PHYSICAL REVIEW B VOLUME 28, NUMBER 4 15 AUGUST 1983

Enhancement of Auger recombination in semiconductors by electron-hole plasma interactions

Masumi Takeshima
Semiconductor Laboratory, Matsushita Electronics Corporation, Takatsuki, Osaka, Japan

(Received 14 April 1983)

I show that electron-hole plasma interaction has a very important effect on band-to-band Auger recombination in semiconductors. The effect is an enhancement, by a factor of about 5, of the Auger recombination rate as compared to the value calculated with the neglect of the electron-hole plasma interaction. Quantitative agreements between theories and experiments in a number of previous papers are fortuitous as a result of overestimation of overlap integrals. By careful estimation of overlap integrals the present theory gives a satisfactory explanation of experiments.

I. INTRODUCTION

The band-to-band Auger recombination (BBAR) of excess carriers in semiconductors is an intrinsic nonradiative process which is important under high concentrations of free carriers. A number of theoretical and experimental investigations[1–4] have been made on the basis of the pure-collision Auger recombination (PCAR) since a successful work by Beatie and Landsberg.[5] This process has offered, for order-of-magnitude estimation, a satisfactory explanation of experiments when at least one of the following conditions is satisfied: a narrow direct-gap material, high temperature, and/or degenerate statistics. To explain experiments under some other conditions, e.g., especially under an indirect-gap material, phonon-assisted Auger recombination (PAAR) has been proposed.[6] Theories of PCAR (Ref. 5) and PAAR (Refs. 7–10) have been based on the first-order and the second-order perturbation treatments, respectively.

Recently, I have given a theory[11] based on the Green's-function formalism through which the effect of energy-level broadening due to some scatterings can be taken into account. The theory is of general use since PCAR is obtained as a special case where the scattering effect is not considered. On the basis of the theory I have studied PAAR (Refs. 12 and 13) and the impurity-assisted Auger recombination[14–16] (IAAR). I have found that the PAAR rate is considerably larger than that based on the second-order perturbation treatment especially at high temperatures as well as the PCAR rate under almost all conditions. This situation is the same for IAAR but the difference between the IAAR rate and the PCAR rate is small under some conditions.

The Green's-function formalism of BBAR starts with the four-particle Green's function. Then the function has been given approximately as a product of four one-particle Green's functions, giving a final formula. The approximation corresponds to neglecting interactions among four particles which intervene between the initial state and the final state for the Auger transition. I have shown[11] that the effect of the neglected interactions on BBAR is unimportant with the exception of the PCAR case. The interactions result in energy shift of the interacting particles on the one hand and in particle rearrangement due to electron-hole plasma interaction on the other hand. All the discussions[11] of the effect of the interactions have been based on the first-order perturbation treatment. Actually, however, the electron-hole plasma interaction should be treated including all series of the expansion. This is a weak point of the treatment in Ref. 11.

The purpose of the present paper is to offer improved treatment of the electron-hole plasma interaction. As a result the BBAR rate in this paper is by a factor of about 5 larger than that in Ref. 11. It has been stated above that the PAAR rate in Ref. 11 is considerably larger than the results of the conventional calculations. In view of this fact, the conventional calculations are also expected to yield quite erroneous numerical results. Despite the expectation these calculations have often been shown to give a satisfactory explanation of experiments. I show that the agreements are fortuitous as a result of overestimation of overlap integrals. I point out that the overlap integrals should carefully be estimated in order to attain good agreement between the present theory and experiments.

II. BASIC FORMULA

In this section we discuss the effect of carrier-carrier interaction on BBAR. We consider the Auger transition shown in Fig. 1(a), where a carrier 1 and carriers 2,3,4 belong to the valence band (VB) and the conduction band (CB), respectively, and in Fig. 1(b), where carriers 1,2,3

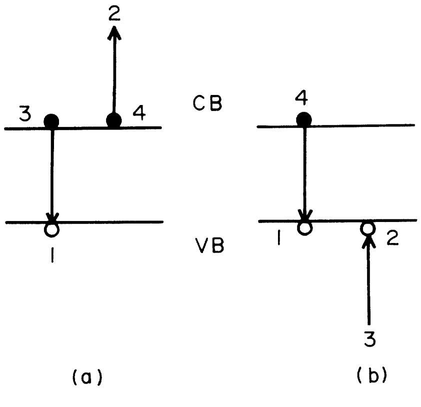

FIG. 1. BBAR in (a) the *VCCC* process and (b) the *VVVC* process.

and a carrier 4 belong to VB and CB, respectively. Let us call the processes shown in Fig. 1(a) and in Fig. 1(b) the *VCCC* process and the *VVVC* process, respectively, in numerical order of the labels 1, 2, 3, and 4 in the figure.

Let us start with quite a general expression for the excess-carrier lifetime τ of BBAR, which is given in Ref. 11 as

$$\frac{1}{\tau}=-\frac{1}{8\hbar n_C V}\sum_{\substack{1,2,3,4,\\5,6,7,8}}\Gamma(1234)\Gamma(5678)\Delta_{1234}\operatorname{Im}G_4^R(\mu_\Delta)\ . \tag{2.1}$$

Here $\hbar$ is the Planck constant divided by 2π, n_C the excess-carrier concentration in CB, and V the crystal volume. The number m $(=1,2,\ldots,8)$ in the summand is the abbreviation of $m\equiv l_m\vec{k}_m\sigma_m$ for a state with the band index l_m, the wave vector $\vec{k}_m$, and the spin σ_m: It should be noted that at present the number m $(=1,2,3,4)$ does not necessarily correspond to the label m in Fig. 1, representing all possible states. We write

$$\begin{aligned}\Delta_{1234}=&\Delta(l_1-l_C)+\Delta(l_2-l_C)\\&-\Delta(l_3-l_C)-\Delta(l_4-l_C)\ ,\end{aligned} \tag{2.2}$$

where l_C denotes CB: With x as a scalar or a vector we define $\Delta(x)=1$ if $x=0$ and $\Delta(x)=0$ otherwise. Assuming that the CB system and the VB system can be described by quasi-Fermi-levels μ_C and μ_V, respectively, we define

$$\mu_\Delta=(\mu_C-\mu_V)\Delta_{1234}\ . \tag{2.3}$$

$\Gamma(1234)$ is related to the Fourier component of the electron-electron screened Coulomb interaction $U(\vec{k})/V$, which is given for the bare potential $\mathcal{V}(\vec{k})/V$, i.e.,

$$\mathcal{V}(\vec{k})=\frac{4\pi e^2}{k^2} \tag{2.4}$$

as

$$U(\vec{k})=\frac{\mathcal{V}(\vec{k})}{\epsilon(\vec{k})}\ . \tag{2.5}$$

In Eqs. (2.4) and (2.5) e is the electronic charge and $\epsilon(\vec{k})$ represents the dielectric screening due to host lattice and free carriers, which is given later. Thus we define

$$\begin{aligned}\Gamma(1234)=&\frac{1}{V}[U(\vec{k}_1-\vec{k}_4)\Delta(\sigma_1-\sigma_4)F_{14}F_{23}\\&-U(\vec{k}_1-\vec{k}_3)\Delta(\sigma_1-\sigma_3)F_{13}F_{24}]\\&\times\Delta(p_1+p_2-p_3-p_4)\ ,\end{aligned} \tag{2.6}$$

where $p_m=\vec{k}_m\sigma_m$,

$$\Delta(p_m-p_n)=\Delta(\vec{k}_m-\vec{k}_n)\Delta(\sigma_m-\sigma_n)\ ,$$

and $F_{mn}=\langle l_m,\vec{k}_m\mid l_n,\vec{k}_n\rangle$ is the overlap integral between the modulating parts of the Block functions $\mid l_m,k_m\rangle$ and $\mid l_n,k_n\rangle$. Use of $\Gamma(1234)$ is the convention to give the Hamiltonian in a convenient symmetric form.

