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Quantum yield of electron-hole pairs in semiconductors

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It is shown that the two existing theories, the "crazy-carpentry" and the probability method, are essentially equivalent in evaluating quantum yield and variance in semiconductors. Quantum yield is determined by an integro-differential equation represented in terms of the density of states, the loss parameter, and the threshold energy. The analytical method used to calculated the relative yield, i.e., the inverse of the average *e-h* pair-creation energy, is developed for the two cases: extended crazy-carpentry and free-particle models. The optical-mode deformation-potential and the polar-mode electrostatic-potential contributions to the phonon loss are taken into account.

I. INTRODUCTION

Quantum yield of electron-hole pairs generated by high-energy electrons or photons in semiconductors is an important factor that determines phosphor efficiency or the characteristic performance of semiconductor devices. Electron-hole pairs are generated in semiconductors by the branching processes of ionization and phonon emission. Yield and Fano factor are largely determined at the final stage of the branching process where secondary electrons and holes have energies a few times the ionization threshold, and where the energy loss by phonons is competing with the energy loss by ionization.[1–5]

van Roosebroeck[2] developed a phenomenological model that describes the statistics of the branching processes independent of the details of the physics. His model, named "crazy carpentry," is represented by two approaches: (1) computer simulation of "board" cutting, and (2) the mathematical formulation in terms of the moment-generating function. His results show that yield is proportional to the energy of the primary particle when this is a few times larger than the threshold energy. A proportionality constant, the limiting relative yield, corresponds to the inverse of the average *e-h* pair-creation energy.

Alig, Bloom, and Struck[6] proposed another approach called "the probability method" to calculate the yield and the Fano factor; the pair-number probability distribution is evaluated recursively. Computer calculations of the first moment $\langle n(E)\rangle$ and the Fano factor have been carried out for a wide variety of semiconductors with the free-particle model and the deformation potential for phonon loss.

This paper demostrates that the crazy-carpentry method and the probability method are equivalent in the sense that the yield and the variance satisfy the common equations for the two methods with exact correspondence between relevant parameters. In other words, the probability method is a natural extension of the crazy-carpentry method to include the effect of nonuniform state density and the energy dependence of the phonon-loss mechanisms. With the analytical method in the present paper the relative yield is determined from the slope of the linear solution of $\langle n(E)\rangle$ for large E in the extended crazy-carpentry model and the free-particle model. The quantum yield is mainly determined by two factors, the loss parameter and the threshold energy. It is found that the energy dependence of the loss parameter is important in determining the slope of the linear solution. The loss parameter is examined in terms of the optical-mode deformation potential and the polar-mode electrostatic potential.

II. THEORETICAL ANALYSIS

A. Reformulation of the probability method

For evaluating yield and variance the probability method is conveniently formulated in terms of the first and the second moments, $\langle n(E)\rangle$ and $\langle n^2(E)\rangle$, rather than the probability distribution. The probability $p_n(E)$ that the primary particle of energy E ultimately produces n ionization events is

described by the recursion relation, Eq. (12) of Ref. 6:

$$p_n(E)=P_0(E)\frac{r_{n-1}(E)}{r(E)} +[1-P_0(E)]p_n(E-\hbar\omega_0)\ ,\quad n\geq 1\ . \tag{1}$$

The first term represents the product of the probability $P_0(E)$ of the primary particle creating ionization before phonon emission and of the probability $r_{n-1}(E)/r(E)$ of the product particles further creating $n-1$ ionizations in total. The second term is the product of the probability $1-P_0(E)$ that the primary particle first creates a phonon and of the probability $p_n(E-\hbar\omega_0)$ that this particle with energy $E-\hbar\omega_0$ further produces n ionizations. The probability $P_0(E)$ that a particle produces the e-h pair prior to phonon emission is given by

$$P_0(E)=\frac{r(E)}{r(E)+w(E)}\ , \tag{2}$$

where $r(E)$ is the scattering rate for ionization and $w(E)$ that for phonon emission.

