Transition rates for acoustic-phonon-hole scattering in *p*-type silicon with nonparabolic bands

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Transition rates for acoustic-phonon – hole interactions in Si are calculated using the deformation-potential scattering theory of Tiersten. No assumptions of band parabolicity have been made. The transition rates incorporating the full nonspherical-nonparabolic nature of the Si band structure have been calculated numerically. As a result, the transition rates are strikingly dependent on energy as well as on incident and scattered directions. We have also found for intraband scattering, as Tiersten did for Ge, that light holes scatter more strongly in the forward direction and heavy holes scatter more strongly in the forward direction and heavy holes scatter more strongly in the backward direction when the forward scattering direction is chosen from the $\langle 100 \rangle$ or $\langle 111 \rangle$ symmetry set. We have also considered the $\langle 110 \rangle$ symmetry set and have found here that as energy increases the trend mentioned above for intraband scattering is no longer true. As a check on our computational procedure we have calculated transition rates for Ge and compared our results to those of Tiersten. The two sets of values are in close agreement.

I. INTRODUCTION

In calculating electronic transport coefficients of semiconductors, it is necessary to obtain transition rates for carriers scattered by various mechanisms. At low temperatures scattering processes are dominated by acoustic-phonon interactions. In the present work we investigate the scattering rates of holes by acoustic phonons in the long-wavelength limit for p-type Si. Although the problem of acoustic mode scattering in the diamond structure has been dealt with in great detail in the past, 1-8detailed comprehensive results have mostly been applied to Ge (Ref. 9) in which the valence-band structure is approximately parabolic. Band nonparabolicity, if accounted for, was usually included in the density of states¹⁰ or in energy correction factors in the calculation of transport coefficients.⁶ However, the transition rates themselves were all calculated based on the scattering between parabolic bands. This is justifiable for Ge in which the valence spin-orbit splitting is relatively large (0.3 eV) and the coupling between the spin-orbit split and the two top valence bands is weak and may be neglected. This approximation is not valid for Si

in which the spin-orbit splitting energy is small (0.044 eV). The coupling is strong and should not be neglected.

Wiley^{7,11} did consider the effects of band nonparabolicity in the calculation of transition rates and displays the results for Si. But, he concerned himself mainly with the direct-gap III-V compounds. Wiley used the wave functions of Kane¹² which were calculated for narrow-gap materials such as InSb, in which the coupling between the conduction and valence bands is very much stronger than the coupling between the spin orbit and the two top valence bands. Consequently, the latter coupling was neglected. Also, in that work the heavy-hole band was treated as parabolic and decoupled from the other bands. This, however, is not the situation in Si. The light and heavy valence bands in Si are coupled to the spin-orbit band much more strongly than they are to the conduction band because the direct gap is large (4.185 eV) relative to the split-off energy.¹³ Also, the heavy-hole band can be quite nonparabolic especially in the $\langle 110 \rangle$ directions. Thus, the application of the narrow-gap wave functions is not warranted for Si.

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Furthermore, Wiley used an expression for the transition rates given by Ehrenreich,¹⁴ which was derived just for intraconduction-band scattering of longitudinal-optical modes coupled to electrons by polar interaction. This expression he then modified to accommodate *p*-type conduction involving both intra- and interband transitions. An essential part of Wiley's analysis was based upon an overlap integral which arises as a distinct factor in the interaction Hamiltonian given by Ehrenreich. The overlap was taken between the periodic parts of the initial and final Bloch states having the same energy. Wiley assumed acoustic mode scattering to be modulated by the same overlap factor. This Costato⁸ explicitly states. In the more complete theoretical models of acoustic-phonon scattering $^{2-5}$ another type of overlap integral occurs. This overlap is not taken between the initial and final Bloch states since they are mediated by a deformation operator. What does occur is an overlap between the initial (final) Bloch states and a complete set of intermedi-

In order to evaluate the overlap, Wiley (and Costato) assumed the incident wave vector parallel to any one principal axis to be representative of any other incident direction. As a result, their transition rates depend only on the scattering angle between the incident and scattered wave vectors and not on the details of the incident and scattered directions relative to the Brillouin-zone axes. Vassell et al.¹⁵ show this assumption to be valid for the Ehrenreich overlap integral in III-V narrowgap semiconductors by using the symmetry properties of the associated Kane wave functions. However, it is quite clear from Tiersten's^{2,3} treatment of acoustic mode scattering in Ge that the transition probabilities are highly dependent on the incident and scattered directions relative to the axes of the Brillouin zone as well as the scattering angle. The same should be particularly true of Si in light of the high anisotropy of its valence band structure.

ate virtual states at different energies.

