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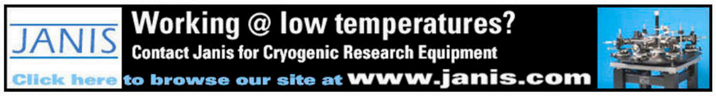

Ultra-low values of the absorption coefficient for band–band transitions in moderately doped Si obtained from luminescence

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The absolute value of the absorption coefficient $\alpha_{bb}(\hbar\omega)$ for band–band transitions near the band edge was determined in moderately doped silicon by photoluminescence spectra analysis. The major advantage of this method in determining $\alpha_{bb}(\hbar\omega)$ is the lack of interference with free carrier absorption, in contrast to conventional methods like transmission or photothermal deflection measurements. We deduce values for $\alpha_{bb}(\hbar\omega)$, which are nearly five orders of magnitude smaller than the absorption coefficient $\alpha_{fc}(\hbar\omega)$ for free carrier absorption. With this method it is possible to examine in detail the influence of doping on the absorption coefficient for band–band transitions near the absorption edge. The appearance of band tails and band-gap narrowing are very well reflected. With conventional methods, which can only detect the overall absorption of the incident radiation, the determination of $\alpha_{bb}(\hbar\omega)$ in the vicinity of the band edge is impossible for moderately and heavily doped silicon, because it is completely masked by the free carrier absorption. © *1996 American Institute of Physics.* [S0021-8979(96)03220-3]

I. INTRODUCTION

The spontaneous emission rate via direct and indirect transitions is described by the generalized Planck radiation law with a non-zero chemical potential μ_γ of the photons.[1] In a recently published paper,[2] this generalized Planck law was used to determine ultra-low values for the absorption coefficient of lightly doped silicon. At a temperature of 90 K, values as small as 10^{-16} cm^{-1} could be obtained from photoluminescence spectra for photon energies well below the band gap. In this paper we want to present a method for the analysis of photoluminescence data, which is especially useful to determine absolute values of the band to band absorption coefficient $\alpha_{bb}(\hbar\omega)$ in the case of moderately and heavily doped silicon for photon energies near and below the indirect band gap.

In the following we will first describe the theory for the analysis of the luminescence spectra and, using thermodynamic arguments, we will show that, as a major advantage of our method, there is no interference with the free carrier absorption in the determination of $\alpha_{bb}(\hbar\omega)$. Like photoluminescence excitation spectroscopy (see, for example, Ref. 3) our method is only sensitive to band–band transitions, but in contrast to these measurements, we are able to determine absolute values for $\alpha_{bb}(\hbar\omega)$ near and well below the band edge by making use of reabsorption processes inside the sample. After these remarks we will take a short look at the experimental setup, which is designed for these transmission photoluminescence measurements and deviates therefore in one special point from the usual setup. Subsequently we will present experimental data of the luminescence spectra of moderately doped silicon and the absorption coefficient $\alpha_{bb}(\hbar\omega)$ derived from these spectra. In this context we will give a short discussion concerning the influence of heavy doping on band-gap narrowing and band tails. Furthermore we want to explain how the different values published for the band-gap narrowing ΔE_g as derived from photoluminescence or transmission experiments can be understood.

II. THEORY

The spontaneous emission rate for band–band transitions $dr_{em}(\hbar\omega)$ of photons with energy between $\hbar\omega$ and $\hbar\omega + d\hbar\omega$ into the solid angle Ω is given by[2]

$$dr_{em}(\hbar\omega) = \alpha_{bb}(\hbar\omega)\frac{c_\gamma D_\gamma \Omega}{\exp\left(\dfrac{\hbar\omega - \mu_\gamma}{kT}\right) - 1}\, d\hbar\omega. \tag{1}$$

$\alpha_{bb}(\hbar\omega)$ is the absorption coefficient for band–band transitions, $c_\gamma = c_0/n$ is the velocity of light in the emitting medium with refractive index n, and $D_\gamma = n^3(\hbar\omega)^2/4\pi^3\hbar^3 c_0^3$ the density of states per solid angle for photons in the medium. The chemical potential μ_γ of the emitted photons is equal to the difference, $\epsilon_{F,C} - \epsilon_{F,V}$, of the quasi-Fermi energies, which describe separately the occupation of states in the conduction and in the valence band. In chemical and thermal equilibrium with the surrounding blackbody radiation of 300 K, $\epsilon_{F,C} - \epsilon_{F,V} = \mu_\gamma = 0$ and Eq. (1) reduces to the original Planck law for thermal radiation. The spontaneous emission rate in Eq. (1) is not directly observable. It has to be integrated over the emitting volume, taking reabsorption into account. Photon recycling[4] is already contained in Eq. (1). Reabsorption of photons can occur through interband transitions, and, especially in heavily doped silicon, also through intraband transitions in the form of free carrier absorption. The process of reabsorption is therefore described by the sum of the absorption coefficients for free carrier and band–band absorption by $\alpha_{\mathrm{tot}}(\hbar\omega) = \alpha_{fc}(\hbar\omega) + \alpha_{bb}(\hbar\omega)$. The spontaneous emission rate, however, is dominated by interband transitions, which are characterized by $\alpha_{bb}(\hbar\omega)$. Free carrier emission as the reversal of free carrier absorption can