The expression for $r_{n-1}(E)$, the ionization rate that the three secondary particles will create $n-1$ ionizations, is calculated by time-dependent perturbation theory with the random-k approximation[7]:

$$r_{n-1}(E)=\frac{2\pi}{\hbar}\frac{\Delta}{V}|M|^2\sum_{i,j}\int dE_f\int dE_e\int dE_h\rho(E_f)\rho(E_e)\rho(E_h)p_i(E_f)p_j(E_e)p_{n-1-i-j}(E_h) \times\delta(E-E_g-E_f-E_e-E_h),\quad E\geq E_{\rm th} \tag{3}$$

with $E_{\rm th}$ being the ionization threshold. Hereafter, $E_{\rm th}$ is taken equal to E_g.

The equation governing the first moment can be derived by multiplying Eq. (1) by n and summing over n. One obtaines after a few rearrangements of the terms,

$$\langle n(E)\rangle=\frac{P_0(E)}{C(E)}\int_0^{E-E_g}dE_f\int_0^{E-E_g-E_f}dE_e\rho(E_f)\rho(E_e)\rho(E-E_g-E_f-E_e) \times[1+\langle n(E_f)\rangle+\langle n(E_e)\rangle+\langle n(E-E_g-E_f-E_e)\rangle] +[1-P_0(E)]\langle n(E-\hbar\omega_0)\rangle,\quad E\geq E_g \tag{4}$$

where

$$C(E)=\int_0^{E-E_g}dE_f\int_0^{E-E_g-E_f}dE_e\rho(E_f)\rho(E_e)\rho(E-E_g-E_f-E_e)\ . \tag{5}$$

Similarly, multiplying Eq. (1) by n^2 and summing over n, one obtains the equation for the second moment:

$$\langle n^2(E)\rangle=\frac{P_0(E)}{C(E)}\int_0^{E-E_g}dE_f\int_0^{E-E_g-E_f}dE_e\rho(E_f)\rho(E_e)\rho(E-E_g-E_f-E_e) \times\{1+\langle n^2(E_h)\rangle+\langle n^2(E_f)\rangle+\langle n^2(E-E_g-E_f-E_e)\rangle +2\langle n(E_f)\rangle\langle n(E_e)\rangle+2[\langle n(E_f)\rangle+\langle n(E_e)\rangle]\langle n(E-E_g-E_f-E_e)\rangle +2[\langle n(E_f)\rangle+\langle n(E_e)\rangle+\langle n(E-E_g-E_f-E_e)\rangle]\} +[1-P_0(E)]\langle n^2(E-\hbar\omega_0)\rangle,\quad E\geq E_g\ . \tag{6}$$

Below the threshold

$$\langle n(E)\rangle=\langle n^2(E)\rangle=0,\quad 0\leq E<E_g\ . \tag{7}$$

Quantum yield, $\langle n(E)\rangle$, and Fano factor

$$F=\frac{\{\langle n^2(E)\rangle-[\langle n(E)\rangle]^2\}}{\langle n(E)\rangle} \tag{8}$$

can be evaluated from the solutions of Eqs. (4) and (6), which are uniquely determined from $\rho(E)$, $P_0(E)$, and E_g.

B. Relation to the crazy-carpentry model

In this model of van Roosbroeck it is assumed that the excess energy of the particle is always divided in a constant ratio between the secondary electron and hole. Let us assume that β and $1-\beta$ fractions of the excess energy is given to the electron and hole, respectively. This corresponds to setting the condition $E_e=\beta(E-E_g-E_f)$ on Eqs. (4) and (6). We further assume that the density of states for both electrons and holes are constant, $\rho(E)=\text{const}$. Then we obtain

$$\langle n(E)\rangle=P_0(E)+[1-P_0(E)]\langle n(E-\hbar\omega_0)\rangle + \frac{P_0(E)}{E-E_g}\int_0^{E-E_g} dE'[\langle n(E')\rangle+\langle n(\beta E')\rangle+\langle n(\gamma E')\rangle],\quad E\geq E_g \tag{9}$$