In Eq. (2.1) $G_4^R(\mu_\Delta)$ is obtained from $G_4^R(\omega)$, where ω is an energy variable. $G_4^R(\mu_\Delta)$ is the four-particle retarded Green's function, which can be related to the four-particle temperature Green's function $\mathcal{G}_4(i\xi)$. Hereafter let $\xi/(\pi T)$ and $\eta/(\pi T)$, where T is the thermal energy, be an even integer and an odd integer, respectively, when ξ and η are used in a temperature Green's function of any kind; thus ξ and η, with suffixes attached to or not, take discrete values. A relation we use is

$$G_4^R(\omega)=\mathcal{G}_4(\omega+i\delta) \tag{2.7}$$

under $\delta\to0^+$. $\mathcal{G}_4(i\xi)$ is the Fourier component of $\mathcal{G}_4(\tau)$, i.e.,

$$\mathcal{G}_4(i\xi)=\int_0^{1/T}d\tau\exp(i\xi\tau)\mathcal{G}_4(\tau)\ , \tag{2.8}$$

where we define

$$\begin{aligned}\mathcal{G}_4(\tau)=-\langle T_\tau(&\tilde{a}_1^\dagger(\tau)\tilde{a}_2^\dagger(\tau)\tilde{a}_3(\tau)\tilde{a}_4(\tau)\\&\times\tilde{a}_5^\dagger(0)\tilde{a}_6^\dagger(0)\tilde{a}_7(0)\tilde{a}_8(0))\rangle\ .\end{aligned} \tag{2.9}$$

In the equation T_τ is the Wick chronological operator,

$$\begin{aligned}\tilde{a}_m^\dagger(\tau)&=\exp(\tau\bar{H}_0)a_m^\dagger\exp(-\tau\bar{H}_0)\ ,\\\tilde{a}_m(\tau)&=\exp(\tau\bar{H}_0)a_m\exp(-\tau\bar{H}_0)\ ,\end{aligned} \tag{2.10}$$

with $\bar{H}_0$ as the Hamiltonian described below, and $\langle\mathcal{F}\rangle=\operatorname{Tr}(\rho_0\mathcal{F})$, where

$$\rho_0=\exp\left[\frac{\Omega-\bar{H}_0}{T}\right] \tag{2.11}$$

under the definition of a constant Ω through $\operatorname{Tr}\rho_0=1$.

We define $\bar{H}_0$ as

$$\bar{H}_0=H_0-\mu_C\hat{N}_C-\mu_V\hat{N}_V\ , \tag{2.12}$$

where H_0 is the Hamiltonian consisting of the unperturbed Hamiltonian for electrons and the perturbations, i.e., the electron-electron interaction and some other scatterings such as the electron-phonon interaction and the electron-impurity interaction: $\hat{N}_C$ and $\hat{N}_V$ are the number operators for the CB system and for the VB system, respectively.

Now our task is to find $\mathcal{G}_4(\tau)$ from Eq. (2.9). Following the procedure in Ref. 11, we use an approximation

$$\begin{aligned}\mathcal{G}_4(\tau)=&-4\mathcal{G}(7,1\tau)\mathcal{G}(8,2\tau)\mathcal{G}(3\tau,5)\mathcal{G}(4\tau,6)-4\mathcal{G}(7,1\tau)\mathcal{G}(3\tau,5)\mathcal{G}_{2A}^b(4,8;2,6{:}\tau)\\&+4\mathcal{G}(7,1\tau)\mathcal{G}(4\tau,5)\mathcal{G}_{2A}^b(3,8;2,6{:}\tau)-4\mathcal{G}(7,2\tau)\mathcal{G}(4\tau,5)\mathcal{G}_{2A}^b(3,8;1,6{:}\tau)\\&+4\mathcal{G}(7,2\tau)\mathcal{G}(3\tau,5)\mathcal{G}_{2A}^b(4,8;1,6{:}\tau)+4\mathcal{G}(7,1\tau)\mathcal{G}(8,2\tau)\mathcal{G}_{2B}^b(3,4;5,6;\tau)\\&+4\mathcal{G}(3\tau,5)\mathcal{G}(4\tau,6)\mathcal{G}_{2B}^b(7,8;1,2{:}-\tau)\ ,\end{aligned} \tag{2.13}$$

where we define

$$\mathcal{G}(m\tau,n)=-\langle T_\tau(\tilde{a}_m(\tau)\tilde{a}_n^\dagger(0))\rangle\ , \tag{2.14}$$

$$\mathcal{G}(m,n\tau)=-\langle T_\tau(\tilde{a}_m(0)\tilde{a}_n^\dagger(\tau))\rangle\ , \tag{2.15}$$

$$\mathcal{G}_{2A}(1,2;3,4{:}\tau)=\langle T_\tau(\tilde{a}_3^\dagger(\tau)\tilde{a}_1(\tau)\tilde{a}_4^\dagger(0)\tilde{a}_2(0))\rangle\ , \tag{2.16}$$

$$\mathcal{G}_{2B}(1,2;3,4{:}\tau)=\langle T_\tau(\tilde{a}_1(\tau)\tilde{a}_2(\tau)\tilde{a}_3^\dagger(0)\tilde{a}_4^\dagger(0))\rangle\ . \tag{2.17}$$

Here $\mathcal{G}$ is the one-particle temperature Green's function, $\mathcal{G}_{2A}$ is the two-particle temperature Green's function describing electron-hole scattering, and $\mathcal{G}_{2B}$ is the two-particle temperature Green's function describing electron (hole)—electron (hole) scattering; the bound parts of $\mathcal{G}_{2A}$ and $\mathcal{G}_{2B}$ are denoted by $\mathcal{G}_{2A}^b$ and $\mathcal{G}_{2B}^b$, respectively. In Eq. (2.13) the first term is the free part and the residual six terms are obtained by decomposing the bound part into all possible combinations of interacting and noninteracting pairs. In Ref. 11 the bound part is neglected and the free part alone is retained.

In order to calculate $\mathcal{G}_4(i\xi)$ from Eq. (2.8) we make use of the following relations:

$$\mathcal{G}(m\tau,n)=\frac{1}{\pi}\int_{-\infty}^{\infty}d\omega[1-\Theta(\omega)]\mathrm{Im}G^R(m,n;\omega)\times\exp(-\omega\tau)\ , \tag{2.18}$$

$$\mathcal{G}(m,n\tau)=-\frac{1}{\pi}\int_{-\infty}^{\infty}d\omega\,\Theta(\omega)\mathrm{Im}G^R(m,n;\omega)\exp(\omega\tau)\ , \tag{2.19}$$

$$\mathcal{G}_2(\tau)=\frac{1}{\pi}\int_{-\infty}^{\infty}d\omega[P(\omega)+1]\mathrm{Im}G_2^R(\omega)\exp(-\omega\tau),\quad \tau>0 \tag{2.20}$$

$$\mathcal{G}_2(\tau)=\frac{1}{\pi}\int_{-\infty}^{\infty}d\omega\,P(\omega)\mathrm{Im}G_2^R(\omega)\exp(-\omega\tau),\quad \tau<0\ . \tag{2.21}$$

Here $\mathcal{G}_2(\tau)$ represents $\mathcal{G}_{2A}(1,2;3,4{:}\tau)$ or $\mathcal{G}_{2B}(1,2;\,3,4{:}\tau)$. $G^R(m,n;\omega)$ and $G_2^R(\omega)$ are the one-particle retarded Green's function and the two-particle retarded Green's function, respectively, which are obtained from

$$G^R(m,n;\omega)=\mathcal{G}(m,n;\omega+i\delta)\ ,$$

and $G_2^R(\omega)=\mathcal{G}_2(\omega+i\delta)$; $\mathcal{G}(m,n{:}i\eta)$ and $\mathcal{G}_2(i\xi)$ are the Fourier components of $\mathcal{G}(m\tau,n)$ $[\mathcal{G}(m,n\tau)]$ and $\mathcal{G}_2(\tau)$, respectively, which are given from Eq. (2.8) by replacing $\mathcal{G}_4$ with the relevant-temperature Green's functions. In Eqs. (2.18)—(2.21) we define

$$\Theta(\omega)=\frac{1}{\exp\left[\dfrac{\omega}{T}\right]+1}\ , \tag{2.22}$$

$$P(\omega)=\frac{1}{\exp\left[\dfrac{\omega}{T}\right]-1}\ . \tag{2.23}$$

As for $\mathcal{G}(m,n;\omega)$ we consider only the intraband, spin conserving, and wave-vector conserving scatterings. These are the cases for the carrier-carrier interaction and the electron-phonon interaction. On the other hand, the wave vector is not conserved for the electron-impurity interaction under random distribution of impurities. However, the wave-vector conservation is restored by considering the ensemble average over all the impurity sites.[14,17,18] We can write

$$\mathcal{G}(m,n;i\eta)=\Delta(\bar{p}_m-\bar{p}_n)\mathcal{G}(m,i\eta)\ , \tag{2.24}$$

where $\bar{p}_m\equiv m=l_m\vec{k}_m\sigma_m$,

$$\Delta(\bar{p}_m-\bar{p}_n)=\Delta(l_m-l_n)\Delta(\vec{k}_m-\vec{k}_n)\Delta(\sigma_m-\sigma_n)\ ,$$

