. We measure and numerically calculate *B* as a function of injection density, and with the gained model we simulate an experiment in order to extract the Coulomb-enhancement of Auger recombination.**

I. Introduction

The quantification of the radiative recombination rate in crystalline silicon is important to the present development of efficient light-emitting devices based on this material. Such devices have reached external quantum efficiencies of near 1% for electroluminescence [1] and over 10% for photoluminescence [2], both of which are noticeably high considering that silicon has an indirect band-gap.

The rate R_{rad} of spontaneous radiative recombination is proportional to the density of free electrons n and free holes p. Considering only excess carriers, there holds

$$R_{rad} = B(np - n_{i,eff}^2)\,, \qquad (1)$$

where the proportionality factor B is the radiative recombination coefficient, and $n_{i,eff}$ is the effective intrinsic carrier density. It has been known since 1974 [3] that B is enhanced by the Coulomb attraction between electrons and holes, which leads to an increased hole density in the vicinity of an electron, and vice versa. This enhancement depends on both temperature [3] and carrier injection level [4]; it varies with the amount of screening among the free carriers. While the temperature-dependence of B has been thoroughly examined [5 and references therein], no quantification of the injection dependence has been made available, although it is the dominant effect in light-emitting devices operated at constant ambient temperature.

II. Measurements

B can be determined experimentally using two different approaches. Firstly, by measuring R_{rad} and the density of excess carriers [3]; and secondly, by measuring the absorption coefficient for band-to-band transitions, α_{bb}, and by applying the van Roosbroeck theory [6] or the generalized Planck equation [5,7].

In the symmetrical plasma (n=p), we determine the injection dependence of B with the first experimental approach, using the well-established data of Schlangenotto et al. [3]. In Fig. 1a, we plot the dependence in terms of B/B_{low} (symbols), where B_{low} is obtained at very low carrier densities. This scaling is done because, in contrast to measurements of B, the determination of B/B_{low} does not require absolute measurements of the emitted photon flux j_γ. The data in Fig. 1a shows that B declines with increasing injection density in a temperature-dependent manner (apart from the scatter above B/B_{low} = 0.8).

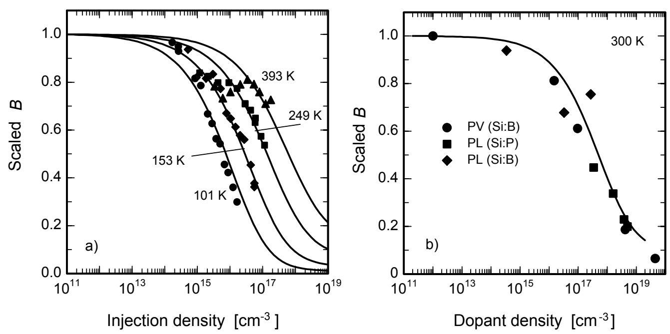

Figure 1a): The scaled radiative recombination coefficient B/B_{low} for a symmetrical plasma (n = p) at various temperatures. B_{low} is obtained at very low carrier densities. Symbols: measurements, as extracted from [3]; lines: our calculations. Fig. 1b): B/B_{low} for the asymmetrical plasma ($n \neq p$) at 300 K. Symbols: our measurements obtained using photovoltaic (PV) and photoluminescence (PL) methods; lines: our calculations.

In the asymmetrical case ($n \neq p$), we determine the injection dependence of B with the second experimental approach. We obtain α_{bb} for various phosphorus or boron dopant densities N_{dop} from photoluminescence spectra in the same way as in [8]. In addition, we obtain the necessary $n_{i,eff}$ via

$$n_{i,eff} = n_i e^{\Delta E_g/(2kT)}\,, \qquad (2)$$

where the intrinsic carrier density n_i is taken from [9], and the band gap shrinkage ΔE_g from [10]. The resulting B/B_{low} values are depicted in Fig. 1b; they decline with increasing hole or electron density. To complement these data, we fabricated solar cells with wafers of various boron dopant densities [11], and we determined α_{bb} with spectral response measurements as in [12,13]. Our results are plotted in Fig. 1b as circles; they coincide with the photoluminescence data shown as squares.