and

$$\begin{aligned}\langle n^2(E)\rangle=&-P_0(E)+2\langle n(E)\rangle+[1-P_0(E)][\langle n^2(E-\hbar\omega_0)\rangle-2\langle n(E-\hbar\omega_0)\rangle]\\&+\frac{P_0(E)}{E-E_g}\int_0^{E-E_g} dE'\{\langle n^2(E')\rangle+\langle n^2(\beta E')\rangle+\langle n^2(\gamma E')\rangle\\&+2\langle n(E')\rangle[\langle n(\beta(E-E_g-E'))\rangle+\langle n(\gamma(E-E_g-E'))\rangle]\\&+2\langle n(\beta E')\rangle\langle n(\gamma E')\rangle\},\quad E\geq E_g\end{aligned} \tag{10}$$

where

$$\beta+\gamma=1\ . \tag{11}$$

Equations (9) and (10) are exactly the same as the equation for the mean yield, $y(L)=L-w(L)$, and the equation for $q(L)\equiv L^2-2Lw(L)+u(L)$, respectively, of the crazy-carpentry model where L is the initial board length, and $w(L)$ and $u(L)$ are the mean "waste" and the second moment, respectively. The equations for $y(L)$ and $q(L)$ are readily obtained from Eqs. (14) and (15) of Ref. 2. There is exact correspondence between the quantities involved in the probability method and the crazy-carpentry method as given in Table I. Thus, the crazy carpentry corresponds to a case of the probability method with the approximations: constant density of states, constant division of the excess energy of the primary particles, and energy-independent $P_0(E)$. The yield and Fano factor have been evaluated by the analytical method and the Monte Carlo method and reported in Ref. 2.

III. LIMITING YIELD

A. Extended crazy-carpentry model

Analytical calculations are made in this section of the quantum yield for the extended crazy-carpentry model. The model is extended such that: (i) The restriction of the constant division of the excess energy of

the primary particle between the electron and hole is removed, and (ii) the energy dependence of phonon emission and ionization rate is taken into account. The density of states is taken to be constant for electrons and holes. For the sake of simplicity, it is assumed that the electrons and holes are equivalent in regard to the densities of states, the ionization rate, and the phonon-emission rate.[8] Equation (4) is thus given by

$$\langle n(E)\rangle = P_0(E) + [1-P_0(E)]\langle n(E-\hbar\omega_0)\rangle + \frac{6P_0(E)}{(E-E_g)^2}\int_0^{E-E_g} dE'(E-E_g-E')\langle n(E')\rangle, \quad E \geq E_g \tag{12}$$

with the condition

$$\langle n(E)\rangle = 0, \quad E < E_g \ . \tag{13}$$

By approximating $\langle n(E-\hbar\omega_0)\rangle$ by the first two terms of the Taylor series for $E >> \hbar\omega_0$, Eq. (12) is reduced to the integro-differential equation

$$\langle n(E)\rangle + K(E)\frac{d\langle n(E)\rangle}{dE} = 1 + \frac{6}{(E-E_g)^2}\int_0^{E-E_g} dE'(E-E_g-E')\langle n(E')\rangle \ , \tag{14}$$

where

$$K(E) = \frac{w(E)}{r(E)}\hbar\omega_0 \ . \tag{15}$$

The scattering rate $r(E)$ for an electron with energy E to create an e-h pair is given by Eq. (3) with $n=1$. With a constant density of states $r(E)$ becomes

$$r(E) = \begin{cases} \dfrac{2\pi}{\hbar}\dfrac{\Delta}{V}|M|^2\dfrac{(E-E_g)^2}{2}, & E > E_g \\ 0, & E \leq E_g \ . \end{cases} \tag{16}$$

Similarly, the scattering rate $w(E)$ for an electron to lose its energy E by phonon emission is calculated using the random-k approximation. For a constant density of states $w(E)$ is independent of the particle energy

$$w(E) = \text{const} \ . \tag{17}$$

Then the loss parameter $K(E)$ varies with E as

$$K(E) = \frac{K_0}{(E-E_g)^2} \ , \tag{18}$$

with the constant parameter K_0.