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be neglected as is shown by the following considerations, which hold for n-type silicon, but are valid for p-type materials as well.

The emission and absorption of photons in the case of interband transitions is described by the following reaction between photons γ, electrons e, holes h, and phonons Γ[2]:

$$\gamma \rightleftharpoons e + h \pm n\Gamma. \tag{2}$$

In indirect materials like silicon, the absorption or emission of a photon γ with energy $\hbar\omega$ in band–band transitions is accompanied by the absorption or emission of at least one phonon for momentum conserving reasons. From thermodynamic arguments the equilibrium of this reaction is given by

$$\mu_\gamma = \eta_e + \eta_h \pm n\mu_\Gamma = \epsilon_{F,C} - \epsilon_{F,V} \pm n\mu_\Gamma . \tag{3}$$

The sum of the electrochemical potentials of electrons and holes $\eta_e + \eta_h$ is equal to the difference of the quasi-Fermi energies. The chemical potential μ_γ of phonons is zero as in thermal equilibrium, because of the large phonon generation and absorption rates, considering phonon lifetimes in the order of 10^{12} s or less.[1]

Intraband transitions of free carriers occur by the absorption or emission of a photon or of a phonon. The fundamental processes are

$$e \pm \gamma \rightleftharpoons e' \quad \text{and} \quad e \pm \Gamma \rightleftharpoons e', \tag{4}$$

with the equilibrium conditions

$$\eta_e + \mu_\gamma = \eta_{e'} \quad \text{and} \quad \eta_e + \mu_\Gamma = \eta_{e'}. \tag{5}$$

Due to the strong electron–phonon interaction, the chemical equilibrium between electrons and phonons is maintained even for excitations by external photons, as long as carrier heating is avoided. Since $\mu_\Gamma = 0$, there is a single Fermi distribution for all electrons in the conduction band $(\eta_e = \eta_{e'})$. This in turn leads to $\mu_\gamma = 0$ of the photons emitted by intraband transitions of electrons, which is room temperature thermal radiation. (The same is of course, true for the valence band.)

In conclusion, radiative intraband transitions lead to the emission of thermal radiation with $\mu_\gamma = 0$, whereas interband transitions lead to luminescence radiation with $\mu_\gamma = \epsilon_{F,C} - \epsilon_{F,V} > 0$. For conditions well below the laser threshold $[\hbar\omega - (\epsilon_{F,C} - \epsilon_{F,V})]/kT \gg 1$[1] the emission formula Eq. (1) can be simplified

$$dr_{em}(\hbar\omega) \simeq \alpha_{bb}(\hbar\omega) c_\gamma D_\gamma \Omega e^{-\hbar\omega/kT} e^{(\epsilon_{F,C} - \epsilon_{F,V})/kT} d\hbar\omega. \tag{6}$$

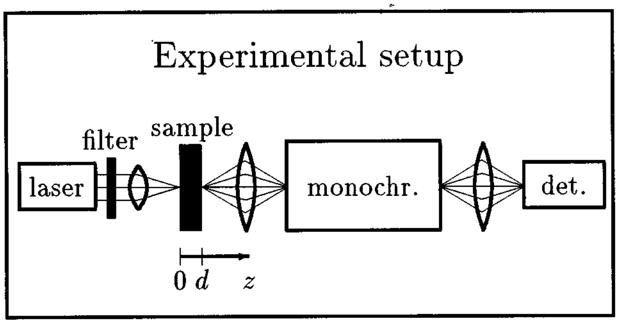

FIG. 1. Experimental setup: The sample is illuminated at one surface $(z=0)$ with a sinusoidally modulated laser diode and the luminescence radiation emitted from the opposite surface at $(z=d)$ is passed through a 1/4 m monochromator and is detected with a LN$_2$ cooled Ge diode.

