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Temperature dependence of the radiative recombination coefficient in crystalline silicon from spectral photoluminescence

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The radiative recombination coefficient $B(T)$ in crystalline silicon is determined for the temperature range 90–363 K, and in particular from 270 to 350 K with an interval of 10 K, where only sparse data are available at present. The band-band absorption coefficient established recently by Nguyen *et al.* [J. Appl. Phys. **115**, 043710 (2014)] via photoluminescence spectrum measurements is employed to compute the values of $B(T)$ at various temperatures. The results agree very well with literature data from Trupke *et al.* [J. Appl. Phys. **94**, 4930 (2003).] We present a polynomial parameterization describing the temperature dependence of the product of $B(T)$ and the square of the intrinsic carrier density. We also find that $B(T)$ saturates at a near constant value at room temperature and above for silicon samples with relatively low free carrier densities. © 2014 AIP Publishing LLC. [<http://dx.doi.org/10.1063/1.4869295>]

Efficiencies of light emitting devices based on crystalline silicon have been improved significantly. Such devices have been demonstrated to have external efficiencies exceeding 10% at low temperature and 6% at room temperature (RT) for photoluminescence (PL).¹ Thus, a comprehensive model accurately describing the temperature dependence of the radiative recombination coefficient $B(T)$ is essential for accurate modelling and simulation of such light emitting devices, and also for silicon solar cells. There have been numerous works in which values of $B(T)$ were determined at different temperatures both theoretically and empirically.^{2–6} These authors determined $B(T)$ via two different methods. The first approach^{2,6} is to measure the spontaneous radiative emission rate R and the carrier densities n and p , then apply the formula $R = B \times n \times p$ to extract B . The second approach^{3–6} is to determine the band-band absorption coefficient and then apply the van Roosbroeck and Shockley theory⁷ or the generalized Planck law.^{8,9} The most recent works carried out by Trupke *et al.*⁵ and Altermatt *et al.*⁶ have established the values of $B(T)$ at different temperatures and free carrier densities, respectively, using the second method. However, data in Trupke *et al.* and Altermatt *et al.* are limited to only a few temperatures due to the limited temperature resolution of the band-band absorption coefficient data.

Recently, the band-band absorption coefficient in crystalline silicon has been reassessed empirically, and its temperature dependence has been formulated by Nguyen *et al.*,¹⁰ courtesy of spectral photoluminescence measurements. In this Letter, we again employ the second approach to determine the values of $B(T)$ across the temperature range of 90–363 K, and in particular around RT with an interval of 10 K, using the experimental values of the band-band absorption coefficient from Nguyen *et al.* We also establish a parameterization of the temperature dependence to allow

accurate interpolation of data in the temperature range of 90–363 K, and find that the radiative recombination coefficient saturates at a near constant value at RT and above for silicon samples with low free carrier densities.

The radiative recombination coefficient in crystalline silicon at a given temperature is determined via the formula^{5,6}

$$B(T) = \frac{1}{n_i^2} \times \frac{1}{\pi^2 \hbar^3 c_0^2} \int_0^\infty \left[n^2 \times (\hbar\omega)^2 \times \alpha_{BB}(\hbar\omega, T) \times \exp\left(\frac{-\hbar\omega}{kT}\right) \times d(\hbar\omega) \right], \quad (1)$$

where c_0 is the speed of light in vacuum, k is Boltzmann's constant, T is the absolute temperature of the sample, n is the refractive index of silicon, $\alpha_{BB}(\hbar\omega, T)$ is the band-band absorption coefficient whose values are a function of energy, and temperature, and n_i is the intrinsic carrier density. The values of n_i depend on the temperature and the free carrier density, and several works have been performed to determine accurate values of this parameter.^{11–15} In this work, to avoid the dependence on the choice of model for the intrinsic carrier density, instead of placing the emphasis on determining values of the radiative recombination coefficient $B(T)$, we will consider the more general parameter $B(T) \times n_i^2$. Multiplying both sides of Eq. (1) with n_i^2 yields

$$B(T) \times n_i^2 = \frac{1}{\pi^2 \hbar^3 c_0^2} \int_0^\infty \left[n^2 \times (\hbar\omega)^2 \times \alpha_{BB}(\hbar\omega, T) \times \exp\left(\frac{-\hbar\omega}{kT}\right) \times d(\hbar\omega) \right]. \quad (2)$$

From Eq. (2), to calculate $B(T) \times n_i^2$, one needs to know the refractive index n and the absorption coefficient $\alpha_{BB}(\hbar\omega, T)$. The refractive index is also a function of energy and temperature, and is extracted from Green.¹⁶ The

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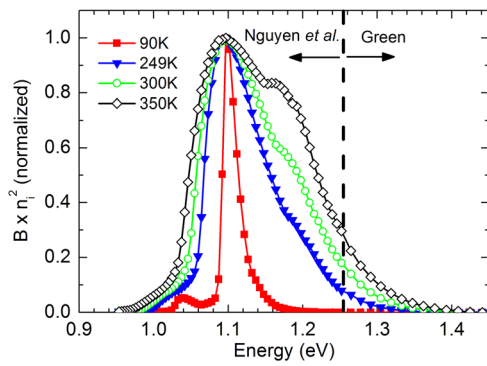


FIG. 1. Normalized $B(\hbar\omega, T) \times n_i^2$ versus energy at various temperatures. The data on the left of the vertical dashed line are calculated from the absorption coefficient in Nguyen *et al.*,¹⁰ and the data on the right are calculated from values in Green.¹⁶

band-band absorption coefficient is obtained from our previous work.¹⁰ The temperatures in Ref. 10 are dense around RT, and thus allow us to establish an accurate temperature parameterization for $B(T) \times n_i^2$.