and $\mathcal{G}(m,i\eta)$ is a newly-defined one-particle temperature Green's function. Using Eqs. (2.18)—(2.24) we obtain $\mathcal{G}_4(i\xi)$, from which $\mathrm{Im}G_4^R(\omega)$ is found using Eq. (2.7) as

$$\mathrm{Im}G_4^R(\omega)=\frac{4}{\pi^3}\left[\exp\left[-\frac{\omega}{T}\right]-1\right]\left[S_0+\sum_{n=1}^{4}(-1)^nS_n\right]\ , \tag{2.25}$$

$$S_0=\Delta(\bar{p}_7-\bar{p}_1)\Delta(\bar{p}_8-\bar{p}_2)\Delta(\bar{p}_5-\bar{p}_3)\Delta(\bar{p}_6-\bar{p}_4)\times\int d\omega_1\int d\omega_2\int d\omega_3\int d\omega_4\delta(\omega_1+\omega_2-\omega_3-\omega_4-\mu_C+\mu_V)\theta_1\theta_2(1-\theta_3)(1-\theta_4)\prod_{m=1}^{4}\mathrm{Im}G^R(\bar{p}_m,\omega_m)\ , \tag{2.26}$$

$$S_1=\Delta(\bar{p}_7-\bar{p}_1)\Delta(\bar{p}_5-\bar{p}_3)\int d\omega_1\int d\omega_3\int d\omega'\delta(\omega+\omega_1-\omega_3-\omega')\theta_1(1-\theta_3)[P(\omega')+1]\times\mathrm{Im}G^R(\bar{p}_1,\omega_1)\mathrm{Im}G^R(\bar{p}_3,\omega_3)\mathrm{Im}G_{2A}^{Rb}(4,8;2,6{:}\omega')\ . \tag{2.27}$$

S_2, S_3, and S_4 are obtained from S_1 under interchanges of suffixes and indices, i.e., $3\rightleftarrows4$ for S_2, $1\rightleftarrows2$ and $3\rightleftarrows4$ for S_3, and $1\rightleftarrows2$ for S_4. We use abbreviation $\theta_m=\Theta(\omega_m)$. G_{2A}^{Rb} is the bound part of G_{2A}^{Rb}. The terms S_0 and S_n come from the first term and the $(n+1)$th term of Eq. (2.13), respectively. The reason why terms corresponding to the sixth and the seventh terms do not appear becomes clear later.

Now we are at the position to find out the expression for $\mathrm{Im}G_{2A}^{Rb}(1,2;3,4{:}\omega)$. We make use of the relation

$$\mathcal{G}_{2A}(1,2;3,4{:}\tau)=T^2\sum_{\eta_1,\eta_3}\exp[-i(\eta_1-\eta_3)\tau]\overline{\mathcal{G}}_{2A}(1,2;3,4{:}i\eta_1,i\eta_3)\ . \tag{2.28}$$

From this we obtain

$$\mathscr{G}_{2A}(1,2;3,4{:}i\xi)=T\sum_{\eta_1}\overline{\mathscr{G}}_{2A}(1,2;3,4{:}i\eta_1,i\eta_1-i\xi)\ . \tag{2.29}$$

The bound part of $\overline{\mathscr{G}}_{2A}$ represents the electron-hole plasma interaction shown by a diagram in Fig. 2(a) in terms of $\gamma(1234)$ describing the interaction between two carriers. Consider an irreducible diagram of $\gamma(1234)$ and let $I(1234)$ be the contribution of these diagrams, called the irreducible interaction of two particles.[19] Then we obtain, neglecting an unimportant term for the free part,

$$\begin{aligned}\overline{\mathscr{G}}_{2A}(1,2;3,4{:}i\eta_1,i\eta_3)=&-\Delta(\bar{p}_1-\bar{p}_4)\Delta(\bar{p}_2-\bar{p}_3)\mathscr{G}(\bar{p}_1,i\eta_1)\mathscr{G}(\bar{p}_3,i\eta_3)\\&-T\mathscr{G}(\bar{p}_1,\eta_1)\mathscr{G}(\bar{p}_3,\eta_3)\sum_{\eta_5,\bar{p}_5,\eta_6,\bar{p}_6}I(1536)\overline{\mathscr{G}}_{2A}(6,2;5,4{:}i\eta_6,i\eta_5)\ .\end{aligned} \tag{2.30}$$

The term of the lowest order in the modified interaction $U(\vec{\mathrm{k}})$ of $I(1234)$ is given as

$$I(1234)=\frac{1}{V}[U(\vec{\mathrm{k}}_1-\vec{\mathrm{k}}_4)\Delta(\sigma_1-\sigma_4)F_{14}F_{23}-\mathscr{V}(\vec{\mathrm{k}}_1-\vec{\mathrm{k}}_3)\Delta(\sigma_1-\sigma_3)F_{13}F_{24}]\Delta(p_1+p_2-p_3-p_4)\ . \tag{2.31}$$

The first term and the second term in the square brackets of the equation represent the Coulomb term and the exchange term, respectively. The exchange term is not modified since $I(1234)$ is irreducible.[20,21] With the use of Eq. (2.31) we find that in Eq. (2.30) the Coulomb term is only an energy correction, which we neglect for the reason described later. We obtain the bound part of $\overline{\mathscr{G}}_{2A}$ as

$$\begin{aligned}\overline{\mathscr{G}}{}^{b}_{2A}(1,2;3,4{:}i\eta_1,i\eta_3)=&-\mathscr{G}(\bar{p}_1,i\eta_1)\mathscr{G}(\bar{p}_3,i\eta_3)\mathscr{H}(\bar{p}_2,\bar{p}_4;i\eta_1-i\eta_3)\frac{1}{V}\frac{\mathscr{V}(\vec{\mathrm{k}}_1-\vec{\mathrm{k}}_3)}{\epsilon(\vec{\mathrm{k}}_1-\vec{\mathrm{k}}_3,i\eta_1-i\eta_3)}\\&\times F_{13}F_{24}\Delta(\sigma_1-\sigma_3)\Delta(p_1+p_2-p_3-p_4)\ ,\end{aligned} \tag{2.32}$$

where

$$\mathscr{H}(\bar{p}_m,\bar{p}_n;i\xi)=T\sum_{\eta'}\mathscr{G}(\bar{p}_m,i\eta')\mathscr{G}(\bar{p}_n,i\eta'+i\xi)\ , \tag{2.33}$$

$$\epsilon(\vec{\mathrm{k}},i\xi)=1-\frac{1}{V}\mathscr{V}(\vec{\mathrm{k}})\sum_{\bar{p}_1,\bar{p}_2}\mathscr{H}(\bar{p}_1,\bar{p}_2;i\xi)\,|\,F_{12}\,|^2\Delta(\sigma_1-\sigma_2)\Delta(\vec{\mathrm{k}}+\vec{\mathrm{k}}_1-\vec{\mathrm{k}}_2)\ . \tag{2.34}$$

With the use of Eq. (2.29) the bound part of $\mathscr{G}_{2A}$ is

$$\mathscr{G}^{b}_{2A}(1,2;3,4;i\xi)=-\frac{1}{V}\frac{\mathscr{V}(\vec{\mathrm{k}}_1-\vec{\mathrm{k}}_3)}{\epsilon(\vec{\mathrm{k}}_1-\vec{\mathrm{k}}_3,i\xi)}F_{13}F_{24}\mathscr{H}(\bar{p}_3,\bar{p}_1;i\xi)\mathscr{H}(\bar{p}_2,\bar{p}_4;i\xi)\Delta(\sigma_1-\sigma_3)\Delta(p_1+p_2-p_3-p_4)\ . \tag{2.35}$$

Transforming the summation of Eq. (2.33) into the contour integration,[17] we obtain under $\xi>0$,

$$\mathscr{H}(\bar{p}_m,\bar{p}_n;i\xi)=-\frac{1}{\pi}\int d\omega\,\Theta(\omega)[\mathrm{Im}G^R(\bar{p}_m,\omega)G^R(\bar{p}_n,\omega+i\xi)+\mathrm{Im}G^R(\bar{p}_n,\omega)\mathrm{Im}G^A(\bar{p}_m,\omega-i\xi)]\ , \tag{2.36}$$

where G^A is the advanced one-particle Green's function. From Eqs. (2.35) and (2.36) we obtain after some manipulations,

$$\begin{aligned}\mathrm{Im}G^{Rb}_{2A}(1,2;3,4{:}\omega)=&\frac{1}{\pi^3V}\frac{\mathscr{V}(\vec{\mathrm{k}}_1-\vec{\mathrm{k}}_3)}{\epsilon(\vec{\mathrm{k}}_1-\vec{\mathrm{k}}_3,\omega)}F_{13}F_{24}\Delta(\sigma_1-\sigma_3)\Delta(p_1+p_2-p_3-p_4)\\&\times\int d\omega_1\int d\omega_2\int d\omega_3\int d\omega_4\frac{1}{\omega_1+\omega_2-\omega_3-\omega_4}[\delta(\omega_1-\omega_3-\omega)-\delta(\omega_4-\omega_2-\omega)]\\&\times(\theta_1-\theta_3)(\theta_2-\theta_4)\prod_{m=1}^{4}\mathrm{Im}G^R(\bar{p}_m,\omega_m)\ .\end{aligned} \tag{2.37}$$

We write hereafter $\epsilon(\vec{\mathrm{k}},\omega+i\delta)$ simply as $\epsilon(\vec{\mathrm{k}},\omega)$.

