# New calculations of the quantum yield of silicon in the near ultraviolet

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The rigorous expression for the quantum yield for electron-hole pair production was simplified using assumptions inspired by Kane's random- $k$  approximation and by recent results of Alig, Bloom, and Struck. The resulting approximation was intuitively satisfying. It required integration with respect to kinetic energy of the product of the joint distribution of the photogenerated electrons and holes and the average number of electron-hole pairs created by the cascade of impact ionizations initiated by a carrier with a given kinetic energy. The first quantity in the integrand was calculated from a self-consistent, first-principles band structure for silicon; the second was obtained from results of Alig, Bloom, and Struck. The results agreed reasonably well with recent experimental measurements of the quantum yield of silicon in the ultraviolet.

#### I. INTRODUCTION

The quantum yield of silicon is of considerable practical interest as an absolute radiometric stand- $\arctan \frac{1}{2}$  It is also interesting from a more fundament point of view, because it is determined by the interaction of fundamental optical and electronic processes in silicon. The absorption of photons having energies in excess of the band-gap energy distributes electrons and holes over the conduction and valence bands (i.e., in kinetic energy), and a fraction of the photogenerated electrons and holes create new electron-hole pairs by impact ionization. This is the process whereby a sufficiently energetic carrier loses energy to a valence-band electron during an Auger transition, which causes the valence-band electron to jump into the conduction band.

Antončík and  $Gaur^2$  (AG) have shown qualitatively how the distribution over the bands of the photogenerated electrons and holes produces features in the quantum-yield spectra of Si and Ge. However, some of the approximations that they used combined to produce rather large errors (quantum yields less than one at some photon energies), so their results are not useful for comparison with recent high-accuracy experimental results<sup>3</sup> for silicon.

In connection with a larger study of ionization scattering that included acceleration of electrons by electric fields, Alig, Bloom, and Struck<sup>4</sup> (ABS) calculated the quantum yield of Si, Ge, InSb, and PbS, using approximations very different from those adopted by AG. As it turns out, the high symmetry

of the band-structure model used by ABS produced a rather conservative lower bound to the quantum yield. $3$  Upper bounds can also be obtained from this model, but real features that are apparent in the experimental spectra of Ref. 3 are beyond the ABS model.

In this paper, we will describe a more accurate approach to quantum-yield calculations. From one point of view, our approach can be considered to be a combination of the approach of AG (to get the features of the quantum-yield spectra) with the approach of ABS (to obtain a manageable approximation to the average number of electron-hole pairs created by an energetic electron or hole). However, we have approached the problem from a somewhat different point of view than either AG or ABS, and we have considered the approximations that we eventually adopted in considerable detail. The remainder of this paper presents the theory of the quantum yield, discusses the simplifying assumptions that we adopt, describes the details of our computational procedure, and discusses our results and their relation to the recent experimental results and the earlier calculations. In particular, we are able to identify the major sources of error in the earlier calculations, and we discuss how we have avoided them.

### II. THEORY

Let  $E_{vi}(\vec{k})$  and  $E_{ci}(\vec{k})$  be the *i*th valence- and the jth conduction-band energies, respectively, at the

point k in the reduced Brillouin zone (BZ), and measure valence-band energy as a positive quantity with its zero at the top of the uppermost valence band, and conduction-band energy as a positive quantity with its zero at the bottom of the lowest conduction band. Thus  $E_{vi}(\vec{k})$  and  $E_{ci}(\vec{k})$  measure the hole and electron kinetic energies, respectively.