Figure 1 shows the calculated values of $B(\hbar\omega, T) \times n_i^2$ versus energy at several intermediate temperatures, based on the energy-dependent absorption coefficient data of Nguyen *et al.*¹⁰ The area under each curve is the total value of $B(T) \times n_i^2$ at a particular temperature. Note that the data in Figure 1 have been normalized to allow comparison. To calculate the absolute total value of $B(T) \times n_i^2$, we use the absolute data of $B(\hbar\omega, T) \times n_i^2$.

In the experiments in Nguyen *et al.*,¹⁰ α_{BB} was determined for wavelengths from 990 to 1300 nm, i.e., for energies from 0.954 to 1.253 eV. Below 0.954 eV, $B(\hbar\omega, T) \times n_i^2$ contributes negligibly to the integration. Above 1.253 eV, $B(\hbar\omega, T) \times n_i^2$ still contributes a significant portion to the

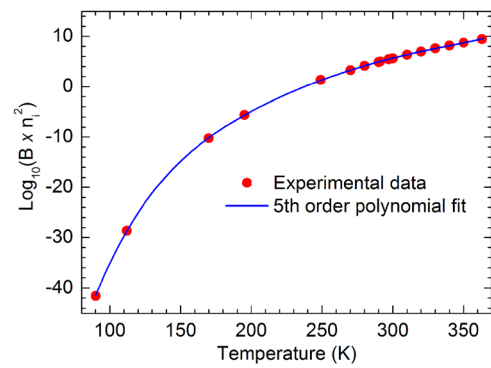


FIG. 2. $\text{Log}_{10}(B(T) \times n_i^2)$ versus temperature and the 5th order polynomial fit given by Eq. (3).

integration around RT, as seen in Figure 1, although at the lower temperature of 90 K it is again insignificant. To correct for this lack of high energy data from the PL spectra, we use the absorption coefficient values from Green¹⁶ to calculate $B(\hbar\omega, T) \times n_i^2$ for energies above 1.253 eV. These values were determined from transmission and reflectance experiments, which in general are more accurate than the PL method at high energies.⁵ The error in these data was estimated to be around 4% by Green.¹⁶ Since this part of the spectrum contributes less than 8% to the area under each curve, the uncertainty due to using absorption data from two different methods is estimated to be only about 0.3%.

Figure 2 plots our data of $\text{Log}_{10}(B(T) \times n_i^2)$ across the temperature range 90–363 K, calculated as described above. We have fitted these points with a 5th order polynomial using the least squares regression method. The formula obtained is given by Eq. (3). Note that $B(T) \times n_i^2$ has the unit of $\text{cm}^{-3} \text{s}^{-1}$.

$$\begin{aligned} \text{Log}_{10}(B(T) \times n_i^2) = & -1.7698 \times 10^2 + 2.68812 \times T - 1.8137 \times 10^{-2} \times T^2 + 6.56769 \times 10^{-5} \times T^3 \\ & - 1.21382 \times 10^{-7} \times T^4 + 8.99086 \times 10^{-11} \times T^5. \end{aligned} \quad (3)$$

Since the values of $B(T) \times n_i^2$ do not depend on n_i and the experimental absorption data in Nguyen *et al.* are not affected by free carriers as long as their density is less than $2 \times 10^{17} \text{cm}^{-3}$ (Refs. 10 and 17), Eq. (3) can be used to extract data for $B(T) \times n_i^2$ at any temperature from 90 to 363 K for samples with free carrier densities below this value. Final values of $B(T)$ can be computed by choosing an appropriate model for the intrinsic carrier density, which can include the temperature and injection level dependence.

Next, to validate our data, we compare them with literature values from Trupke *et al.*⁵ Since Trupke *et al.* calculated $B(T)$, we need to divide our data by n_i^2 . To permit a direct comparison, we employ the same n_i model as used by those authors⁵

$$n_i(T) = 2.9135 \times 10^{15} \times T^{1.6} \times \exp\left(-\frac{E_g(T)}{2kT}\right), \quad (4)$$

with $E_g(T)$ the band-gap energy of silicon at a specific temperature in accordance with Ref. 18. Equation (4) describes the relationship between the intrinsic carrier density and the temperature, including the temperature dependence of the band-gap energy. However, this expression does not include the effect of band-gap narrowing due to free carriers.¹⁹ Therefore, the values of $B(T)$ in Trupke *et al.*⁵ reflect conditions of relatively low densities of free carriers, where the band-gap narrowing effect is insignificant. The values of n_i^2 start increasing, and therefore the values of $B(T)$ decrease, as demonstrated by Altermatt *et al.*,⁶ when the free carrier densities approach approximately 10^{14}cm^{-3} .