It is possible to calculate $\langle n(E)\rangle$ from Eq. (14) stepwise at each interval of E_g by performing integration with boundary condition Eq. (13) and the solution obtained from the preceding step. However, the calculations are not feasible when E rises to a few times E_g. The limiting value of $\langle n(E)\rangle$ at large E is approximately evaluated as follow.

Since $K(E)$ decreases with $(E-E_g)^{-2}$ as E increase, Eq. (14) has a linear solution in the limit of large E where $K(E)$ is negligible:

$$\langle n(E)\rangle = A_1 E + A_2 \ . \tag{19}$$

The limiting relative yield, which is the inverse of the average pair-creation energy for large E, is given by

$$Y = \frac{\langle n(E)\rangle}{E} = A_1 \ . \tag{20}$$

To determine the constants A_1 and A_2, Eq. (14) is solved for large E by first introducing the linear solution of $\langle n(E)\rangle$ into the left side of Eq. (14). The integral on the right side of Eq. (14) is then performed in the three intervals between E_g, $2E_g$, pE_g, and $E-E_g$ with p an integer greater than 2. The solutions of $\langle n(E)\rangle$ at each interval are the exact solution,

TABLE I. Comparison of the crazy-carpentry and probability models.

Crazy-carpentry model	Probability model
L	E/E_g
$y(L)=L-w(L)$	$\langle n(E)\rangle$
$q(L)\equiv L^2-2Lw(L)+u(L)$	$\langle n^2(E)\rangle$
$1-r$	$P_0(E)$
x_r	$\hbar\omega_0/E_g$

$$\langle n(E)\rangle = 1-\exp\left[-\int_{E_g}^{E}\frac{dE'}{K(E')}\right], \quad E_g \le E < 2E_g \tag{21}$$

which follows from Eqs. (13) and (14), the trial solution

$$\langle n(E)\rangle = aE^2+bE+c, \quad 2E_g \le E < pE_g \tag{22}$$

and the linear solution (19) for $E \ge pE_g$. There are five relations that determine the constants A_1, A_2, a, b, and c. The condition that the solutions (21) and (22) are continuous at $E=2E_g$, and that (22) and (19) are continuous at $E=pE_g$, give the two relations

$$b=\frac{1}{(p-2)E_g}\left[pA_1E_g+A_2-1+\exp\left[-\frac{E_g^3}{3K_0}\right]\right]-(p+2)aE_g, \tag{23}$$

and

$$c=\frac{1}{p-2}\left[-2pA_1E_g-2A_2+p-p\exp\left[-\frac{E_g^3}{3K_0}\right]\right]+2paE_g^2. \tag{24}$$

The requirement that the solutions (19), (21), and (22) satisfy Eq. (14) gives the three other relations. By integrating the right side of Eq. (14) it becomes a quadratic form in $(E-E_g)^{-1}$. The conditions for the constant, the $(E-E_g)^{-1}$ and the terms to vanish lead to

$$A_1E_g-2A_2-1=0, \tag{25}$$

$$\frac{5p+2}{4}A_1E_g+\frac{(p-2)^3}{6}aE_g^2=\tfrac{1}{4}(3p-2)+\frac{2-p}{2}\exp\left[-\frac{E_g^3}{3K_0}\right]+\frac{1}{E_g}\int_{E_g}^{2E_g}dE'\left[1-\exp\left[-\frac{(E'-E_g)^3}{3K_0}\right]\right], \tag{26}$$

and

$$\frac{1}{12}\left[\frac{2K_0}{E_g^3}-5p^2-10p-4\right]A_1E_g-\frac{(p-2)^3(p+2)}{12}aE_g^2 = \tfrac{1}{2}(2-p)-\frac{p^2}{4}+\tfrac{1}{6}(p-2)(p+4)\exp\left[-\frac{E_g^3}{3K_0}\right]-\frac{1}{E_g^2}\int_{E_g}^{2E_g}dE'E'\left[1-\exp\left[-\frac{(E'-E_g)^3}{3K_0}\right]\right], \tag{27}$$