Let  $N_{vi}(\vec{k})$  and  $N_{cj}(\vec{k})$  be the average number of electron-hole pairs created by the cascade of impact ionizations initiated by a hole with momentum  $\vec{k}$  in

$$
\Delta \eta(h\nu)\alpha(h\nu) = \sum_{i,j} \int_{BZ} d^3k \mid M \mid^2 \delta(h\nu - E_G - E_{vi}(\vec{k}) - E_{cj}(\vec{k}))[N_{vi}(\vec{k}) + N_{cj}(\vec{k})], \qquad (2)
$$

and

$$
\alpha(h\nu) = \sum_{i,j} \int_{BZ} d^3k \mid M \mid^2 \delta(h\nu - E_G - E_{vi}(\vec{k}))
$$
  
-
$$
E_{cj}(\vec{k}))
$$
 (3)

In Eqs. (2) and (3),  $M$  is the matrix element for the direct, interband transition, and the product of  $|M|^{2}$  and the  $\delta$  function describes the relative density of electron-hole pairs created by the photogeneration process at the point  $\vec{k}$ . Thus  $\alpha(h\nu)$  is proportional to the absorption coefficient of the material in question.

The interpretation of Eqs.  $(1)$ – $(3)$  is straightforward. The quantum yield is equal to 1 (electronhole pair created directly by the absorption process) plus the number of electron-hole pairs created by the cascade of impact ionizations initiated by the distribution of electrons and holes in the BZ that results from the absorption process.

It turns out that  $N_{vi}(\vec{k})$  and  $N_{cj}(\vec{k})$  derive most of their  $\vec{k}$  dependence implicitly from the kinetic energy of the carriers at the point k in the ith valence and jth conduction band, respectively. Therefore, it is convenient to decompose them into the sums of implicit functions of k and explicit functions of k as shown below, where we will later assume that the

the ith valence band and by an electron with momentum k in the *j*th conduction band, respectively. In terms of the above quantities, the quantum yield for electron-hole pair production (which is defined as the average number of electron-hole pairs created per absorbed photon of energy  $h\nu$ ) is given by

$$
\eta(h\nu) = 1 + \Delta \eta(h\nu) \tag{1}
$$

where

contribution from the explicit functions of  $\vec{k}$  are negligible. Let

$$
N_{vi}(\vec{k}) = N_v(E_{vi}(\vec{k})) + \Delta N_{vi}(\vec{k}) , \qquad (4)
$$

where

$$
N_v(E) = [\rho_v(E)]^{-1}
$$
  
 
$$
\times \sum_i \int_{BZ} d^3k \, N_{vi}(\vec{k}) \delta(E_{vi}(\vec{k}) - E) \quad (5)
$$

is the average over the BZ of the number of electron-hole pairs created by the cascade of impact ionizations initiated by a hole with kinetic energy  $E$ , and where

$$
\rho_v(E) = \int_{BZ} d^3k \, \delta(E_{vi}(\vec{k}) - E) \tag{6}
$$

is proportional to the valence-band density of states. Replacement of  $v$  by  $c$  and  $i$  by  $j$  at all occurrences in Eqs. {4}—(6) produces the equivalent decomposition of  $N_{ci}(\vec{k})$ .

Substitution of Eq. (4) and its equivalent for elec-<br>
ons into Eq. (2), and use of the  $\delta$ -function theorem<br>  $N_v(E_{vi}(\vec{k})) = \int dE N_v(E) \delta(E_{vi}(\vec{k}) - E)$  (7) trons into Eq.  $(2)$ , and use of the  $\delta$ -function theorem

$$
N_v(E_{vi}(\vec{k})) = \int dE \, N_v(E) \delta(E_{vi}(\vec{k}) - E) \tag{7}
$$

and its equivalent for  $N_c(E_{cj}(\vec{k}))$ , allow Eq. (2) to be rewritten as

$$
\Delta \eta(h\nu) = \int dE[N_{\nu}(E)P_{\nu}(h\nu,E) + N_c(E)P_c(h\nu,E)]
$$
  
+ 
$$
[\alpha(h\nu)]^{-1} \sum_{i,j} \int_{BZ} d^3k |M|^2 \delta(h\nu - E_G - E_{\nu i}(\vec{k}) - E_{cj}(\vec{k})) [\Delta N_{\nu i}(\vec{k}) + \Delta N_{cj}(\vec{k})],
$$
 (8)

where

$$
P_v(hv,E) = [\alpha(hv)]^{-1} \sum_{i,j} \int_{BZ} d^3k |M|^2 \delta(hv - E_G - E_{vi}(\vec{k}) - E_{cj}(\vec{k})) \delta(E_{vi}(\vec{k}) - E)
$$
\n(9)

and the equivalent expression for  $P_c(hv, E)$  describe the distributions of holes and electrons, respectively, over kinetic energy  $E$  resulting directly from the absorption of photons of energy  $h\nu$ .