Now we give a brief discussion of $\mathscr{G}^{b}_{2B}(1,2;3,4{:}\tau)$ in Eq. (2.13). Consider the Fourier component $\overline{\mathscr{G}}{}^{b}_{2B}(1,2;3,4{:}i\eta_1,i\eta_2)$. Noting that this represents the electron (hole)—electron (hole) interaction as shown in Fig. 2(b), we obtain[17]

$$\overline{\mathscr{G}}{}^{b}_{2B}(1,2;3,4{:}i\eta_1,i\eta_2)=\mathscr{G}(\bar{p}_1,i\eta_1)\mathscr{G}(\bar{p}_2,i\eta_2)T\sum_{\eta_5,\bar{p}_5,\eta_6,\bar{p}_6}I(1256)\overline{\mathscr{G}}{}^{b}_{2B}(5,6;3,4{:}i\eta_5,i\eta_6)\ , \tag{2.38}$$

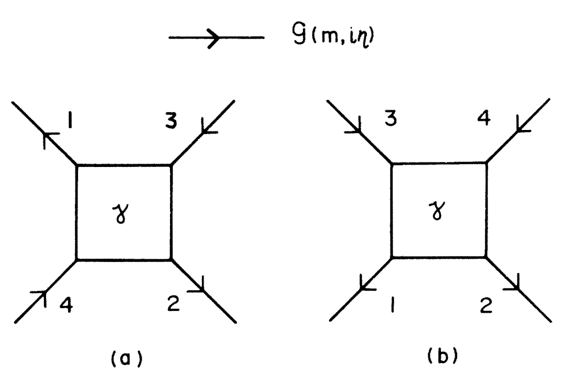

FIG. 2. Diagrams representing (a) the electron-hole interaction and (b) the electron (hole)—electron (hole) interaction.

where we take $I(1234)=\Gamma(1234)$ as the term of the lowest order in $U(\vec{k})$. We find that $\overline{\mathscr{G}}^{b}_{2B}(1,2;3,4:i\eta_1,i\eta_2)$ gives an energy correction in $\mathscr{G}_{2B}(1,2;3,4:i\eta_1,i\eta_2)$ so that we omit $\overline{\mathscr{G}}^{b}_{2B}$. As a result the sixth and the seventh terms in Eq. (2.13) are omitted. Modification to BBAR comes essentially from the electron-hole plasma interaction.

Here we discuss the terms giving energy corrections which have been neglected in the equations for $\mathscr{G}_{2A}$ and $\mathscr{G}_{2B}$. Those terms lead to modification of the free part of $\mathscr{G}_4$ on the one hand and to that of the dielectric screening constant on the other hand. The modification of the free part of $\mathscr{G}_4$ has been fully discussed in a previous paper,[11] showing that the effect is negligible except in the case of PCAR. The modification of the dielectric screening constant, which appears only in relation to $\mathscr{G}_{2A}$, is given in terms of a renormalized energy, which replaces the bare particle band energy. In BBAR the screening effect due to free carriers is negligible while that due to the host lattice is important. The screening due to the host lattice comes in large part from states of large energy so that the effect of the renormalization is negligibly small.

Let us discuss $\epsilon(\vec{k},\omega)$, which is implicitly involved in $\mathrm{Im}G_4^R(\mu_\Delta)$. We take into account the fact that practically the energy ω in $\epsilon(\vec{k},\omega)$ is found to be the band-gap energy in the case of BBAR. Then we can put $\omega=0$ and neglect the imaginary part of $\epsilon(\vec{k},\omega)$. With the use of Eqs. (2.34) and (2.36) under the neglect of the imaginary part of $\epsilon(\vec{k},\omega)$ we obtain

$$\epsilon(\vec{k},\omega)=1-\frac{1}{V}\mathscr{V}(\vec{k})\sum_{\bar{p}_1,\bar{p}_2} H_r(\bar{p}_1,\bar{p}_2;\omega)\,|F_{12}|^2\Delta(\sigma_1-\sigma_2)\Delta(\vec{k}+\vec{k}_1-\vec{k}_2)\,, \tag{2.39}$$

where

$$H_r(\bar{p}_1,\bar{p}_2;\omega)=\frac{1}{\pi^2}\int d\omega_1\int d\omega_2\frac{\theta_1-\theta_2}{\omega_1-\omega_2+\omega}\mathrm{Im}G^R(\bar{p}_1,\omega_1)\mathrm{Im}G^R(\bar{p}_2,\omega_2)\,. \tag{2.40}$$

Actually we use $\epsilon(\vec{k},\omega)=\epsilon(\vec{k},0)=\epsilon(\vec{k})$, where $\epsilon(\vec{k})$ has been defined in Eq. (2.5).

Use of Eqs. (2.1), (2.25), and (2.37) leads, after some manipulation, to

$$\begin{aligned}\frac{1}{\tau}=\frac{2}{\hbar\pi^3 n_C V}&\left[\exp\left[\frac{\mu_C-\mu_V}{T}\right]-1\right]\\ &\times\sum_{1,2,3,4}{}'\int d\omega_1\int d\omega_2\int d\omega_3\int d\omega_4\delta(\omega_1+\omega_2-\omega_3-\omega_4-\mu_C+\mu_V)\theta_1\theta_2(1-\theta_3)(1-\theta_4)\\ &\qquad\times\left[Q_0+2\sum_{n=1}^{4}Q_n\right]\prod_{m=1}^{4}\mathrm{Im}G^R(\bar{p}_m,\omega_m)\,,\end{aligned} \tag{2.41}$$

where

$$Q_0=|\Gamma(1234)|^2\,, \tag{2.42}$$

$$Q_1=\frac{1}{V}U(\vec{k}_4-\vec{k}_1)\sum_{\bar{p}_5,\bar{p}_6}\mathrm{Re}[\Gamma(1234)\Gamma(3516)F_{42}F_{65}]H_r(\bar{p}_6,\bar{p}_5;\omega_4-\omega_2)\Delta(\sigma_4-\sigma_2)\Delta(p_4+p_6-p_2-p_5)\,. \tag{2.43}$$

Q_2, Q_3, and Q_4 are obtained from Q_1 under interchanges of subscripts, i.e., $3\rightleftarrows4$ for Q_2, $1\rightleftarrows2$ and $3\rightleftarrows4$ for Q_3, and $1\rightleftarrows2$ for Q_4, noting the relations

$$\Gamma(1234)=-\Gamma(2134)=-\Gamma(1243)=\Gamma(2143)\,.$$

We have also used $\Gamma(3412)=\Gamma(1234)^*$, $\epsilon(\vec{k},\omega)=\epsilon(\vec{k})$, and Eq. (2.5). It is to be noted that $\sum'$ in Eq. (2.41) means the restricted summation over the states $1234=VC'CC$ or $VVV'C$, where C' and V' represent energetic states for an electron in CB and for a hole in VB, respectively. The terms Q_0 and Q_n correspond to the first term and the $(n+1)$th term of Eq. (2.13), respectively. Thus Q_0 represents the BBAR rate in an approximation of noninteracting carriers and Q_n the correction arising from the electron-hole scattering. We write

$$\frac{1}{\tau}=\frac{1}{\tau_0}+\frac{1}{\tau_{\mathrm{cor}}}\,, \tag{2.44}$$

where τ_0 and τ_{cor} come from Q_0 and $\sum_n Q_n$, respectively. Thus τ_0 is the conventional BBAR lifetime used in previ-

TABLE I. Properties of Q_n's

Process	Term	Interacting states	Relevant bands	Note
VCCC	$Q_1=Q_2$	2–3 2–4	C'B-CB	Neglected
	$Q_3=Q_4$	1–3 1–4	CB-VB	
VVVC[a]	$Q_1=Q_4$	1–4 2–4	CB-VB	
	$Q_2=Q_3$	1–3 2–3	V'B-VB	Neglected

[a]We consider *HHVC*.

ous papers[12–16] and τ_{cor}^{-1} is the correction to τ_0^{-1}, whose discussion is the central subject in the following sections.