This means that a difference in the quasi-Fermi energies leads to an exponential increase of the emission rate for interband transitions by the factor $\exp[(\epsilon_{F,C} - \epsilon_{F,V})/kT]$. In the experiments described below, the emitted luminescence radiation exceeds the thermal radiation approximately by a factor of 1×10^{16}.[5] Under these conditions the spontaneous emission rate in heavily doped silicon is dominated by interband transitions, although the absorption coefficient for band–band transitions may be orders of magnitude smaller than the absorption coefficient for free carrier absorption. By neglecting free carrier emission, we can determine the emitted energy current density in a photoluminescence experiment by integrating the emission rate over the emitting volume, taking reabsorption processes and multiple reflections into account. For a planar slab with lateral dimensions large compared to its thickness, which is homogeneously illuminated at the rear surface at $z=0$ (see Fig. 1), the energy current density dj_E emitted in the interval $d\hbar\omega$ from the front surface into a hemisphere is found by integrating Eq. (1)[2,8]:

$$\begin{aligned} dj_E(\hbar\omega) = {} & \alpha_{bb}(\hbar\omega) M(\hbar\omega) c_0 / n^3 \pi D_\gamma(\hbar\omega) \\ & \times e^{-\alpha_{\text{tot}}(\hbar\omega)d} e^{-\hbar\omega/kT} d\hbar\omega \int_0^d [e^{\alpha_{\text{tot}}(\hbar\omega)z} \\ & + R(\hbar\omega) e^{-\alpha_{\text{tot}}(\hbar\omega)z}] e^{[\epsilon_{F,C}(z) - \epsilon_{F,V}(z)]/kT} dz, \end{aligned} \tag{7}$$

for

$$\{\hbar\omega - [\epsilon_{F,C}(z) - \epsilon_{F,V}(z)]\}/kT \gg 1$$

with

$$M(\hbar\omega) = \frac{1 - R(\hbar\omega)}{1 - R^2(\hbar\omega)\exp[-2\alpha_{\text{tot}}(\hbar\omega)d]}.$$

In general the difference and its spatial variation of the quasi-Fermi energies in the emitting volume is unknown and the integration cannot be carried out. In two special cases this integration is however quite simple:

$$\epsilon_{F,C}(z) - \epsilon_{F,V}(z) = \text{const}, \tag{8}$$

$$dj_E(\hbar\omega) = C_1 M(\hbar\omega) a(\hbar\omega)(\hbar\omega)^3 e^{-\hbar\omega/kT} d\hbar\omega, \tag{9}$$

$$\epsilon_{F,C}(z) - \epsilon_{F,V}(z) \simeq C_2 \delta(z), \tag{10}$$

$$\begin{aligned} dj_E(\hbar\omega) \simeq {} & C_3 M(\hbar\omega) \alpha_{bb}(\hbar\omega) e^{-\alpha_{\text{tot}}(\hbar\omega)d} (\hbar\omega)^3 \\ & \times e^{-\hbar\omega/kT} d\hbar\omega, \end{aligned} \tag{11}$$

$a(\hbar\omega)$ is the absorptivity of the sample.

The first case occurs for a homogeneous distribution of electrons and holes, which is present, if the diffusion length of the minority carriers is much larger than the sample thickness d and if the surface recombination velocity $S \ll d/D$,[9] where D is the ambipolar diffusion coefficient. This relationship has been used to determine ultralow values for $\alpha_{bb}(\hbar\omega)$ for lightly doped high quality silicon.[2]

In the following we will focus on the second case, which occurs for example in our experiments with moderately doped silicon. We illuminate the slab with strongly absorbed laser light. Since the diffusion length of the minority carriers is very short (some microns), a remarkable difference of the quasi-Fermi energies exists only in the vicinity of $z=0$ and is approximated by a delta function. Because the front and back surfaces are parallel and polished (no scattering), only photons emitted into the small solid angle of π/n^2 directed perpendicular to the front surface can escape through this surface without total internal reflection.[8] Since n is large ($\simeq 3.5$), the optical path length for all photons in the escape cone is the same, independent of their place of origin near the back surface, and it does not matter whether the illumination is homogeneous or not. For a larger luminescence signal a focused laser beam can be used without any change in the luminescence spectra, as long as the generated carriers are thermalized before they undergo radiative recombination. As already mentioned above, the emission rate is solely determined by $\alpha_{bb}(\hbar\omega)$, whereas for reabsorption processes free carrier absorption has to be taken into account. The absorption coefficient for free carrier absorption is modeled by the following relations, which fit the experimental values of Schmid[11] quite well ($N_0=1\times10^{18}$ cm^{-3}):

$$\alpha_{fc}(\hbar\omega)\simeq 3.5\frac{N_A}{N_0}\left(\frac{\hbar\omega}{eV}\right)^{-2}\text{cm}^{-1}$$