#### III. SIMPLIFYING ASSUMPTIONS

So far, the development has been rigorous within the framework of a band structure. Of course, to

simplify the computation of  $\eta(h\nu)$ , we must make a number of simplifying assumptions. Foremost among these is the assumption that the second integral on the right-hand side of Eq. (8) is negligible compared to the first. We also assume that  $N_{\nu}(E)=N_{c}(E)=N(E)$ , where  $N(E)$  is derived from an approximate treatment of impact ionization that uses both a highly simplified band-structure model and the random-k approximation to the transition rate for impact ionization. However, it turns out that the errors introduced by all of these assumptions are small compared to those associated with poor approximations for  $P_v(hv, E)$  and  $P_c(hv, E)$ , so we employ a rather sophisticated band-structure model to evaluate the first term in Eq. (8). We turn now to a detailed discussion of the major assumptions that we make.

The functions  $N_{vi}(\vec{k})$  and  $N_{cj}(\vec{k})$  are determined in a rather complicated way by the ratio of the transition rate for phonon emission by a carrier at the point  $E_{vi}(\mathbf{k})$  or  $E_{ci}(\mathbf{k})$  in the BZ to that for impact ionization by a carrier at the same point in the BZ. As might be guessed, it is useful to decompose the transition rate for impact ionization into implicit and explicit functions of k, for example,

$$
r_{cj}(\vec{k}) = r_c(E_{cj}(\vec{k})) + \Delta r_{cj}(\vec{k}), \qquad (10)
$$

where

$$
r_c(E) = [\rho_c(E)]^{-1}
$$
  
 
$$
\times \sum_j \int_{BZ} d^3k \ r_{cj}(\vec{k}) \delta(E_{cj}(\vec{k}) - E) \quad (11)
$$

is the average over the BZ of the transition rate for impact ionization by electrons with kinetic energy E. Replacement of  $c$  and  $j$  by  $v$  and  $i$  at all occurrences gives the similar expressions for holes.

Calculation of  $r_{ej}$ (k) is quite difficult because an integration is needed over the final states of the electron and hole created by the impact ionization, as well as over the final states of the excited carrier. This involves a nine-dimensional integral in k space. The calculation defined in Eq.  $(11)$  is even more difficult, involving integration over twelve dimensions. However, Kane<sup>5</sup> and Geist and Gladden<sup>6</sup> have shown that the random-k approximation to  $r_c(E)$ , which requires integration over only three dimensions in energy space, is surprisingly accurate.

Furthermore, Kane's results imply that  $\Delta r_{cj}(k)$ carries very little information not already available from  $r_c(E_{cj}(k))$ . To be specific, Kane used a Monte Carlo procedure to evaluate the twelve-dimensional integral in Eq.  $(11)$  for energetic electrons in silicon, and he found that  $r_c(E)$  increased by about 5 orders of magnitude from about 1.3 to 6.9 eV. Over the same range of  $E$ , he found that the variation in

 $\Delta r_{cj}(\vec{k})/r_c(E_{cj}(\vec{k}))$  that is caused by the variation in the matrix elements for impact ionization at constant energy but at different locations in the BZ was less than 307o.