where b and c have been eliminated with Eqs. (23) and (24). Finally, the limiting yield is given by

$$Y=A_1=E_g^{-1}\left\{3p^2+12-2(p-2)^2\exp\left[-\frac{E_g^3}{3K_0}\right]+\frac{12}{E_g}\int_{E_g}^{2E_g}dE'\left[(p+2)-\frac{2E'}{E_g}\right]\left[1-\exp\left[-\frac{(E'-E_g)^3}{3K_0}\right]\right]\right\}\Big/\left[5p^2+16p+4+\frac{4K_0}{E_g^3}\right]. \tag{28}$$

In the absence of phonon loss, $K_0=0$, Eq. (28) gives

$$Y=\frac{3(p^2+4p)}{5p^2+16p+4}E_g^{-1} \quad \text{for integer } p>2. \tag{29}$$

For very large K_0, Y approaches

$$E_g^{-1}(p^2+8p+4)/(5p^2+16p+4+4K_0/E_g^3).$$

Figure 1 plots $\langle n(E)\rangle$ vs E for different values of K_0 and $p=4$. The relative yield Y is plotted as a function of K_0/E_g^3 in Fig. 2.

B. Free-particle model

For $\rho(E_e)=\rho(E_h)=d\sqrt{E}$, Eq. (4) reduces to

$$\langle n(E)\rangle+K(E)\frac{d\langle n(E)\rangle}{dE}=1+\frac{315}{16(E-E_g)^{7/2}}\int_0^{E-E_g}dE'\sqrt{E'}(E-E_g-E')^2\langle n(E')\rangle,\quad E\geq E_g \tag{30}$$

with the condition

$$\langle n(E)\rangle=0\,,\quad E<E_g \tag{31}$$

where $K(E)$ is given by Eq. (15) and the assumption $\hbar\omega_0<<E$ is again used to expand $\langle n(E-\hbar\omega_0)\rangle$ by a Taylor series. The random-k approximation is used to calculate the single ionization scattering rate $r(E)$ as before. On the other hand, momentum conservation is explicitly taken into account to calculate the scattering rate $w(E)$ by phonon emission.

Evaluation of $w(E)$ is made in Ref. 9 using time-dependent perturbation theory for the deformation potential and the polar-mode electrostatic potential in the free-electron model. The loss parameter $K(E)$ has the energy dependence.

$$K(E)=\frac{1}{2\pi}\frac{105}{(E-E_g)^{7/2}}\left[S_1(E-\hbar\omega_0)^{1/2}+S_2\frac{(\hbar\omega_0)^2}{\sqrt{E}}\ln\left|\frac{\sqrt{E}+\sqrt{E-\hbar\omega_0}}{\sqrt{E}-\sqrt{E-\hbar\omega_0}}\right|\right]. \tag{32}$$

The first and the second terms arise from the optical-mode deformation potential and the polar-mode electrostatic potential, respectively, with S_1 and S_2 given in terms of the material constants. The symbol ω_0 denotes the optical-phonon frequency.

The relative yield Y for the present case is calculated with less accuracy than for the previous case because of the complicated expression (32) for $K(E)$. One seeks the linear solution (19) of Eq. (30). The integral on the right-hand side is divided into three parts between E_g, $2E_g$, pE_g, and $E-E_g$, for which the solutions (21), (22), and (19) are used as before. Equation (30) for large E turns out to be a finite series of $(E-E_g)^{-1/2}$, involving a constant, $(E-E_g)^{-3/2}$, $(E-E_g)^{-5/2}$, $K(E)$, and $(E-E_g)^{-7/2}$ terms. We use the approximation that Eqs. (21) and (19) satisfy Eq. (30) to the extent that the constant and the terms $(E-E_g)^{-3/2}$ and $(E-E_g)^{-5/2}$ vanish. Then