$$p\text{-type}(N_A<20\times10^{18}\ \text{cm}^{-3}), \quad (12)$$

$$\alpha_{fc}(\hbar\omega)\simeq 5.9\frac{N_D}{N_0}\left(\frac{\hbar\omega}{eV}\right)^{-2.88}\text{cm}^{-1}$$

$$n\text{-type}(N_D<15\times10^{18}\ \text{cm}^{-3}). \quad (13)$$

The deviation from the expected $(1/\hbar\omega)^2$-dependence in the case of n-type silicon can be explained by direct transitions between two conduction bands.[12] However the influence of the free carrier absorption on the shape of the photoluminescence spectra is nearly negligible, because it is almost constant in the considered energy interval, whereas the absorption coefficient for band–band transitions varies by orders of magnitude. The same is true for the reflectivity $R(\hbar\omega)$, which varies only a little in the energy range of interest $[R(\hbar\omega)\simeq 0.31]$[13] and has only a small dependence on doping.[11]

A detailed analysis of the emission formula (11) shows that for the geometry discussed above a relative measurement of the emitted current density $dj_E(\hbar\omega)$ is sufficient for an absolute determination of the absorption coefficient $\alpha_{bb}(\hbar\omega)$. From Eq. (11) one can build the function

$$f(\hbar\omega)=\frac{dj_E(\hbar\omega)}{d(\hbar\omega)(\hbar\omega)^3}e^{\hbar\omega/kT}$$

$$\simeq C_3M(\hbar\omega)e^{-\alpha_{fc}(\hbar\omega)d}e^{-\alpha_{bb}(\hbar\omega)d}\alpha_{bb}(\hbar\omega). \quad (14)$$

This function has a maximum as a function of $\hbar\omega$ near the band edge. Because $\partial\alpha_{fc}(\hbar\omega)/\partial(\hbar\omega)\ll\partial\alpha_{bb}(\hbar\omega)/\partial(\hbar\omega)$, $R(\hbar\omega)\simeq$const. and $R^2(\hbar\omega)\ll 1$ one finds for the position of this maximum

$$\alpha_{bb}(\hbar\omega_{\max})\simeq 0.989/d. \quad (15)$$

TABLE I. Details of the investigated samples.

Identification	Thickness (μm)	Doping density (cm^{-3})	Type
A	250	1.3×10^{14}	p (Si:B)
B	610	3.4×10^{17}	n (Si:P)
C	640	1.6×10^{18}	n (Si:P)
D	535	5.0×10^{18}	p (Si:B)

This relation makes the analysis of the photoluminescence signal quite simple. First one takes the measured values of $dj_E(\hbar\omega)$ and calculates $f(\hbar\omega)$. From the maximum of $f(\hbar\omega)$ one finds the photon energy $\hbar\omega_{\max}$, where the absorption coefficient is given by Eq. (15). With this value, the constant C_3 in Eq. (11) is fixed, and the absorption coefficient for band–band transitions can be determined in the whole energy range of the photoluminescence spectrum.

III. EXPERIMENT

For a demonstration of the efficiency of this new method in determining $\alpha_{bb}(\hbar\omega)$, we have examined Si:P and Si:B doped samples in the doping range from 3.4×10^{17} cm^{-2} to 5×10^{18} cm^{-3}. This doping range is especially interesting, because the exciton binding energy of 14.7 meV[14] for nearly intrinsic silicon is dramatically reduced due to screening effects, and vanishes at a doping concentration of approximately 5×10^{18} cm^{-3}.[15] Furthermore it is interesting to examine the influence of band tails and band-gap narrowing on $\alpha_{bb}(\hbar\omega)$ in the case of moderately doped silicon.

We have investigated samples with polished surfaces, which were grown by the Czochralski method. Details are listed in Table I. Samples B and C were covered with a native oxide. The surfaces of the samples A and D were passivated with a thermally grown oxide of 105 nm thickness to reduce surface recombination and to increase the small photoluminescence intensity of sample D with the highest doping concentration and the smallest minority carrier lifetime. In this case the reflectivity $R(\hbar\omega)$ is determined by the refractive indices of Si[13] and SiO$_2$,[16] and the thickness of the oxide (see for example Ref. 17).

The experimental setup is shown in Fig. 1. It deviates from usual setups by the fact that we illuminate our sample on the opposite surface from which we detect the emitted luminescence radiation, i.e., our experimental setup is similar to a transmission experiment. Due to reabsorption processes over the thickness of the sample, we are able to determine the absolute value of $\alpha_{bb}(\hbar\omega)$ by a relative measurement of the emitted luminescence intensity. Usually only the emission rate $dr_{em}(\hbar\omega)$ is detected, and reabsorption is avoided by a setup, which is similar to a reflection measurement, i.e., the sample is excited at the same surface from which the luminescence radiation is detected.