Our calculated values of $B(T)$ using the experimental data for the absorption coefficient in Nguyen *et al.*,¹⁰ along with the values in Trupke *et al.*,⁵ are plotted in Figure 3. While the data of Trupke *et al.* cover the region 90–300 K, this work extends the measurement of $B(T)$ to the higher temperature limit of 363 K, with very dense data points

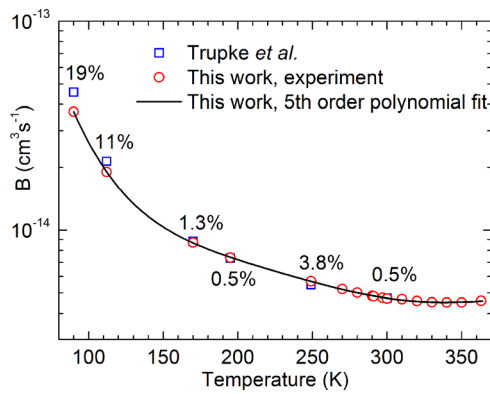


FIG. 3. Comparison of radiative recombination coefficient between this work and Trupke *et al.*⁵ The inserted numbers are the relative deviation between the two works.

around room temperature. The two data sets match very well, except for the value at 90 K where the relative deviation is approximately 20%. The fact that the PL spectra are very sharp at low temperatures¹⁰ contributes to the uncertainties in the measurements of Nguyen *et al.* This is caused by the impact of the limited wavelength resolution on the integration, which in turn affects the absorption data and the integration of $B(T) \times n_i^2$ (see curve 90 K in Figure 1 for example), and thus $B(T)$ in this study. In the same way, the data of Trupke *et al.* were likely subject to similar uncertainties in their low temperature PL measurements. This may be the reason for the 20% relative deviation at 90 K in Figure 3. We also note that the radiative recombination coefficient saturates at a near constant value at RT and above, a conclusion which could not be made on the basis of the relatively sparse data published previously.

Finally, with the same method used for $B(T) \times n_i^2$, we also establish a formula to compute $B(T)$ using the n_i model of Eq. (4) at any temperature from 90–363 K and low free carrier densities, as shown in Eq. (5). In fact, we fitted our data with different methods including the fifth order polynomial, the first and the second order exponential functions and found the best fit with this polynomial function. Note that $B(T)$ has the unit of $\text{cm}^3 \text{s}^{-1}$, and the experimental data of both $B(T) \times n_i^2$ and $B(T)$ in this work are also given in Table I.

$$\begin{aligned} \text{Log}_{10} B(T) = & -9.65614 - 8.05258 \times 10^{-2} \times T \\ & + 6.02695 \times 10^{-4} \times T^2 - 2.29844 \times 10^{-6} \times T^3 \\ & + 4.31934 \times 10^{-9} \times T^4 - 3.16154 \times 10^{-12} \times T^5. \end{aligned} \quad (5)$$

In summary, based on recent band-band absorption data, we have proposed and calculated a general parameter which incorporates both the radiative recombination coefficient and the intrinsic carrier density in crystalline silicon, and have established a polynomial parameterization to describe the temperature dependence for this quantity based on experimental data. This formula, along with a model for the

TABLE I. Experimental values of $B(T) \times n_i^2$ and $B(T)$ in this work.

Temperature (K)	$B(T) \times n_i^2$ ($\text{cm}^{-3} \text{s}^{-1}$)	$B(T)$ ($\text{cm}^3 \text{s}^{-1}$)
90	2.846×10^{-42}	3.697×10^{-14}
112	2.547×10^{-29}	1.902×10^{-14}
170	6.114×10^{-11}	8.722×10^{-15}
195	2.639×10^{-6}	7.384×10^{-15}
249	2.169×10^1	5.689×10^{-15}
270	1.991×10^3	5.220×10^{-15}
280	1.361×10^4	5.023×10^{-15}
290	8.203×10^4	4.847×10^{-15}
291	9.763×10^4	4.835×10^{-15}
297	2.703×10^5	4.750×10^{-15}
300	4.428×10^5	4.705×10^{-15}
310	2.205×10^6	4.680×10^{-15}
320	9.840×10^6	4.587×10^{-15}
330	4.053×10^7	4.526×10^{-15}
340	1.558×10^8	4.511×10^{-15}
350	5.592×10^8	4.513×10^{-15}
363	2.713×10^9	4.592×10^{-15}

intrinsic carrier density, can be used to extract accurate values of the radiative recombination coefficient from 90 to 363 K. Our data are shown to match very well with literature data from Trupke *et al.* Moreover, the radiative recombination coefficient is found to saturate at room temperature and above, for samples with relatively low free carrier densities.

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