In light of the above, it seems quite reasonable to assume that  $\Delta r_{cj}(\vec{k}) = 0$ , and to use the randomapproximation to  $r_c(E)$ . The saving in time is enormous, while the error incurred is modest. Alig, Bloom, and Struck<sup>4</sup> have generalized these ideas considerably, and applied them to a study of ionization scattering in semiconductors and insulators. They used an exceedingly simple band-structure model for all materials, as well as the random- $k$  approximation to the transition rate for impact ionization. Their band-structure model consisted of a parabolic conduction band with the free-electron effective mass, a parabolic valence band with the negative free-electron effective mass, a direct gap of energy  $E_G$ , and a threshold energy for impact ionization  $E_{\text{th}}$ .

ABS used the same ratio of the average matrix element for phonon emission to that for impact ionization for both electrons and holes, and they used an elaborate iterative procedure to calculate  $N_c(E)=N_v(E)=N(E)$  from the random-k approximation to  $r_c(E)=r_v(E)=r(E)$ , and a similar approximation to the transition rate for phonon emission. They chose the ratio of the matrix elements such that the large energy limit of  $E/N(E)$  was equal to the pair-creation energy for silicon, and obtained good agreement with a variety of experimental results on a number of materials. Apparently,  $N_c(E)$  and  $N_v(E)$  are quite insensitive to the details of the band structure, so that the three parameters,  $E_G$ ,  $E_{th}$ , and the average pair-creation energy are sufficient to determine the shape and the absolut value of  $N_c(E)$  and  $N_v(E)$ .<sup>6</sup> To the extent that this is true, materials that have nearly identical thresholds for impact ionization by energetic electrons and by energetic holes will have  $N_c(E) \sim N_v(E)$ , and the procedure of ABS will work well.

We then substitute the approximation that  $N_c(E)=N_c(E)=N(E)$  into Eq. (8), ignore the integral over the BZ for the reasons stated earlier, and combine the result with Eq. (1) to obtain

$$
\eta(h\nu) = 1 + \int dE P(h\nu, E) N(E) , \qquad (12)
$$

where

$$
P(h\nu,E) = P_v(h\nu,E) + P_c(h\nu,E) \tag{13}
$$

Equations (12) and (13) constitute the approximate expression for the quantum yield that we actually evaluated.

The function  $P(hv, E)$ , which is just the joint distribution of photogenerated electrons and holes over

the kinetic energy  $E$  as a function of photon energy,  $h\nu$ , has a number of interesting properties. Conservation of energy of the absorbed photons requires that  $P(hv, E)$  be zero for the kinetic-energy interval  $E \geq h\nu - E_G$ , and that it be symmetric about the midpoint energy  $(hv - E_G)/2$ . It is normalized such that its integral over kinetic energy is 2 (one electron plus one hole per pair), and the broader it is in  $E$ space at a given  $h\nu$ , the greater the value of the quantum yield. This last property results from the preceding constraints on  $P(hv, E)$  in combination with the fact that  $d^2N(E)/dE^2 \gg 0$  near to (but above) the threshold for impact ionization. The net effect is that the quantum yield is very sensitive to the details of  $P(hv, E)$  but rather insensitive to those of  $N(E)$ .

### IV. CALCULATION DETAILS

We approximated  $N(E)$  in Eq. (12) by

$$
N(E) = 1 - p_0(E) \t{,} \t(14)
$$

where  $p_0(E)$  is the probability that a carrier of kinetic energy  $E$  will cause no impact ionizations. The right-hand side of Eq. (14) constitutes the first two terms of the rigorous expression

$$
N(E) = 1 - p_0(E) + \sum_{n=2}^{\infty} (n-1)p_n(E) , \qquad (15)
$$

where  $p_n(E)$  is the probability that exactly n electron-hole pairs will be created by the cascade of impact ionizations initiated by a carrier of kinetic energy  $E$ . Equation (15) is a straightforward result of the definition of  $N(E)$  in terms of  $p_n(E)$ , namely,

$$
N(E) = \sum_{n=1}^{\infty} n p_n(E) , \qquad (16)
$$

and the requirement that the probability of all possible events be unity, that is,

$$
\sum_{n=0}^{\infty} p_n(E) = 1 \tag{17}
$$

Equation  $(14)$  is an excellent approximation<sup>4</sup> to Eq. (15) for  $E \leq 4$  eV or  $h\nu \leq 5.1$  eV, and is only 10% low at  $hv=6$  eV. For  $p_0(E)$  in Eq. (14), we used the same values that ABS derived to give the correct pair-creation energy for silicon.<sup>7</sup>