The samples were illuminated by a laser diode emitting at 790 nm. The penetration depth at the laser wavelength is about 11 μm. All investigated samples have a thickness $d\geqslant 250$ μm, therefore the samples act as an effective filter, and prevent any laser light from reaching the detector. Low intensity emission of the laser at longer wavelengths, which would be transmitted by the samples, was blocked by an interference filter centered at the laser wavelength. The laser beam was focused on the sample surface, and the absorbed energy current was about 20 mW.

The photoluminescence radiation was passed through a 1/4 m monochromator with a grating blazed at 1000 nm, and was detected by a liquid-N_2 cooled Ge *p-i-n* diode. The spectral response of the whole detection unit was determined with a calibrated blackbody radiator. The intensity of the laser diode was modulated sinusoidally at 565 Hz and the detector signal was measured with a current–voltage converter and a lock-in amplifier. The overall wavelength resolution was 7 nm.

The validity of the approximation $\exp(\epsilon_{F,C}-\epsilon_{F,V}) \simeq C_2\delta(z)$ is fulfilled quite well for the investigated samples for the following reasons:

(1) Due to the large absorption coefficient for the incident laser light, all photons are absorbed within a few microns.

(2) Illuminating the sample with a focused laser beam leads to a three-dimensional carrier distribution, falling off within a characteristic depth L, which is markedly smaller than the diffusion length L_{diff} of the minority carriers.

(3) All samples are grown by the Czochralski method, resulting in a rather small minority carrier lifetime and diffusion length.

It was impossible to measure these lifetimes with conventional methods like photoconductivity decay (PCD) or surface photovoltage (SPV) measurements, because of the relative high doping level and the low minority carrier concentration. However, with photoluminescence measurements we were able to determine these quantities. From the absolute photoluminescence intensity,[10] the luminescence phase delay,[19–21] and spatially resolved photoluminescence measurements[22,23] an upper limit for the diffusion lengths in our samples was determined. We found $L_{\text{diff}} \leqslant 20$ μm for sample B, $L_{\text{diff}} \leqslant 12$ μm for sample C and in the case of sample D the diffusion length is even smaller, but we were unable to determine the exact value.

For an error estimation due to the δ-function approximation we made a worst case calculation with a one-dimensional carrier distribution, taking the exponential decay of the incident photon current density, carrier diffusion and surface recombination into account.[18] In this special case ($L_{\text{diff}} \ll d$), however, only the number of the emitted photons depends on the surface recombination velocity, but not the shape of the luminescence spectrum. We use the values published by Keevers and Green[24] for $\alpha_{bb}(\hbar\omega)$ in our calculations of $dj_E(\hbar\omega)$ and $f(\hbar\omega)$ [see Eq. (15)]. With a diffusion length of 20 μm and a sample thickness of 610 μm for these simulations we estimated, that the maximum error in the determination of $\hbar\omega_{\max}$ is smaller than 1 meV with respect to the δ-function approximation. This means, that in the case of a large absorption coefficient for the incident laser radiation, small carrier diffusion lengths and thick samples ($d \gg L_{\text{diff}}$) our method is very well suited for an absolute determination of $\alpha_{bb}(\hbar\omega)$. The knowledge of the complex three dimensional carrier distribution, which is difficult to simulate because the exact values of L_{diff} and S are usually unknown, is irrelevant.

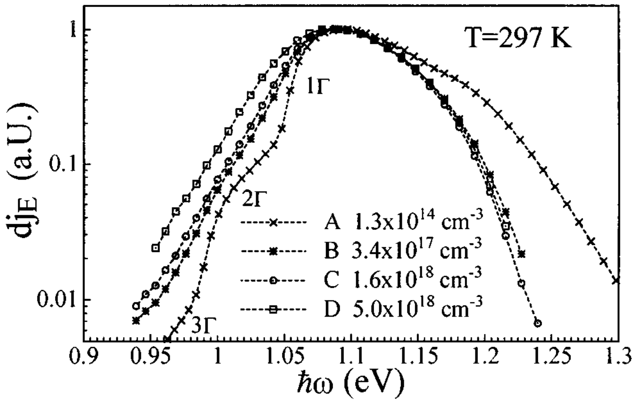

FIG. 2. Photoluminescence spectra of the samples A–D, measured at room temperature. The high energy range reflects the influence of the spatial distribution of the carriers due to reabsorption processes, whereas the low energy part is dominated by the spontaneous emission rate $dr_{em}(\hbar\omega)$. The influence of increasing doping concentration is especially noticeable for photon energies below the maximum of the luminescence spectrum.