Finally, Wiley's results of the overlap analysis for interband scattering are in contradiction with those of the more complete theories of acoustic mode scattering,¹⁻³ since the former predicts zero forward and backward scattering. The work on Ge by Ehrenreich and Overhauser¹ and Tiersten³ clearly shows nonzero transition rates for forward and backward interband acoustic-phonon scattering. Ehrenreich and Overhauser used both a rigid-ion model and a deformable-ion model, while Tiersten used a deformation-potential model.

In this paper we use the deformation-potential

scattering theory of Tiersten,² and apply it to Si. Tiersten's theory is reviewed in Sec. II.

Because of the complicated nature of the wave functions away from $\vec{k} = 0$, they were generated numerically. As we will show in Sec. III, the incorporation of band nonparabolicity results in transition rates which are strikingly dependent on energy as well as on incident and scattered directions. Also, in Sec. III, we have applied our computational procedure to Ge and have compared the results to those of Tiersten. The two sets of results are in close agreement.

II. A REVIEW OF THE THEORY

The theory of phonon-hole interactions in semiconductors is directly connected with the theory of strain-induced effects. The operator \hat{D} which effects the transition between Bloch states is precisely the operator that arises when considering the effect of a small homogeneous strain.^{4,16} It is

$$\hat{D} = \sum_{i,j}^{3} D^{ji} \epsilon_{ij} . \qquad (2.1)$$

Here, the sum is over the Cartesian coordinates x, y, and z. D^{ji} is an element of the tensor deformation potential operator and is discussed by Whitfield.⁵ ϵ_{ij} is an element of the strain tensor $\dot{\epsilon}$.

The operator \hat{D} arises by requiring the potential of the strained crystal to have the same periodicity as the potential of the unstrained crystal. Consequently, the Bloch modulating functions also have the same periodicity, which is desirable if perturbation theory is to be used. When the appropriate coordinate transformation^{4,16} $\vec{r}' \simeq (\vec{1} - \vec{\epsilon}) \cdot \vec{r}$, which assures the periodicity condition, is substituted into the $\vec{k} \cdot \vec{p}$ Hamiltonian, it causes

$$\hat{H} \rightarrow \hat{H} + \hat{D}$$
 (2.2)

In particular, for Si

$$\hat{H} = \hat{H}_0 + \hat{H}_{\vec{k} \cdot \vec{p}} + H_{SO}$$
, (2.3)

where \hat{H}_0 is the unperturbed Hamiltonian operator made up of the kinetic energy part plus the periodic lattice potential. The eigenvalue equation for \hat{H}_0 is satisfied by the functions $|\epsilon_1\rangle$, $|\epsilon_2\rangle$, and $|\epsilon_3\rangle$ at $\vec{k} = 0$. These functions transform as a basis of the Γ'_{25} representation of the cubic group.¹⁷ Including spin, the top of the valence-band structure is sixfold degenerate. The next term, $\hat{H}_{\vec{k}\cdot\vec{p}}$, is due to the $\vec{k}\cdot\vec{p}$ perturbation. This term splits the de<u>24</u>

generacy, away from $\vec{k} = 0$, yielding three twofold degenerate bands. Lastly, \hat{H}_{SO} is the kindependent part of the spin-orbit interaction. Its effect is to split off one of the degenerate bands at $\vec{k} = 0$ by an amount Δ (=0.0441 eV for Si). The $\vec{k} \cdot \vec{p}$ theory, including the effects of a spin-orbit perturbation, for Si is discussed thoroughly by Kane.¹³ Once the eigenfunctions of \hat{H} are known, the calculation of the probability of transition of an electron between states due to the perturbation \hat{D} may be carried out.

The transition matrix element for phonon-hole scattering between Bloch states of bands n and m, wave vectors \vec{k} and $\vec{k'}$, and phonon states characterized by occupation numbers N and N', as given by Tiersten² [Eq. (3.1)], is

$$\langle n \vec{\mathbf{k}}, N \mid T \mid m \vec{\mathbf{k}}', N' \rangle$$

= $\frac{1}{2} \sum_{i,j}^{3} \langle n \vec{\mathbf{k}}, N \mid S_{ij} D^{ji} + D^{ji} S_{ij} \mid m \vec{\mathbf{k}}', N' \rangle$, (2.4)

where S_{ij} is an element of the displacement tensor and can be written as

$$S_{ij} = \frac{\partial u_j}{\partial x_i} . \tag{2.5}$$

That is, S_{ij} is the change in the *j*th component of

the local lattice displacement \vec{u} with respect to the *i*th direction. The insertion of S_{ij} into Eq. (2.4) comes about since the strain tensor ϵ_{ij} in Eq. (2.1) can be written as the symmetric part of the displacement tensor S_{ii} . Also,