We calculated  $P_v(hv, E)$  and  $P_c(hv, E)$  in Eq. (13) by assuming that  $|M|^2$  is independent of  $\vec{k}$  in Eq.  $(9)$ , and using the theorem that

$$
\int d^3x \, \delta(f(\vec{x}))\delta(g(\vec{x})) = \int \frac{dl}{|\vec{\nabla}f(\vec{x})| |\vec{\nabla}_f g(\vec{x})|},
$$

$$
f(\vec{x}) = g(\vec{x}) = 0 \quad (18)
$$

where  $\vec{\nabla}_f$  indicates the component of the gradient along the surface  $f = 0$ , and where dl is integrated along the line of intersection of the two surfaces defined by  $f = g = 0$ . The assumption that the matrix elements are independent of k could have been avoided, but it produces less error than many of the other assumptions already adopted.<sup>8</sup>

To evaluate the line integral in Eq. (18) numerically,  $f(\vec{x})$  was treated as in the linear-analytictetrahedron method for evaluating the density of states in three-dimensional Brillouin zones.<sup>9</sup> That is, the irreducible wedge of the BZ was divided into tetrahedra, and  $f(\vec{x})$  was approximated by  $f(\vec{x})$ , which is a linear function of  $\vec{x}$  over each tetrahedron such that  $\tilde{f}(\vec{x})=f(\vec{x})$  at the corners of the tetrahedra. As a result,  $\vec{\nabla} \cdot \vec{f}(\vec{x})$  is a constant over each tetrahedron, and  $\tilde{f}(\vec{x})=0$  is a continuous surface consisting of three or less triangles per tetrahedron. Next,  $g(\vec{x})$  was treated as in the analytictriangular-linear-energy method<sup>10</sup> for evaluating the density of states in a two-dimensional Brillouin zone. The end result is that the line integral in Eq. (18} is evaluated as a sum of analytic expressions, which are stated in Ref. 10, that depend only upon the values of  $f(\vec{x})$  and  $g(\vec{x})$  at a small number of points in the BZ.

The band structure that we used in Eq. (9) and its equivalent for  $P_c(hv,E)$  is that described by Wang<br>and Klein.<sup>11</sup> It is a state-of-the-art application of and Klein.<sup>11</sup> It is a state-of-the-art application of local-density theory employing a fully selfconsistent, first-principles calculation. It suffers from the well-known problem of describing the excitation spectrum using single-particle energies from local-density theory. For instance, the silicon band gap is calculated to be 0.67 eV rather than the experimentally determined value of 1.12 eV. We corrected for this error by a rigid displacement of all of the conduction bands to higher energy by 0.45 eV. With this change, the direct gap occurs near 3.<sup>1</sup> eV rather than 3.4 eV.

#### **V. RESULTS**

The result of our calculation is shown in Fig. 1, where it is compared with recent experimental results for the quantum yield of  $p^+$ -type silicon. Figure <sup>1</sup> also shows upper and lower bounds for the quantum yield, and an improved approximation still within the framework of the ABS model.