$$A_1E_g-2A_2-1=0\,, \tag{33}$$

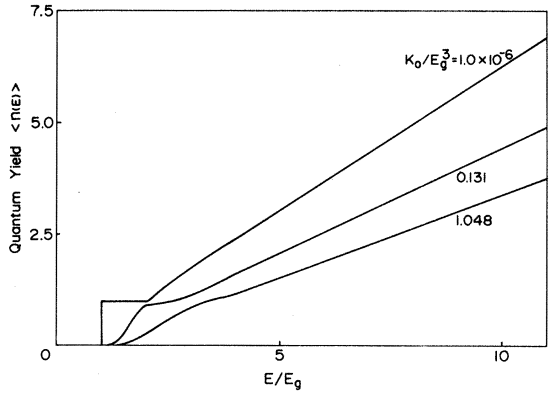

FIG. 1. Quantum yield $\langle n(E)\rangle$ vs E/E_g for different values of the loss parameter K_0/E_g^3 calculated from Eqs. (21), (22), and (19) with (18) and $p=4$.

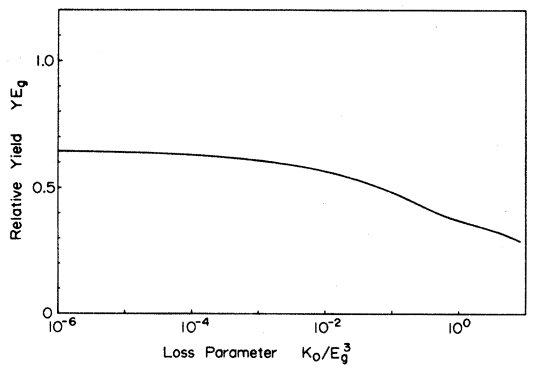

FIG. 2. Dependence of relative yield Y on the loss parameter K_0/E_g^3 calculated from Eq. (28) with $p=4$.

$$Y=\frac{1}{D(p)E_g}\{35(4p^{9/2}/63-8p^{7/2}/35+32\sqrt{2p}\,/35-64\sqrt{2}/63)$$
$$\times[15(p-2)I_{1/2}+2p^{5/2}-8\sqrt{2}+(4p^{5/2}-20\sqrt{2}p+24\sqrt{2})F(2E_g)]$$
$$-15(4p^{7/2}/35-8p^{5/2}/15+16\sqrt{2}p/15-32\sqrt{2}/35)$$
$$\times[35(p-2)I_{3/2}+2p^{7/2}-16\sqrt{2}+(4p^{7/2}-56\sqrt{2}p+80\sqrt{2})F(2E_g)]\}\,, \tag{34}$$

where

$$D(p)=35(4p^{9/2}/63-8p^{7/2}/35+32\sqrt{2}p/35-64\sqrt{2}/63)(10p^{5/2}-16\sqrt{2}p-8\sqrt{2})$$
$$-15(4p^{7/2}/35-8p^{5/2}/15+16\sqrt{2}p/15-32\sqrt{2}/35)(10p^{7/2}-32\sqrt{2}p-16\sqrt{2})\,, \tag{35}$$

$$I_{n/2}=E_g^{-(n/2+1)}\int_{E_g}^{2E_g}dE'(E')^{n/2}F(E')\,, \tag{36}$$

$$F(E)=1-\exp\left[-\int_{E_g}^{E}\frac{dE'}{K(E')}\right]. \tag{37}$$

In the absence of phonon loss $K(E)=0$, Eq. (34) gives $Y=0.652$. In Fig. 3, $\langle n(E)\rangle$ is plotted versus E for different parameter values S_1 and $S_2=0$, with $p=4$. Figure 4(a) gives the relative yield Y as a function of S_1 for different values of S_2. Figure 4(b) gives Y as a function of S_2 for different values of S_1. The present results are compared with the computer calculations in Ref. 6 which give $Y=0.617\ E_g^{-1}$ for no phonon loss, i.e., $S_1=S_2=0$, and $Y=0.30\ E_g^{-1}$ for $S_1/E_g^4=0.21$ and $S_2=0$.[10] The analytical result (34), however, approaches a finite value, 0.298, in the limit of very large S_1 or S_2. This occurs because $\langle n(E)\rangle$ is approximated by the linear solution in the low-energy region down to $E=4E_g$. The region where the linear solution holds shifts toward higher energy as the phonon loss parameter S_1 or S_2 increases. Thus, the preceding approximation for