$$|n\vec{\mathbf{k}},N\rangle = |\xi_{n\vec{\mathbf{k}}}\rangle e^{i\vec{\mathbf{k}}\cdot\vec{\mathbf{r}}}|N\rangle , \qquad (2.6)$$

where $|N\rangle$ is a phonon state, which can be written as a product of quasistationary-phonon states $|N_{\vec{q},s}\rangle$ of wave vector \vec{q} and polarization *s*, each satisfying the harmonic oscillator equation. $|\xi_{n\vec{k}}\rangle$ is the periodic part of the Bloch state. It may be expanded in terms of the original unperturbed degenerate set of eigenfunctions of \hat{H}_0 , then becoming

$$|\xi_{n\vec{k}}\rangle = \sum_{r=1}^{\circ} A_{nr}(\vec{k}) |\epsilon_{r}\rangle . \qquad (2.7)$$

The expansion coefficients A_{nr} are obtained directly by diagonalization of \hat{H} in Eq. (2.3). These are the quantities that we treat numerically throughout the calculation. The first index n on A_{nr} labels the band, the second index r labels the spin state, r=1,2,3 \uparrow , r=4,5,6 \downarrow .

Inserting a complete set of states between the first pair of operators S_{ij} and D^{ji} of Eq. (2.4) and noting that D^{ji} does not operate on phonon states we get

$$\langle n\vec{\mathbf{k}}, N | S_{ij}D^{ji} | m\vec{\mathbf{k}}', N' \rangle = \sum_{N'} \sum_{n', \vec{\mathbf{k}}'} \langle n\vec{\mathbf{k}}, N | S_{ij} | n'\vec{\mathbf{k}}', N' \rangle \langle n'\vec{\mathbf{k}}' | D^{ji} | m\vec{\mathbf{k}}' \rangle , \qquad (2.8)$$

since D^{ji} is diagonal in \vec{k}' , but not in the band index.⁵

The matrix element for just S_{ij} is

$$\langle n\vec{\mathbf{k}}, N | S_{ij} | n'\vec{\mathbf{k}}', N' \rangle = \int d^3r \langle N | S_{ij} | N' \rangle \exp[-i(\vec{\mathbf{k}} - \vec{\mathbf{k}}') \cdot \vec{\mathbf{r}}] \xi_{n\vec{\mathbf{k}}}^*(\vec{\mathbf{r}}) \xi_{n'\vec{\mathbf{k}}'}(\vec{\mathbf{r}}) .$$

$$(2.9)$$

The displacement field \vec{u} of Eq. (2.5) can be Fourier analyzed into phonon states, and thus S_{ij} may be written as

$$S_{ij} = i \sum_{\vec{q},s} p_j(\vec{q},s) q_i Q(\vec{q},s) \exp(i \vec{q} \cdot \vec{r}) .$$
(2.10)

Here p_j is the *j*th component of the phonon polarization vector \hat{p} and $Q(\hat{q},s)$ are the Fourier-Euler coefficients. Inserting Eq. (2.10) into Eq. (2.9) we obtain

$$\langle n\vec{\mathbf{k}}, N | S_{ij} | n'\vec{\mathbf{k}}', N \rangle = i \sum_{\vec{q},s} p_j(\vec{q},s) q_i \langle N | Q(\vec{q},s) | N' \rangle \delta_{\vec{q},\vec{\mathbf{k}}-\vec{\mathbf{k}}'} I_{nn'}(\vec{\mathbf{k}},\vec{\mathbf{k}}') , \qquad (2.11)$$

where $I_{nn'}(\vec{k},\vec{k}') = \langle \xi_{n\vec{k}} | \xi_{n'\vec{k}'} \rangle$ is the overlap integral between the periodic parts of the Bloch states. Because we are considering long-wavelength phonons umklapp processes are comparatively uncommon and have been neglected in the Kronecker delta.