With  $N(E)$  fixed in Eq. (12),

$$
P(hv, E) = 2\delta(hv - E_G - 2E)
$$
 (19)

and

$$
P(hv,E) = \delta(E) + \delta(hv - E_G - E) , \qquad (20)
$$

provide respective lower and upper bounds to the



FIG. 1. Comparison of various expressions for the quantum yield of silicon with experimental values from Ref. 3. The lower bound (which was used as a quantumyield approximation in Ref. 4) is obtained from the assumption that the photon energy in excess of the bandgap energy is divided equally between the photogenerated hole and electron; the upper bound from the assumption that all of the excess energy is given to one or the other of the two photogenerated carriers. A more realistic generic distribution of the photogenerated carriers over kinetic energy gives curve 1, and the distribution of photogenerated carriers obtained from the self-consistent, first-principles band structure of Ref. 11 gives curve 2.

quantum yield subject to the constraints imposed on  $P(hv, E)$  by conservation of energy. Equation (19) describes a band structure in which the photon energy in excess of the band-gap energy is divided equally between the photogenerated electrons and holes at all photon energies. This does not happen in real band structures, of course, but it does occur with direct transitions in the highly symmetric ABS model band structure. This is the reason that ABS reported such a low quantum yield for silicon near threshold. To improve the approximation obtained from the ABS approach,  $\text{Alig}^7$  has suggested that a random-k approximation to the photogeneration process similar to that used for the impact ionization process (i.e., indirect transitions involving phonons of negligible energy) might produce a more realistic estimate of the quantum yield within the framework of the ABS model. Indeed, this seems to be the case.

Equation (20) describes a band structure in which

all of the excess photon energy is given to one of the photogenerated carriers, the kinetic energy of the other carrier remaining zero. A flat valence band would produce this result.

Real distributions of the photogenerated carriers over kinetic energy vary between these extremes subject to the earlier mentioned constraints that we repeat here.  $P(hv, E)$  is nonzero only for E in the interval from 0 to  $h\nu - E_G$ , it is symmetric about the midpoint of that interval, and its integral over  $E$  is 2.

Figure 2 shows  $P(3.13 \text{ eV}, E)$ , which is approaching the extreme of Eq. (20), while Fig. 3 shows a more intermediate distribution over kinetic energy, namely  $P(4.55 \text{ eV}, E)$ . For the band structure that we used, most of the direct transitions at 3.13 eV occur from very near the top of the valence band to deep within the conduction band. Thus, at this photon energy, the photogenerated electrons are receiving almost all of the excess photon energy and the photogenerated holes almost none, and the calculated quantum yield approaches its upper bound.

The same feature would not be expected to occur in the experimental curve until about 3.4 eV, and if it is there, it is not obvious. There are two explanations for this, but the relative role of each is somewhat uncertain at this time. First, the experimental curve was derived from measurements on  $p^+$ -type silicon, and the strength of the direct transition from regions very near the top of the uppermost valence band is reduced by the decreased electron population there. Second, by what might be called coincidence, three different regions of the BZ have the same approximate direct gap of about 3.4 eV.



FIG. 2. Distribution  $P(hv, E)$  of photogenerated electrons and holes over the kinetic energy  $E$  in the band structure of Ref. 11 for a photon energy  $h\nu$  of 3.13 eV.



FIG. 3. Distribution  $P(hv, E)$  of electrons and holes over the kinetic energy  $E$  in the band structure of Ref. 11 for a photon energy  $h\nu$  of 4.55 eV.

As a result, the feature in the silicon absorption spectrum near 3.4 eV is a composite associated with transitions from these different regions of the BZ. The total contribution from the region very near the top of the valence band is quite small.<sup>12</sup> On the other hand, the contributions from all of these regions are resolved into three separate features stretching from 3.<sup>1</sup> to 3.4 eV by the band structure that we used.<sup>13</sup> Apparently the feature near 3.1 eV has very little contribution other than that arising very near the top of the valence band. It is to be noted that features in the absorption coefficient spectra need not appear in the quantum-yield spectra, and vice versa. Only those involving transitions from the band edges will be prominent in the quantum yield spectra. Thus reducing the theoretical absorption spectrum at 3.<sup>1</sup> eV by moving contributions from parts of the BZ other than the vicinity of point  $\Gamma$  to higher photon energies, actually increases the quantum-yield spectrum at 3.<sup>1</sup> eV, as can be seen in Fig. 1.