Note that $G^R(\bar{p}_m,\omega_m)$ in Eq. (2.41) is the complete Green's function, through which all scattering effects such as the phonon scattering effect, impurity scattering effect, and carrier-carrier scattering effect can be taken into account in terms of the self-energy $\Sigma(\bar{p}_m,\omega_m)$. Let us expand G^R in a power series of Σ as

$$G^R=G_0^R+G_0^R\Sigma G_0^R+\cdots \,, \tag{2.45}$$

where G_0^R is the free-particle Green's function. We consider the phonon scattering effect as an example. We use Eq. (2.45) in Eq. (2.41) and give $\prod_{m=1}^{4}\operatorname{Im}G^R(\bar{p}_m,\omega_m)$ in a power series of Σ. Then τ^{-1} can be given as a sum of inverse lifetimes for PCAR in the first-order perturbation theory, for PAAR in the second-order perturbation theory, and for terms in the higher-order perturbation theory. If the higher-order terms can be neglected, we obtain PCAR and PAAR as independent events. Therefore, the correction due to the electron-hole scattering is prerequisite for all types of calculations.

III. CORRECTION TERMS

In this section we discuss the corrections Q_n's in Eq. (2.41) with particular attention to CB, the heavy-hole band (HB), the light-hole band (LB), and the spin-splitoff band (SB) as states 1,2,3,4 in Fig. 1. Those bands are denoted by l_C, l_H, l_L, and l_S, respectively, and let E_G and Δ_0 be the band-gap energy and the spin-splitoff energy, respectively. As for the *VVVC* process we consider only the *HHVC* process, which is usually of practical importance. Some properties of Q_n's are shown in Table I. Equalities in the second column come from equivalent roles of electrons 3 and 4 in Fig. 1(a) and of holes 1 and 2 in Fig. 1(b) in BBAR. The terms in the first and fourth rows are neglected because scatterings are for energetic carriers.

First we consider Q_1 for the *HHVC* process. It is convenient to define

$$\Gamma(1234)=(f_1,g_1)=\frac{1}{V}[f_1\Delta(\sigma_1-\sigma_4)-g_1\Delta(\sigma_1-\sigma_3)]\Delta(p_1+p_2-p_3-p_4)\,, \tag{3.1}$$

where f_1 and g_1 are found from Eq. (2.6). Similarly we define $\Gamma(3516)=(f_2,g_2)$. By performing a summation over spin states, we obtain for Q_1

$$\begin{aligned}S_\Gamma&=\sum_{\text{spin}}\Gamma(1234)\Gamma(3516)F_{42}F_{65}\Delta(\sigma_4-\sigma_2)\Delta(\sigma_4+\sigma_6-\sigma_2-\sigma_5)\\&=2(f_1-2g_1)f_2-2g_2)F_{42}F_{65}\Delta(\vec{k}_1+\vec{k}_2-\vec{k}_3-\vec{k}_4)\Delta(\vec{k}_3+\vec{k}_5-\vec{k}_1-\vec{k}_6)\,.\end{aligned} \tag{3.2}$$

From close similarity between the expressions for τ and τ_0 we can make use of an approximation adopted usually for τ_0: Quantities other than the statistical factor are evaluated under the threshold condition of BBAR and taken out of the summation and the integral. Let us assume that some scatterings such as phonon scattering are present. A scattering effect on BBAR is to relax the momentum-conservation requirement in PCAR. The threshold condition[11] is

$$\begin{aligned}&\text{(a)}\ \ \vec{k}_1=\vec{k}_3,\ \ \vec{k}_2=\vec{k}_4=0\\&\text{or}\\&\text{(b)}\ \ \vec{k}_2=\vec{k}_3,\ \ \vec{k}_1=\vec{k}_4=0\,,\end{aligned} \tag{3.3}$$

where $\vec{k}_3$ is the wave vector at the threshold for an energetic hole: We assume that k_3 is of significant magnitude. The two conditions (a) and (b) come from equivalent roles of 1 and 2. For Q_1 we need to know S_Γ under both $\vec{k}_4+\vec{k}_6-\vec{k}_2-\vec{k}_5=0$ and the condition (3.3). We find $S_\Gamma=0$ under the condition (a) and $S_\Gamma\neq 0$ under the condition (b). On the average over both cases we obtain

$$\begin{aligned}S_\Gamma=&(4|g_1|^2|F_{65}|^2-2g_1f_2F_{42}F_{65})\\&\times\Delta(\vec{k}_1+\vec{k}_2-\vec{k}_3-\vec{k}_4)\Delta(\vec{k}_3+\vec{k}_5-\vec{k}_1-\vec{k}_8)\end{aligned} \tag{3.4}$$

under the condition (b). It is important to note that the threshold condition has been considered for the states 1,2,3,4 but not for the intermediate states 5 and 6. Thus $\bar{p}_5$ and $\bar{p}_6$ can still cover all possible states allowable for $\vec{k}_4+\vec{k}_6-\vec{k}_2-\vec{k}_5=0$.

In order to consider S_Γ under the threshold condition (3.3) we make use of an approximate form[22]

$$\langle l,\vec{k}_m\,|\,l_H,\vec{k}_n\rangle=\vec{\xi}_{lH}\cdot(\vec{k}_m-\vec{k}_n)\,, \tag{3.5}$$

where l_H denotes HB and l denotes CB, LB, or SB. $\vec{\xi}_{lH}$ is given by Kane's $\vec{k}\cdot\vec{p}$ method[23] in a form

$$\vec{\xi}_{lH}=\xi_l(\hat{e}_x+i\hat{e}_y)\,, \tag{3.6}$$

where $\hat{e}_x$ and $\hat{e}_y$ are unit vectors in the x and y directions, respectively, and ξ_l is a material parameter. Hereafter let us assume spherical energy surfaces for all bands. Since all quantities other than S_Γ in Eq. (2.41) are spherically symmetric with respect to $\vec{k}_3$, we give S_Γ by taking an angular average over $\vec{k}_3$. Then the second term of Eq. (3.4) vanishes so that we obtain

$$\begin{aligned}S_\Gamma=4\,|g_1|^2\,|F_{65}|^2\Delta(\vec{k}_1+\vec{k}_2-\vec{k}_3-\vec{k}_4)\\ \times\Delta(\vec{k}_3+\vec{k}_5-\vec{k}_1-\vec{k}_6)\,.\end{aligned} \tag{3.7}$$

Next we consider Q_3 for the *HCCC* process. Assuming also that some scatterings are present, the threshold condition[11] is

$$\vec{k}_1=-\vec{k}_2,\ \ \vec{k}_3=\vec{k}_4=0\,, \tag{3.8}$$

where $\vec{k}_2$ is the wave vector at the threshold for an energetic electron. By the discussion similar to that given above,

$$\begin{aligned}S_\Gamma=\sum_{\text{spin}}\Gamma(1234)\Gamma(4526)F_{31}F_{65}\\ \times\Delta(\sigma_3-\sigma_1)\Delta(\sigma_3+\sigma_6-\sigma_1-\sigma_5)\end{aligned} \tag{3.9}$$

for Q_1 is rewritten as

$$\begin{aligned}S_\Gamma=4\,|g_1|^2\,|F_{65}|^2\Delta(\vec{k}_1+\vec{k}_2-\vec{k}_3-\vec{k}_4)\\ \times\Delta(\vec{k}_3+\vec{k}_6-\vec{k}_1-\vec{k}_5)\,.\end{aligned} \tag{3.10}$$