Lastly, $\langle N | Q | N' \rangle$ must be evaluated. This can be accomplished by quantizing the Fourier-Euler coefficients $Q(\vec{q},s)$ in terms of a normalized set of creation and annihilation operators. When this is done the only surviving terms are

$$\langle N | Q(\vec{q},s) | N' \rangle = \begin{cases} \left[\frac{\hbar(N+1)}{2\rho V \omega(\vec{q},s)} \right]^{1/2} & \text{for emission} \\ \left[\frac{\hbar N}{2\rho V \omega(\vec{q},s)} \right]^{1/2} & \text{for absorption} \end{cases}$$

where ρ is the mass density of the crystal, V is its volume, and $\omega(\vec{q},s)$ is the angular frequency of the elastic wave. \hbar is Planck's constant divided by 2π . Now,

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$$N = \left[\exp\left[\frac{\hbar\omega(\vec{q},s)}{k_B T}\right] - 1 \right]^{-1} \simeq \frac{k_B T}{\hbar\omega(\vec{q},s)}$$
(2.13)

with k_B being the Boltzmann constant and T the absolute temperature. We assume that $\hbar\omega(\vec{q},s) << k_B T$, which is valid for all but the lowest of temperatures and hence the equipartition of energy among phonon modes. With this assumption $N + 1 \simeq N$, and emission and absorption may be considered to have equal weight.

The same analysis can be carried out on the second pair of operators in Eq. (2.4) with similar results. Then, for either emission or absorption, the transition matrix element for a particular branch of polarization becomes

$$T_{nm}^{s}(\vec{k},\vec{k}') = \frac{i(k_{B}T)^{1/2}}{2(\rho V)^{1/2}} \sum_{i,j}^{3} \frac{q_{i}p_{j}(\vec{q},s)}{qc_{s}(\vec{q})} B_{nm}^{ji}(\vec{k},\vec{k}') , \qquad (2.14)$$

where $c_s(\vec{q}) [=\omega(\vec{q},s)/q]$ is the speed of an elastic wave with polarization *s*, and

$$B_{nm}^{ji}(\vec{k},\vec{k}') = \sum_{n'} \left[I_{nn'}(\vec{k},\vec{k}') \langle \xi_{n'\vec{k}'} | D^{ji} | \xi_{m\vec{k}'} \rangle + \langle \xi_{n\vec{k}} | D^{ji} | \xi_{n'\vec{k}} \rangle I_{n'm}(\vec{k},\vec{k}') \right].$$
(2.15)

Note that the sum over n' is, in principle, over all the bands at \vec{k} (and $\vec{k'}$) but for Si we choose $1 \le n' \le 6$, corresponding to the doubly degenerate set of the top two valence and one spin-orbit bands. These are coupled to each other much more strongly than to other bands as \vec{k} and $\vec{k'} \rightarrow 0$.

With the aid of Eq. (2.7) B^{ji} may be rewritten in terms of the original unperturbed degenerate set of eigenfunctions. The overlap integral takes the form

$$I_{nn'}(\vec{k},\vec{k}') = \sum_{p=1}^{6} A_{np}^{*}(\vec{k}) A_{n'p}(\vec{k}') , \qquad (2.16)$$

while the matrix element for D^{ji} becomes

$$D_{n'm}^{ji} = \langle \xi_{n'k'} | D^{ji} | \xi_{m\vec{k}'} \rangle$$

= $\sum_{c,d}^{6} A_{n'c}^{*}(\vec{k}') A_{md}(\vec{k}') \langle \epsilon_{c} | D^{ji} | \epsilon_{d} \rangle$.
(2.17)

Recalling that $|\epsilon_r\rangle$ and $|\epsilon_{r+3}\rangle$, r=1,2,3, have the same transformation properties except for spin we write the deformation potentials¹⁸

$$l = \langle \epsilon_i \pm | D^n | \epsilon_i \pm \rangle ,$$

$$m = \langle \epsilon_j \pm | D^{ii} | \epsilon_j \pm \rangle ,$$

$$n = 2 \langle \epsilon_i \pm | D^{ji} | \epsilon_i \pm \rangle ,$$

(2.18)

where the + and - signs indicate spin up and spin down, respectively.

By using the symmetry properties of the $|\epsilon_r\rangle$ (Ref. 17) and those of the operator⁵ D^{ji} Eq. (2.17) reduces to

$$D_{n'm}^{ii} = F_{n'm}^{ii} l + (F_{n'm}^{jj} + F_{n'm}^{kk})m, \ i \neq j \neq k$$
(2.19)

with

$$F_{n'm}^{ii} = A_{n'i}^{*}(\vec{k}')A_{mi}(\vec{k}') + A_{n'i+3}^{*}(\vec{k}')A_{mi+3}(\vec{k}') , \qquad (2.20)$$

or

$$D_{n'm}^{ji} = [A_{n'j}^{*}(\vec{k}')A_{mi}(\vec{k}') + A_{n'j+3}^{*}(\vec{k}')A_{mi+3}(\vec{k}') + A_{n'i}^{*}(\vec{k}')A_{mj+3}(\vec{k}')]\frac{n}{2}$$

$$i \neq j.$$
(2.21)