Due to the small minority carrier lifetime, it was impossible to measure the photoluminescence signal of more highly doped silicon samples than sample D with our equipment. Sample A, with the absorption coefficient of high resistivity silicon, was included for comparison. In this case the minority carrier diffusion length $L_{\text{diff}} \gg d$, so that the emitted current density for this homogeneously excited sample is given by Eq. (9), from which the absorption coefficient $\alpha_{bb}(\hbar\omega)$ was determined.[2]

IV. RESULTS

Figure 2 shows the measured photoluminescence spectra for the different samples, all measurements were carried out at room temperature. Due to the indirect band gap in silicon, radiative transitions require the simultaneous absorption or emission of at least one phonon for momentum conserving reasons. Since the band gap of intrinsic silicon at room temperature is 1.124 eV,[25] the emission of a photon for photon energies below the luminescence maximum is accompanied by the emission of at least one phonon, whereas for the absorption of a photon at the same energy the absorption of at least one phonon is necessary. Although the phonons are involved differently, the emission rate $dr_{em}(\hbar\omega)$ is determined by the absorption coefficient $\alpha_{bb}(\hbar\omega)$ at the same energy, due to the generalized Planck radiation law for indirect transitions.[1]

The structure on the low energy side of the luminescence spectrum is characterized by the simultaneous emission of up to three phonons Γ,[2,26] whereas the high energy side is mainly influenced by the absorption of the transversal optical phonon ($\hbar\Omega \simeq 57.3$ meV[27]). Figure 2 shows, that especially the low energy transitions are influenced by increasing doping concentrations. From these luminescence spectra we have calculated the absorption coefficient $\alpha_{bb}(\hbar\omega)$ according to the method described above, the analysis of the high resistivity sample was carried out as explained in detail in Ref. 2.

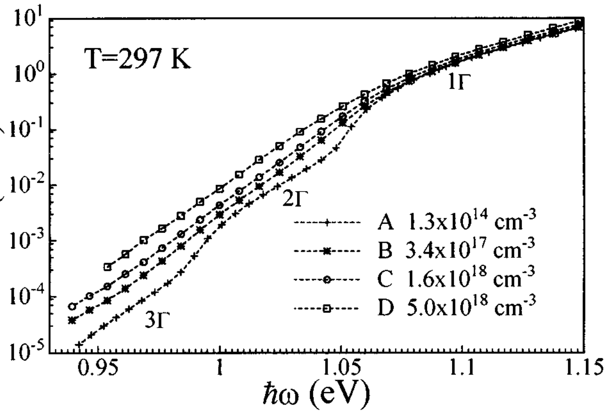

FIG. 3. Absorption coefficient α_{bb} for band–band transitions of silicon at 297 K as a function of photon energy $\hbar\omega$, obtained from a detailed analysis of the photoluminescence spectrum. A relative measurement of the photoluminescence intensity is sufficient for an absolute determination of the absorption coefficient $\alpha_{bb}(\hbar\omega)$. The influence of doping is much greater for multi-phonon than for single-phonon transitions.

Figure 3 shows the result of these calculations in the low energy range. It is possible to determine values for $\alpha_{bb}(\hbar\omega)$ as small as 10^{-4} cm^{-1} for the moderately doped samples, at energies well below the band gap. It is obvious that the multiphonon structure is smeared out with increasing doping concentration, and it becomes invisible for a boron concentration of 5×10^{18} cm^{-3}. For higher photon energies the influence of doping on the absorption coefficient is much weaker. For optical transitions involving a single phonon $\alpha_{bb}(\hbar\omega)$ is not affected by doping up to doping densities of 3.4×10^{17} cm^{-3}. For higher doping densities the $\alpha_{bb}(\hbar\omega)$ curve is shifted slightly towards lower photon energies.

In Fig. 4 the results for the sample with the highest doping level are shown separately, together with values for the overall absorption coefficient $\alpha_{\text{tot}}(\hbar\omega)=\alpha_{bb}(\hbar\omega)+\alpha_{fc}(\hbar\omega)$, determined by ordinary transmission experiments.[11] We have used the low energy part of these data, where free carrier absorption is dominant, to extrapolate $\alpha_{fc}(\hbar\omega)$ into the energy range where the absorption coefficient is composed of $\alpha_{fc}(\hbar\omega)$ and $\alpha_{bb}(\hbar\omega)$. By subtracting the extrapolated values of $\alpha_{fc}(\hbar\omega)$ from $\alpha_{\text{tot}}(\hbar\omega)$, it is possible to determine $\alpha_{bb}(\hbar\omega)$ from the results of a transmission measurement. This, however, is possible only for energies where band–band transitions contribute markedly to the overall absorption coefficient $\alpha_{\text{tot}}(\hbar\omega)$. It is impossible to determine values for $\alpha_{bb}(\hbar\omega)$ from transmission, which are smaller than 2 cm^{-1} for a doping level $N_D\geqslant5\times10^{18}$cm^{-3}.