Let us rewrite Q_1 and Q_3 with the use of Eqs. (3.7) and (3.10). Since Q_1 and Q_3 represent the electron-hole interaction, for intermediate states 5 and 6 we have $l_5=l_C$ when $l_6=l_V$, and vice versa where l_V denotes VB. It should be noted that l_5 and l_6 cover all bands. Here we make use of Eq. (2.39) noting that $\epsilon(\vec{k},\omega)$ can be written as

$$\epsilon(\vec{k},\omega)=\epsilon_0(\vec{k},\omega)+\epsilon_f(\vec{k},\omega)\,, \tag{3.11}$$

where $\epsilon_0(\vec{k},\omega)$ and $\epsilon_f(\vec{k},\omega)$ represent the dielectric screening due to the host lattice and free carriers, respectively; $\epsilon_0(\vec{k},\omega)$ is obtained from Eq. (2.39) by restricting the summation over $\bar{p}_1$ and $\bar{p}_2$ to $(l_1=l_C,\ l_2=l_V)$ and $(l_1=l_V,\ l_2=l_C)$: Summation over all other possible states gives $\epsilon_f(\vec{k},\omega)$. With the use of Eqs. (2.39), (3.7), (3.10), and (4.11) we obtain

$$\begin{aligned}Q_1&=-4\,|g_1|^2\frac{\epsilon_0-1}{\epsilon(\vec{k}_4-\vec{k}_1)}\quad(\text{for } HHVC)\,,\\ Q_3&=-4\,|g_1|^2\frac{\epsilon_0-1}{\epsilon(\vec{k}_3-\vec{k}_1)}\quad(\text{for } HCCC)\,.\end{aligned} \tag{3.12}$$

Here we have neglected the ω and $\vec{k}$ dependence of $\epsilon_0(\vec{k},\omega)$. This is approximately equal to $\epsilon_0(0,0)\equiv\epsilon_0$ since in BBAR we have $\omega\sim E_G$ and $\vec{k}$ is nearly at the center of the first Brillouin zone especially for direct-gap materials.

As for Q_0 we obtain

$$\sum_{\text{spin}}|\Gamma(1234)|^2=2(\,|f_1|^2+|g_1|^2+|f_1-g_1|^2)\,. \tag{3.13}$$

This becomes $4|f_1|^2$, $4|g_1|^2$, and $2(\,|f_1|^2+|g_1|^2)$ under the conditions (3.3a), (3.3b), and (3.8). Since we find $f_1=g_1$ for the threshold conditions, we finally obtain

$$\frac{1}{\tau}=\left[1+\frac{4(\epsilon_0-1)}{\epsilon(\vec{k}_T)}\right]\frac{1}{\tau_0}\,, \tag{3.14}$$

where $\vec{k}_T$ is the threshold value of $\vec{k}_2$ for the *HCCC* process and $\vec{k}_3$ for the *HHVC* process, respectively. Here we have used the relations $\epsilon(\vec{k},\omega)=\epsilon(-\vec{k},-\omega)$, $\vec{k}_4-\vec{k}_2=-\vec{k}_3$ under the condition (3.3b), and $\vec{k}_3-\vec{k}_1=\vec{k}_2$ under the condition (3.8).

The Thomas-Fermi approach gives

$$\epsilon(\vec{k})=\epsilon_0\left[1+\frac{\lambda^2}{k^2}\right]\,, \tag{3.15}$$

where λ is the inverse screening length. Usually we have $k_T\gg\lambda$ so that to take $\epsilon(\vec{k}_T)=\epsilon_0$ is a good approximation. We see that Eq. (3.14) gives the BBAR rate larger by a factor of about 5 than the conventional one, noting that we have $\epsilon_0\sim 10$.

Although the discussion has been given for the case where some scatterings are present, we find that Eq. (3.14) is also useful under the threshold condition of PCAR. Thus Eq. (3.14) is useful in almost all cases where τ_0 is calculated on the basis of the first-order perturbation treatment, of the second-order perturbation treatment, and of the complete Green's-function formalism. This point has been stressed just below Eq. (2.45). The only case where Eq. (3.14) is not useful is the *HHSC* process under $E_G\lesssim\Delta_0$, where Δ_0 is the spin-splitoff energy. In this case we have $k_3\simeq 0$ at the threshold and we cannot give S_Γ in a tractable form.

IV. DISCUSSION OF OVERLAP INTEGRALS

In this section we discuss how we attain a satisfactory explanation of experiments on the basis of Eq. (3.14). The discussion is necessary since some of the previous calculations[13,24–29] have shown agreements between the conventional theories and experiments. I point out that the agreements are fortuitous as a result of the fact that the overlap integrals have been overestimated[13,26–29] or as a result of the fact that the screened exchange term in $\Gamma(1234)$ has been replaced by the unscreened one[24,25] although accurate estimation of the overlap integrals has been done.[30] As for the latter case I have pointed out[29] that the replacement is incorrect; the screened exchange term should be used, as is done in this paper.

Let us consider the overlap integrals by restricting the discussion to the *HCCC* process and the *HHSC* process. We define the wave-vector-dependent effective masses m_2 and m_3 as follows. $\hbar^2k_2{}^2/(2m_2)$ is the energy of a state 2 for the *HCCC* process shown in Fig. 1(a), which is measured upward from the CB edge. On the other hand, $\hbar^2k_3{}^2/(2m_3)$ is the energy of a state 3 for the *HHSC* process shown in Fig. 1(b), which is measured downward from the SB edge. Practically we use m_2 and m_3, which are estimated at the threshold values of $\vec{k}_2$ and $\vec{k}_3$, respectively, for BBAR. Taking into account the threshold conditions, dependence of τ_0 on the overlap integrals is given in a form $\tau_0^{-1} \propto P$, where

$$P = |\langle l_C,\vec{0}\,|\,l_H,\vec{k}_2\rangle|^2\,|\langle l_C,\vec{0}\,|\,l_C,\vec{k}_2\rangle|^2$$

for the *HCCC* process and

$$P = |\langle l_C,\vec{0}\,|\,l_H,\vec{k}_3\rangle|^2\,|\langle l_H,\vec{0}\,|\,l_S,\vec{k}_3\rangle|^2$$

for the *HHSC* process. Hereafter let $\vec{k}$ represent $\vec{k}_2$ or $\vec{k}_3$.

According to Kane's $\vec{k}\cdot\vec{p}$ method,[23] we obtain the wave functions $|l,\vec{k}\rangle$ for $l=l_C$, $l=l_L$, and $l=l_S$ as

$$|l,\vec{k}\rangle = a_l(\vec{k})\,|is\uparrow\rangle + b_l(\vec{k})\,|(x+iy)/\sqrt{2}\downarrow\rangle + c_l(\vec{k})\,|z\uparrow\rangle\,, \tag{4.1}$$

where $|is\uparrow\rangle$, $|(x+iy)/\sqrt{2}\downarrow\rangle$, and $|z\uparrow\rangle$ are the wave functions at $\vec{k}=0$ in the s-p subspace. The energy of the band l and the relevant coefficients $\vec{a}_l(\vec{k})$, $b_l(\vec{k})$, and $c_l(\vec{k})$ are calculated from characteristic equations of the $\vec{k}\cdot\vec{p}$ method, which represent direct coupling among CB, LB, and SB. To these bands is coupled HB indirectly only through interaction with bands outside the s-p subspace. We can calculate $\langle l_C,\vec{0}\,|\,l_C,\vec{k}\rangle$ simply from Eq. (4.1) but we have

$$\langle l_C,\vec{0}\,|\,l_H,\vec{k}\rangle = \langle l_H,\vec{0}\,|\,l_S,\vec{k}\rangle = 0$$

if the effect of the bands outside the s-p subspace is neglected as in Eq. (4.1). An alternative procedure of calculating $\langle l_C,\vec{0}\,|\,l_H,\vec{k}\rangle$ and $\langle l_H,\vec{0}\,|\,l_S,\vec{k}\rangle$ is based on the use of the oscillator strength,[22] of which a careful discussion is given below.