III. CALCULATIONS

The Coulomb attraction between the electrons and holes increases the band-to-band recombination coefficient from its hypothetical free-carrier value B_0 to the empirical value $B = g_{eh}B_0$. The factor g_{eh} accounts for the enhanced probability of finding an electron and a hole in the immediate vicinity of each other, and is given by the pair correlation function at zero interparticle distance. Denoting the radial s-wave functions for the relative motion of the two charge carriers by $R_{\nu 0}(r)$, there holds

$$g_{eh} = \frac{\Lambda_{eh}^3}{4\pi} \sum_{\nu} \left| R_{\nu 0}(0) \right|^2 \exp(-E_{\nu 0} / kT) \,, \qquad (3)$$

where $\Lambda^2_{eh} = h^2/2\pi kTm_{eh}$ is the thermal wavelength squared, and m_{eh} is the reduced electron-hole mass. The summation index ν comprises both discrete and continuous quantum numbers. We incorporate screening effects by employing the Debye potential. Hence, the energy levels $E_{\nu 0}$ and wave functions $R_{\nu 0}(r)$ in Eq. (3) vary with the inverse screening length κ, so that g_{eh} depends not only on the temperature T but also on the particle densities. In particular, when Boltzmann statistics can be applied, one has $\kappa^2 \propto (1/kT)\cdot(n + p)$, i.e., the enhancement factor becomes a function of $n + p$. From Eq. (3) and the Boltzmann expression for κ given above, it can be seen that the decrease of g_{eh} sets in at lower carrier densities when T is reduced. The theoretical curves are shown in Figs. 1a and 1b as lines and describe the experiments well within the measurements' precision.

We parameterize our calculations using the asymmetrical logistical equation

$$\frac{B}{B_{low}} = b_{\min} + \frac{b_{\max} - b_{\min}}{1 + \left(n + p / b_1\right)^{b_2} + \left(n + p / b_3\right)^{b_4}} \,, \qquad (4)$$

where

$$b_{\min} = r_{\max} + \frac{r_{\min} - r_{\max}}{1 + (T / r_1)^{r_2}} \,,$$

$$b_1 = s_{\max} + \frac{s_{\min} - s_{\max}}{1 + (T / s_1)^{s_2}} \,, \; b_3 = w_{\max} + \frac{w_{\min} - w_{\max}}{1 + (T / w_1)^{w_2}} \,.$$

The parameters are given in the table below, and were obtained with nonlinear regression. The parameters were truncated such that the reduced χ^2 did not surpass 10^{-5} in the temperature range from 77 K to 400 K and in the injection range from 10^{11} cm^{-3} to 10^{19} cm^{-3}. This means that the above analytical fit deviates from our calculations by less than the line thickness in Figs. 1a and 1b. In order to obtain the absolute values of B, Eq. (4) needs to be multiplied with the experimentally determined B_{low} values published in [5].

b_{max} =	1.00			b_2 =	0.54	b_4 =	1.25
r_{max} =	0.20	r_{min} =	0.00	r_1 =	320	r_2 =	2.50
s_{max} =	1.5×10^{18}	s_{min} =	1×10^{7}	s_1 =	550	s_2 =	3.00
w_{max} =	4.0×10^{18}	w_{min} =	1×10^{9}	w_1 =	365	w_2 =	3.54

IV SIMULATIONS

We implement the parameterization (4) into the leading device simulator Dessis and simulate a classic experiment [14], designed for determining the Auger-lifetime limit of silicon. This experiment has been difficult to interpret: the silicon sample was immersed in hydrofluoric acid during lifetime measurements, and hence its optical properties could not be optimized. This caused a significant amount of light-trapping and re-absorption of the emitted radiation. For the first time, we are able to take these effects into account, so we can extract the Auger-lifetime limit with unprecedented precision. Details about these simulations and the results will be presented at the conference.

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