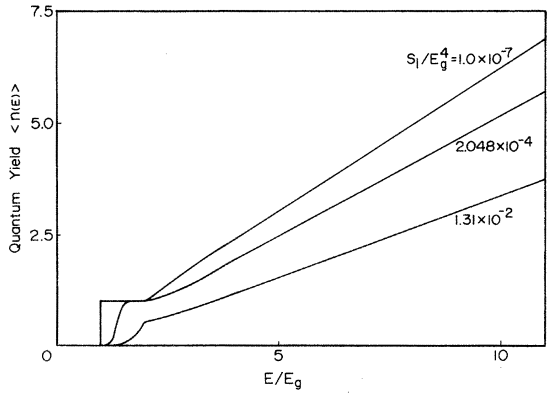

FIG. 3. Quantum yield $\langle n(E)\rangle$ vs E/E_g for different values of the loss parameter S_1/E_g^4 with $S_2/E_g^3=0$ and $\hbar\omega_0/E_g=0.025$ calculated from Eqs. (21), (22), and (19) with (32) and $p=4$.

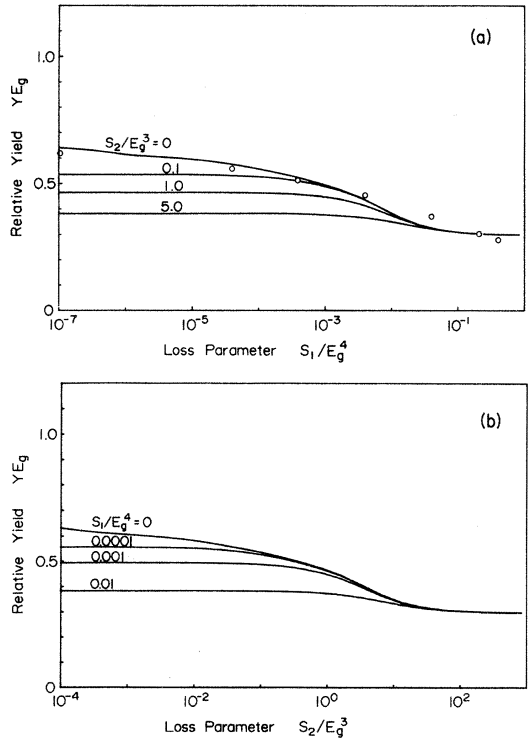

FIG. 4. Relative yield Y is plotted as a function of S_1/E_g^4 in (a) and as a function of S_2/E_g^3 in (b). Calculations done with $\hbar\omega_0/E_g=0.025$ and $p=4$ from Eq. (34). Computer calculations marked by open circles for $S_2=0$ were taken from Fig. 3 of Ref. 6.

solving the limiting yield for large phonon loss becomes inadequate. In actual semiconductors, the parameter S_1/E_g^4 is smaller than 0.5 and S_2/E_g^3 smaller than 500, values for which the analytical method gives reasonable results in agreement with the results of Ref. 6 for $S_2=0$. Agreement is within 10%.