In a similar way, the feature near 4.4 eV that occurs in both curves includes some transitions occurring from deep within the valence band near  $X_4$  to near the bottom of the conduction band near  $X_1$ . The significantly greater value of the peak in the calculated curve is explained primarily by the fact that these transitions occur at about 0.<sup>1</sup> eV greater photon energies in the band structure that we

used than in the real silicon band structure. The really significant difference is the width and depth of the minimum that follows the maximum near 4.4 eV. We do not know the details of the explanation, but assume that it has to do with either the differences between the calculated and true band structure, or the assumption of constant matrix elements for the absorption process.

## VI. DISCUSSION

ABS did not calculate the quantum yield in the same way that we did, but their procedure is equivalent to using Eq. (19) for  $P(hv, E)$ . It was pointed out earlier that when  $N(E)$  is specified, use of Eq.  $(19)$  produces the lowest possible value for the quantum yield that is consistent with the physical constraints on  $P(hv, E)$ . This is the reason that the quantum yields reported by ABS were so low.

Use of a more realistic, generic  $P(hv, E)$  distribution will produce a more realistic quantum yield in the ABS procedure. For instance, the random- $k$  approximation to the absorption process with the ABS band structure produces a fairly good result for silicon as shown in Fig. 1. This does not mean that indirect transitions are actually being invoked. It is just an artifact to compensate for the very high symmetry of the ABS band structure.

Turning attention to the calculation by AG, we first observe that their procedure was much more similar to ours. However, the actual computation was done in the form

$$
\eta(h\nu) = \int dE P(h\nu, E)g(E)
$$
  
=  $\frac{1}{2} \int dE P(h\nu, E)$   
+  $\int dE P(h\nu, E)N(E)$ , (21)

where  $g(E) = \frac{1}{2} + N(E)$ . While this is formally equivalent to our Eq.  $(12)$ , it is not computationally equivalent to it. The first term in both Eqs. (12) and (21) should be identically equal to one (electron-hole pair created directly as the result of the annihilation of one photon). This, of course, is the case with Eq. (12). However, any errors in the normalization of  $P(hv, E)$  show up in Eq. (21) in the value of the first term, which should be 1 as well as in  $\Delta \eta(h v)$  [compare Eqs. (1), (12), and (21)]. Thus the propagation of error is worse with Eq. (21) than with Eq. (12). This would not be a serious problem if  $P(hv, E)$ were accurately normalized. Unfortunately, this was not the case with the calculation by AG.

AG considered only two valence and two conduction bands, and these were not sufficient to account for all of the absorption by silicon in the  $(3-6)-eV$ spectral region. This is clear from Fig. <sup>1</sup> of their paper, where they plotted the relative probability of a photon being absorbed by a transition from the ith valence band to the jth conduction band. The sum over the four transitions that they considered does not equal one.

However, AG normalized  $P(hv, E)$  to the true absorption coefficient rather than the absorption coefficient that describes the four transitions that they actually considered. The net effect was to impose structure on the quantum yield that is related to the ratio of the absorption coefficient for the four transitions to that for all transitions. Therefore, this structure, which is quite evident in the AG curves, is an artifact. The only structure that the quantum yield actually shows is associated with the shape of  $P(hv, E)$ , and this structure is pronounced only when the absorption coefficient contains a large contribution from transitions involving the top of the uppermost valence band or the bottom of the lowest conduction band.

Finally, we observe that AG did not know what

value to use for the ratio of the average matrix element for impact ionization to that for phonon emission. Therefore, they calculated a family of curves in which this ratio was systematically varied for both holes and electrons, and the resulting curves were compared with Christensen's<sup>14</sup> experimental results, which were the best in existence at that time. However, the later investigation by ABS suggests that it is possible to derive a quite satisfactory value for this ratio from the average pair-creation energy at high energy.

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