We first consider $\langle l_C,\vec{0}\,|\,l_H,\vec{k}\rangle$. If we make a $\vec{k}\cdot\vec{p}$ perturbation expansion of $|l_H,\vec{k}\rangle$ starting with $|l_H,\vec{0}\rangle$ as the zeroth-order function, we obtain

$$|\langle l_C,\vec{0}\,|\,l_H,\vec{k}\rangle|^2 = \frac{\hbar^2k^2/2m_0}{E_C(0)-E_H(0)} f_{CH}(0) \tag{4.2}$$

with the oscillator strength given by

$$f_{CH}(0) = \tfrac{1}{3}\,|a_C(0)|^2 \frac{E_p}{E_C(0)-E_H(0)}\,. \tag{4.3}$$

Here the subscripts C and H are used for l_C and l_H, respectively, $E_l(\vec{k})$ is an energy for the band l, E_p a matrix element with dimension of energy,[31] and m_0 the electron mass in the free space. We have $a_C(0)=1$ and $E_C(0)-E_H(0)=E_G$, giving $f_{CH}(0)=E_p/(3E_G)$. The overlap integral $\langle l_C,\vec{0}\,|\,l_H,\vec{k}\rangle$ also appears in the theory of PCAR. In a good deal of the literature[5,12,14,15,26–28,32] the estimation based on Eqs. (4.2) and (4.3) has been done or seems to have been done. I have pointed out[13,29] that this estimation is incorrect since HB and LB are degenerate at $\vec{k}=0$: We cannot calculate $|l_H,\vec{k}\rangle$ starting simply with $|l_H,\vec{0}\rangle$. Agreements which are found in some cases[26–28] between the theory based on Eqs. (4.2) and (4.3) and experiments can be ascribed to the use of the PCAR theory; actually PAAR and/or IAAR should be taken into account. A simple alternative method which I have used[13,29] is to give $|l_C,\vec{0}\rangle$ starting with $|l_C,\vec{k}\rangle$ as the zeroth-order function by the $\vec{k}\cdot\vec{p}$ perturbation expansion. We obtain

$$|\langle l_C,\vec{0}\,|\,l_H,\vec{k}\rangle|^2 = \frac{\hbar^2k^2/2m_0}{E_C(\vec{k})-E_H(\vec{k})} f_{CH}(\vec{k})\,, \tag{4.4}$$

with

$$f_{CH}(\vec{k}) = \tfrac{1}{3}\,|a_C(\vec{k})|^2 \frac{E_p}{E_C(\vec{k})-E_H(\vec{k})}\,. \tag{4.5}$$

The equations give a value of $|\langle l_C\vec{0},\,|\,l_H,\vec{k}\rangle|^2$ smaller by 1 order of magnitude than the value given by Eqs. (4.2) and (4.3). Here we give

$$E_C(\vec{k})-E_H(\vec{k}) \simeq E_C(\vec{k})-E_H(0)$$

as $2E_G$ for the *HCCC* process and

$$E_G+(E_G-\Delta_0)m_3/m_C(\vec{k}_3)$$

for the *HHSC* process, where $m_C(\vec{k}_3)$ is the CB mass at k_3.

Actually I have given Eq. (4.4) approximately as

$$|\langle l_C,\vec{0}\,|\,l_H,\vec{k}\rangle|^2 = \frac{\hbar^2k^2}{2m_0E_G} f_{CH}(\vec{k})$$

in the literature[13,16,29] in accordance with the convention and have found fortuitously good agreement between the theory of τ_0 and experiments. For this calculation we write $|\langle l_C,\vec{0}\,|\,l_H,\vec{k}\rangle|_b^2$ while we write $|\langle l_C,\vec{0}\,|\,l_H,\vec{k}\rangle|_a^2$ for the calculation based on Eqs. (4.2) and (4.3).

Equation (4.5) is still not a rigorous expression for the oscillator strength since the momentum matrix element $\langle l_C,\vec{k}\,|\,\vec{p}\,|\,l_H,\vec{k}\rangle$ in $f_{CH}(\vec{k})$ has been given under an approximation $|l_H,\vec{k}\rangle = |l_H,\vec{0}\rangle$: Thus we have neglected the effect of the bands outside the s-p subspace. A rigorous calculation of $|\langle l_C,\vec{0}\,|\,l_H,\vec{k}\rangle|^2$ has been done by Lochmann[30] from the first principle using the full-zone double-group $\vec{k}\cdot\vec{p}$ method. Since this calculation is too tedious for a practical purpose, we adopt a simpler method of solving Kane's 4×4 matrix,[23] which is obtained by taking into account the bands outside the s-p subspace but neglecting the spin-orbit interaction: This neglect is a good approximation under $E_G \gg \Delta_0$ and $\hbar^2k^2/(2m_0) \gg \Delta_0$. In this method we obtain a form

$$|l_H\vec{k}\rangle = \alpha_H(\vec{k})\,|s\uparrow\rangle + \beta_H(\vec{k})\,|x\uparrow\rangle + \gamma_H(\vec{k})\,|y\uparrow\rangle + \delta_H(\vec{k})\,|z\uparrow\rangle \tag{4.6}$$

for HB, where the coefficients $\alpha_H(\vec{k})$, $\beta_H(\vec{k})$, $\gamma_H(\vec{k})$, and $\delta_H(\vec{k})$ are determined using the 4×4 matrix. Since the coefficients are dependent on the direction of $\vec{k}$, we consider averages such as $\langle|\alpha_H(\vec{k})|^2\rangle_{\mathrm{av}}$ over all directions. We find

$$\langle|\beta_H(\vec{k})|^2\rangle_{\mathrm{av}} = \langle|\gamma_H(\vec{k})|^2\rangle_{\mathrm{av}} = \langle|\delta_H(\vec{k})|^2\rangle_{\mathrm{av}} \simeq \tfrac{1}{3} \gg \langle|\alpha_H(\vec{k})|^2\rangle_{\mathrm{av}}$$

for various III-V compounds. The value of $\langle|\alpha_H(\vec{k})|^2\rangle_{\mathrm{av}}$ may be sensitive to the spin-orbit splitting which is neglected for the 4×4 matrix. In fact $\langle|\alpha_H(\vec{k})|^2\rangle_{\rm av}$ is too small especially if $E_G \lesssim \Delta_0$. Therefore, it is inadequate to use the direct relation $|\langle l_C,\vec{0}\,|\,l_H,\vec{k}\rangle|^2=\langle|\alpha_H(\vec{k})|^2\rangle_{\rm av}$. Instead of using the relation we calculate the momentum matrix element $\langle l_C,\vec{k}\,|\,\vec{p}\,|\,l_H,\vec{k}\rangle$ in $f_{\rm CH}(\vec{k})$ using Eqs. (4.1) and (4.6). We obtain

$$f_{CH}(\vec{k})=\tfrac{1}{3}\,|a_C(\vec{k})|^2\,|b_H(\vec{k})|^2\frac{E_p}{E_C(\vec{k})-E_H(\vec{k})}\,, \qquad (4.7)$$

where we define

$$|b_H(\vec{k})|^2=3\left\langle\left|\frac{\beta_H(\vec{k})k_x+\gamma_H(\vec{k})k_y+\delta_H(\vec{k})k_z}{k}\right|^2\right\rangle_{\rm av}. \qquad (4.8)$$

For the calculation based on Eqs. (4.4), (4.7), and (4.8) we write $|l_C,\vec{0}\,|\,l_H,\vec{k}\rangle|^2_C$. We consider this to offer the most rigorous calculation.

Next we consider $\langle l_H,\vec{0}\,|\,l_S,\vec{k}\rangle$. Discussions are analogous to those for $\langle l_C,\vec{0}\,|\,l_H,\vec{k}\rangle$. To obtain the expressions for $\langle l_H,\vec{0}\,|\,l_S,\vec{k}\rangle$ the subscripts C and H in Eqs. (4.2)–(4.8) are replaced by the subscripts H and S, respectively, with the exception of $b_H(\vec{k})$ which is common to $f_{CH}(\vec{k})$ and $f_{HS}(\vec{k})$. We write $|\langle l_H,\vec{0}\,|\,l_S,\vec{k}\rangle|^2_a$, $|\langle l_H,\vec{0}\,|\,l_S,\vec{k}\rangle|^2_b$, and $|\langle l_H,\vec{0}\,|\,l_S,\vec{k}\rangle|^2_c$ for the calculations based on the pairs of equations corresponding to Eqs. (4.2) and (4.3), Eqs. (4.4) and (4.5), and Eqs. (4.4) and (4.7), respectively. We have $|\langle l_H,\vec{0}\,|\,l_S,\vec{k}\rangle|^2_a=0$ because of $a_S(0)=0$. Conventionally $|\langle l_H,\vec{0}\,|\,l_S,\vec{k}\rangle|^2_b$ has been used. However, $|\langle l_H,\vec{0}\,|\,l_S,\vec{k}\rangle|^2_c$ offers the most rigorous calculation based on $f_{HS}(\vec{k})$.