IV. DISCUSSION

An analytical approach to calculate the quantum yield of *e-h* pairs in semiconductors has been developed based on the probability method. The relative quantum yield, which is equal to the inverse of the average pair-creation energy, is given by the slope of the asymptotic linear solution of $\langle n(E)\rangle$ for large E. The slope is determined by making use of the solutions for small E regions. An alternative method to determine the slope is to make use of the exact solution of $\langle n(E)\rangle$ at one point in the linear region obtained by computer calculations. Since $K(E)$ in general decreases as E increases, the relation $A_1E_g-1=2A_2$, as given by Eqs. (25) and (33), holds irrespective of the details of the band structure and the state densities. Then, from Eq. (19) the limiting yield is evaluated by

$$Y=A_1=\frac{2\langle n(E)\rangle+1}{2E+E_g}\ , \tag{38}$$

in terms of $\langle n(E)\rangle$ in the linear region. The validity of Eq. (38) can easily be checked with the results of computer calculations of $\langle n(E)\rangle$. The slope in the linear region is 0.39 E_g^{-1} for CdS ($E_g=2.41$ eV) and 0.48 E_g^{-1} for ZnO ($E_g=3.35$ eV) [see Figs. 9(a) and 9(b) of Ref. 6]. From Eq. (38) one obtains $Y=0.40\ E_g^{-1}$ with the computer solution $\langle n(E)\rangle=2.27$ at $E=15$ eV for CdS, and $Y=0.49E_g^{-1}$ with $\langle n(E)\rangle=2.0$ at $E=17$ eV for ZnO, both in reasonable agreement with the computer results. In fact, the alternative method is more accurate than the method presented in the preceding section for the case of large phonon loss. In contrast, the assumption of an energy-independent loss parameter $K=$const, as used in the original crazy-carpentry model, leads to the relation $(E_g+K)A_1-1=2A_2$. This in turn gives

$$Y=\frac{2\langle n(E)\rangle+1}{2E+E_g+K}\ . \tag{39}$$

The denominator involves the loss parameter K to deduce the value of Y. Thus, the assumption of constant K tends to overestimate the phonon loss contrary to the fact that it is dominant only in the energy region a few times above threshold, and consequently gives a smaller quantum yield in the higher-energy region.

The loss-parameter constant, K_0 of Eq. (18) in the extended crazy-carpentry model, and S_1 and S_2 of Eq. (32) in the free-particle model, can be described in terms of the physical properties of the materials.[11] In semiconductors, the phonon loss is contributed by the deformation potential and the polar-mode electrostatic potential. Using the time-dependent perturbation theory with the random-k approximation one obtains

$$K_0=\frac{1}{\Delta(N/W)^2\,|M|^2}\times\left[\frac{4\pi^2\hbar^2}{\rho a^2}\,|E_d|^2+\frac{3a^2e^2}{\pi\epsilon^*}(\hbar\omega_0)^2\right]\ , \tag{40}$$

where the first and the second terms arise from the deformation potential and the polar-mode electrostatic potential, respectively. The notations are as follows: W is the bandwidth, M is the matrix element of the screened Coulomb interaction, ρ is the density of the lattice, a is the lattice constants, E_d is the deformation-potential parameter, $\epsilon^*=(\epsilon_\infty^{-1}-\epsilon_0^{-1})^{-1}$ with ϵ_∞ and ϵ_0 being the high-frequency and static dielectric constants, and ω_0 is the frequency of the longitudinal-optical phonon.

Similarly, S_1 and S_2 of Eq. (32) are given by

$$S_1=\frac{\pi^6\hbar^8\,|E_d|^2}{4\Delta\,|M|^2V^2\rho m^3a^2}\ ,$$

and

$$S_2=\frac{\pi^5\hbar^8e^2}{64\Delta\,|M|^2V^2m^4}\ . \tag{41}$$

As is clear from Eq. (40) for the constant density of states, and Eqs. (32) and (41) for the free-particle model, the term of the deformation potential in the loss parameter is insensitive to the optical-phonon frequency ω_0, whereas the term from the polar-mode electrostatic potential increases as ω_0^2. Therefore, the polar semiconductors with higher polar-mode optical phonons have greater phonon loss and a smaller yield. The empirical correlation between a high ir optical-phonon frequency and a poor cathodoluminescent efficiency for a group of oxyanion phosphors seems to indicate that the polar-mode electrostatic potential dominates the deformation potential as a cause of phonon loss in these materials.

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