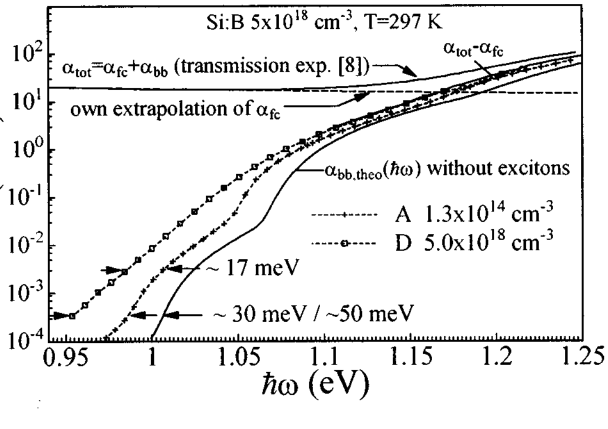

FIG. 4. Comparison of the results for the determination of $\alpha_{bb}(\hbar\omega)$ from transmission and photoluminescence experiments (Si:B, 5×10^{18} cm^{-3}). With our new method we could determine values for $\alpha_{bb}(\hbar\omega)$, which are nearly five orders of magnitude smaller than the absorption coefficient for free carrier absorption $\alpha_{fc}(\hbar\omega)$. For a better understanding of the difficulties in determining ΔE_g, we have added $\alpha_{bb}(\hbar\omega)$ for the high resistivity sample A, and theoretical values of $\alpha_{bb}(\hbar\omega)$, neglecting the excitonic part of the absorption coefficient. In the low energy range any value between 17 meV and 50 meV for ΔE_g is possible.

By comparison, the great advantage of photoluminescence measurements becomes obvious. With our method we can determine values of $\alpha_{bb}(\hbar\omega)$ which are nearly 5 orders of magnitude smaller than the absorption coefficient for free carrier absorption. In the high energy range, our data agree quite well with those extracted from the published data of the transmission experiment.

The influence of heavy doping on the band structure of silicon is often described by a single parameter ΔE_g, named band-gap narrowing. This band-gap narrowing has been investigated by many authors with different techniques like photoluminescence, optical absorption, or electrical transport measurements on device structures, a good summary and a comparison of the different methods is given by Wagner and del Alamo.[28] However, an exact description of the influence of heavy doping on the band structure of silicon with only one parameter is not possible, because there are at least two points which have to be taken into account. The first is a rigid shift of valence and conduction band towards one another and the second is the formation of band tails with increasing doping density (see for example Ref. 29). Band tails, in particular, play an important role for the interpretation of luminescence data, because low energy emission resulting from transitions near the band edge is preferred as predicted by the generalized Planck radiation law. Transmission experiments, however, are not sensitive to these transitions, because $\alpha_{bb}(\hbar\omega)$ is very small and $\alpha_{\text{tot}}(\hbar\omega)$ is dominated by $\alpha_{fc}(\hbar\omega)$. This has been pointed out by Dumke[30] and by Pantelides *et al.*[31]

Comparing the results of transmission and conventional photoluminescence experiments concerning band-gap narrowing, a precise analysis of the photoluminescence line shape is necessary. Values for the band-gap narrowing in heavily doped silicon were already determined by, for example, Dumke[30] and Wagner.[32] Well below the laser threshold the spontaneous emission rate is given in Eq. (6). For photon emission under phonon emission a spectrum of the form

$$dr_{em}(\hbar\omega)\propto(\hbar\omega-\hbar\Omega-E_g)^2\hbar\omega e^{-\hbar\omega/kT}d\hbar\omega, \qquad (16)$$

is obtained from Eq. (6), if only one phonon branch is considered and if parabolic bands are assumed and excitonic effects are neglected.[33] This is the exact expression for the spontaneous emission rate under the assumptions made above, and it is quite different from the one used for example, by Dumke[30] for his determination of band-gap nar-

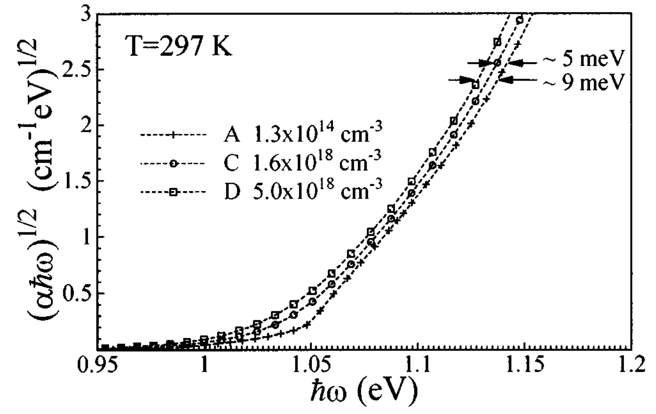

FIG. 5. The function $\sqrt{\alpha_{bb}(\hbar\omega)\times\hbar\omega}$ shows a more or less rigid shift towards lower photon energies with increasing doping level. However, this is only true for one-phonon transitions and if band tails are not involved in the absorption processes (see Figs. 3 and 4).