The value of $|b_H(\vec{k})|^2$, which is commonly involved in the expressions of $|\langle l_C,\vec{0}\,|\,l_H,\vec{k}\rangle|^2_c$ and $|\langle l_H,\vec{0}\,|\,l_S,\vec{k}\rangle|^2_c$, is calculated under the threshold conditions of the *HCCC* process and the *HHSC* process. Materials $\mathrm{Ga}_{1-x}\mathrm{Al}_x\mathrm{As}$, $\mathrm{InAs}_x\mathrm{P}_{1-x}$, $\mathrm{In}_{1-x}\mathrm{Ga}_x\mathrm{As}_y\mathrm{P}_{1-y}$, and GaSb are taken as examples. For these materials and for both the *HCCC* and *HHSC* (under $E_G>\Delta_0$) processes we find $|b_H(\vec{k})|^2=0.89\pm0.06$. Table II shows the calculated results of the products

$$P_a=|\langle l_C,\vec{0}\,|\,l_H,\vec{k}_2\rangle|^2_a\,|\langle l_C,\vec{0}\,|\,l_C,\vec{k}_2\rangle|^2\,,$$

$$P_b=|\langle l_C,\vec{0}\,|\,l_H,\vec{k}_2\rangle|^2_b\,|\langle l_C,\vec{0}\,|\,l_C,\vec{k}_2\rangle|^2\,,$$

and

$$P_c=|\langle l_C,\vec{0}\,|\,l_H,\vec{k}_2\rangle|^2_c\,|\langle l_C,\vec{0}\,|\,l_C,\vec{k}_2\rangle|^2$$

for the *HCCC* process, and the products

$$P_a=|\langle l_C,\vec{0}\,|\,l_H,\vec{k}_3\rangle|^2_a\,|\langle l_H,\vec{0}\,|\,l_S,\vec{k}_3\rangle|^2_b\,,$$

$$P_b=|\langle l_C,\vec{0}\,|\,l_H,\vec{k}_3\rangle|^2_b\,|\langle l_H,\vec{0}\,|\,l_S,\vec{k}_3\rangle|^2_b\,,$$

and

$$P_c=|\langle l_C,\vec{0}\,|\,l_H,\vec{k}_3\rangle|^2_c\,|\langle l_H,\vec{0}\,|\,l_S,\vec{k}_3\rangle|^2_c$$

for the *HHSC* process. In the table we also show

$$P_c'=[1+4(\epsilon_0-1)/\epsilon_0]P_c\,.$$

It should be noted that P_a, P_b, and P_c correspond to τ_0^{-1} and P_c' corresponds to τ^{-1} in Eq. (3.14). We see that P_a is quite incorrect as compared to P_c even though this has frequently been used for the calculation based on the conventional formulas. Although P_b is a result of the improved calculation, P_b is larger than P_c. However, it is of special importance that P_c' fairly agrees with P_b, since the calculations of τ_0 based on P_b have given a satisfactory explanation of experiments for *p*-type GaAs (Refs. 13 and 16) and *n*-type InAs.[13,29] This shows that τ, i.e., Eq. (3.14), gives an accurate description of experiments. Discussion concerning the overestimation of the overlap integrals has also been given from a different view point in Ref. 33.

In conclusion, although a number of calculations of the BBAR rate have led to agreements between theories and experiments, the agreements are fortuitous as long as the calculations have been based essentially on τ_0. We should

TABLE II. Values of P_a, P_b, P_c, and P_c'.

Process	Material	P_a	P_b	P_c	P_c'
HCCC	GaAs	0.72	0.23	0.10	0.48
	$\mathrm{Ga_{0.8}Al_{0.2}As}$	0.84	0.27	0.11	0.52
	InP	0.77	0.23	0.097	0.46
	$\mathrm{InAs_{0.6}P_{0.4}}$	0.61	0.19	0.083	0.39
	InAs	0.68	0.20	0.095	0.45
	GaSb	0.70	0.22	0.087	0.36
	$\mathrm{In_{0.91}Ga_{0.09}As_{0.2}P_{0.8}}$	0.69	0.23	0.10	0.47
	$\mathrm{In_{0.72}Ga_{0.28}As_{0.6}P_{0.4}}$	0.64	0.22	0.10	0.47
	$\mathrm{In_{0.53}Ga_{0.47}As}$	0.64	0.22	0.10	0.47
HHSC	GaAs	0.081	0.035	0.019	0.087
	$\mathrm{Ga_{0.8}Al_{0.2}As}$	0.083	0.039	0.020	0.095
	InP	0.088	0.037	0.018	0.082
	$\mathrm{InAs_{0.6}P_{0.4}}$	0.073	0.031	0.016	0.075
	$\mathrm{InAs_{0.8}P_{0.2}}$	0.10	0.018	0.0090	0.042
	$\mathrm{In_{0.91}Ga_{0.09}As_{0.2}P_{0.8}}$	0.098	0.042	0.021	0.099
	$\mathrm{In_{0.72}Ga_{0.28}As_{0.6}P_{0.4}}$	0.092	0.040	0.022	0.10
	$\mathrm{In_{0.53}Ga_{0.47}As}$	0.071	0.029	0.015	0.070

use Eq. (3.14) for a rigorous calculation under a careful estimation of the overlap integrals. This is important especially at the present stage when a discussion of semiconductor laser operation requires a high-accuracy calculation of the BBAR rate. In order to find the overlap integrals, use of the oscillator strength under $|b_H(\vec{k})|^2=0.89$ is recommended for practical purposes.

ACKNOWLEDGMENTS

I wish to express my appreciation to Dr. G. Kano, Dr. I. Teramoto, and Dr. H. Mizuno for their constant encouragement.

---

[1] P. T. Landsberg, Phys. Status Solidi A 41, 457 (1970).

[2] A. Haug, in *Festköperprobleme XII, Advances in Solid State Physics,* edited by O. Madelung (Pergamon, Braunschweig, 1972), p. 411.

[3] R. Conradt, in *Festkörperprobleme XII, Advances in Solid State Physics,* edited by O. Madelung (Pergamon, Braunschweig, 1972), p. 449.

[4] P. T. Landsberg and M. J. Adams, J. Lumin. 7, 3 (1973).

[5] A. R. Beatie and P. T. Landsberg, Proc. R. Soc. London, Ser. A 249, 16 (1959).

[6] R. Conradt, Z. Phys. 209, 445 (1968).

[7] L. Huldt, Phys. Status Solidi A 33, 607 (1976).

[8] W. Lochmann, Phys. Status Solidi A 40, 285 (1977).

[9] W. Lochmann, Phys. Status Solidi A 42, 181 (1977).

[10] W. Lochmann, Phys. Status Solidi A 45, 423 (1978).

[11] M. Takeshima, Phys. Rev. B 26, 917 (1982).

[12] M. Takeshima, Phys. Rev. B 23, 6625 (1981).

[13] M. Takeshima, Jpn. J. Appl. Phys. 22, 491 (1983).

[14] M. Takeshima, Phys. Rev. B 23, 771 (1981).

[15] M. Takeshima, Phys. Rev. B 25, 5390 (1982).

[16] M. Takeshima, Phys. Rev. B 27, 2387 (1983).

[17] S. Doniach and E. H. Sondheimer, in *Green's Function for Solid State Physicists* (Benjamin, Boston, 1974).

[18] V. L. Bonch-Bruevich, in *Semiconductors and Semimetals,* edited by R. K. Willardson and A. C. Beer (Academic, New York, 1966), Vol. 1, Chap. 4.

[19] P. Nozières, *Theory of Interacting Fermi Systems* (Benjamin, New York, 1964).

[20] Y. Abe, Y. Osaka, and A. Morita, J. Phys. Soc. Jpn. 17, 1576 (1962).

[21] L. J. Sham and T. M. Rice, Phys. Rev. 144, 708 (1966).

[22] E. Antončik and P. T. Landsberg, Proc. Phys. Soc. London 82, 337 (1963).

[23] E. O. Kane, in *Semiconductors and Semimetals,* edited by R. K. Willardson and A. C. Beer (Academic, New York, 1966), Vol. 1, Chap. 3.

[24] W. Lochmann and A. Haug, Solid State Commun. 35, 553 (1980).

[25] W. Lochmann and A. Haug, J. Phys. Soc. Jpn. 49, 643 (1980).

[26] A. Sugimura, Appl. Phys. Lett. 39, 21 (1981).

[27] A. Sugimura, IEEE J. Quantum Electron. QE-17, 441 (1981).

[28] A. Sugimura, IEEE J. Quantum Electron. QE-17, 627 (1981).

[29] M. Takeshima, Phys. Rev. B 26, 3192 (1982).

[30] W. Lochmann, Ph.D. thesis, Technische Universität, Berlin, 1978 (unpublished).

[31] P. Lawaetz, Phys. Rev. B 4, 3460 (1971).

[32] M. Takeshima, J. Appl. Phys. 49, 6118 (1978).

[33] M. G. Burt, Electron. Lett. 18, 806 (1982).