rowing in p-type silicon by an analysis of the photoluminescence data of Schmid *et al.*[34] Connecting the spontaneous emission rate with the absorption coefficient for band–band transitions brings up another important point which has been overlooked so far. Band-gap narrowing extracted from transmission experiments is deduced from a comparison with the absorption coefficient of high resistivity silicon where excitonic absorption plays an important role,[33] whereas it is negligible in the heavy doping range.[15] However, the parameter ΔE_g extracted from luminescence data results from a line shape analysis without any exciton contribution,[30,32] which is correct only in the case of heavy doping. Even for nearly intrinsic silicon this way of luminescence data analysis would result in a band-gap narrowing of about the excitonic binding energy (14.7 meV[14]), which is obviously wrong. Furthermore it is difficult to model multiphonon transitions in a line shape analysis, because they follow a quite different energy dependence than one-phonon transitions,[23,35] but they are important for a correct description of the luminescence lineshape, and for determining ΔE_g. In a detailed line shape analysis additional problems arise through the unknown position of the Fermi level which is linked to the unknown densities of states at the band edges, especially in heavily doped silicon. None of these difficulties occurs by using our method. By taking advantage of the geometry of our experiment, we use the reabsorption inside the sample to determine the absolute value of $\alpha_{bb}(\hbar\omega)$ with a relative measurement of the photoluminescence intensity so we are able to investigate in detail both parts of the absorption spectrum, the low energy part which is characterized by multiphonon absorption and the influence of band tails (Figs. 3 and 4), and the higher energy part which is described by one-phonon absorption and a more or less rigid shift of the densities of states. If the absorption process is dominated by a single phonon branch with energy $\hbar\Omega$ and if excitonic transitions are neglected, indirect transitions follow the relation $\sqrt{\alpha_{bb}(\hbar\omega)\hbar\omega} \propto \hbar\omega - E_g \pm \hbar\Omega + \Delta E_g$.[33,36] This is pointed out in Fig. 5, which shows selected data for $\sqrt{\alpha_{bb}(\hbar\omega)\hbar\omega}$ as a function of $\hbar\omega$. In the energy interval shown in Fig. 5, the absorption of a photon with $\hbar\omega > 1.09$ eV is dominated by the absorption of the TO phonon, whereas for photon energies $\hbar\omega < 1.05$ eV the absorption of a photon is accompanied by the simultaneous absorption of two phonons.[36]

For the rigid shift in the high energy regime we find 5 and 9 meV for the samples C and D, with respect to the data of the high resistivity sample A. These values are in good agreement with those determined by Schmid with transmission measurements.[11]

Now we come back to Fig. 4, where we have added calculated values for $\alpha_{bb}(\hbar\omega)$, neglecting the excitonic part of the absorption coefficient.[23,36,37] It is obvious that there is a great difference in the determination of ΔE_g depending on the selected energy interval and the model for the analysis of the experimental data. Any value between 50 meV and 9 meV (Fig. 5) is possible. A band-gap narrowing of 50 meV for a doping concentration of $N_D = 5\times10^{18}$ cm^{-3} was determined by Wagner,[32] using a line shape analysis of his photoluminescence data.

V. CONCLUSIONS

We have developed a method for the absolute determination of the band–band absorption coefficient for moderately doped silicon, based on a relative measurement of the emitted photoluminescence intensity and the validity of the generalized Planck radiation law. The absorption coefficient can be extracted directly from the emission spectra without any assumption concerning the density of states at the band edge or the position of the Fermi energy. The influence of the free carrier absorption is very small, and can easily be taken into account. With this method it is possible to determine absolute values of the absorption coefficients for band–band transitions $\alpha_{bb}(\hbar\omega)$ which are up to five orders of magnitude smaller than the absorption coefficient for free carrier absorption $\alpha_{fc}(\hbar\omega)$. These measurements will help to understand the discrepancies in the determination of the band-gap narrowing, ΔE_g, derived from the analysis of photoluminescence spectra and transmission experiments. This method is not restricted to the examined doping range and it can easily be applied to higher doping levels and other direct and indirect semiconductor materials.

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