It is convenient at this point to change notation slightly. Since each band is twofold degenerate, we group the band indices into degenerate sets. Thus for the spin-orbit bands $n=1,2\rightarrow N=S$, the lighthole bands $n=3,4\rightarrow N=L$, and for the heavy-hole bands $n=5,6\rightarrow N=H$. Now the transition probability per unit time is written as

(2.12)

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$$W_{NM}(\vec{\mathbf{k}},\vec{\mathbf{k}}')=2\left[\frac{2\pi}{\hbar}\right]\sum_{s=1}^{3}|T_{NM}^{s}(\vec{\mathbf{k}},\vec{\mathbf{k}}')|^{2}$$
$$\times\delta(E_{N\vec{\mathbf{k}}}-E_{M\vec{\mathbf{k}}'}),$$

(2.22)

where the initial factor of 2 arises because emission and absorption have been given equal weight and both processes have been included in Eq. (2.22).

If W_{NM} is to be used in transport calculations we must recognize that the collision term of the Boltzmann equation does not distinguish between degenerate states. This means that $|T_{NM}^s|^2$ is not just $|T_{nm}^s|^2$ summed over the degenerate states associated with N and M. What must be done is a sum over the degenerate final states and an average over the initial states,^{1,3,14} thus yielding.

$$T_{NM}^{s}(\vec{k},\vec{k}') |^{2} = \frac{1}{2} \sum_{n(N)} \sum_{m(M)} |T_{nm}^{s}(\vec{k},\vec{k}')|^{2}.$$
(2.23)

It is Eq. (2.22), along with Eq. (2.23), whose evaluation will be the focus of the next section.

III. CALCULATION OF MATRIX ELEMENTS AND DISCUSSION

In order to calculate the matrix elements T we require the phonon polarization vectors $\hat{p}(\vec{q},s)$. Since we are concerned with the long-wavelength limit we assume the solid can be treated as elastically isotropic, so that longitudinal and transverse waves will be independent of direction, but in general are not equal to each other. The set of polarization vectors we use are those given by Ehrenreich and Overhauser.¹ They are

$$\hat{p}(\vec{q},l) = \frac{1}{q} \begin{vmatrix} q_{x} \\ q_{y} \\ q_{z} \end{vmatrix},$$

$$\hat{p}(\vec{q},t_{1}) = (q_{x}^{2} + q_{y}^{2})^{-1/2} \begin{vmatrix} q_{y} \\ -q_{x} \\ 0 \end{vmatrix}, \qquad (3.1)$$

$$\hat{p}(\vec{q},t_{2}) = q^{-1}(q_{x}^{2} + q_{y}^{2})^{-1/2} \begin{vmatrix} q_{x} \\ -q_{x} \\ q_{y} q_{z} \\ -(q_{x} + q_{y}) \end{vmatrix},$$

where l stands for longitudinal and t_1 and t_2 refer to the two transverse polarization branches.

Isotropic phonon velocities c_s may be obtained from spherically averaged elastic coefficients. They are given by Wiley¹¹ for Si as

$$\overline{C}_{44} = \rho c_t^2 = 6.804, \ \overline{C}_{11} = \rho c_l^2 = 17.262$$
 (3.2)

in units of 10^{11} dyne/cm².

Two sets of other quantities are needed to complete the calculation. They are the valence-band parameters¹⁰ (in a.u.)

$$L = -6.53, M = -4.64, N = -8.75$$
 (3.3)

and the deformation potentials^{18,11} (in eV)

$$a = 2.1, b = -2.2, d = -5.3$$
. (3.4)

We now have the necessary ingredients to calculate the transition rates W of Eq. (2.22). To illustrate the effect of band nonparabolicity on the transition rates, the transition rates are plotted as a function of energy for several sets of directions in Figs. 1(a), 1(b), and 1(c). Some insight into the structure of these plots may be obtained by simultaneously viewing the energy-band diagram of Fig. 2. There we have plotted energy versus wave vector squared for the valence bands, so that regions of nonparabolicity may be readily identified.

Figure 1(a) shows both intra- and interband scattering between the [100] and [001] directions with forward scattering being in the [100] direction. We first note that the heavy-hole to heavyhole $(H \rightarrow H)$ scattering is constant as a function of energy. The band diagram shows that the heavyhole (HH) band for the $\langle 100 \rangle$ set of directions is parabolic. As a consequence of band parabolicity the eigenfunctions of \hat{H} depend only on the direction of k and not its magnitude. It may then be expected that transitions between two bands which are parabolic would depend only on the directions of \vec{k} and \vec{k}' and not on their magnitudes. This kind of behavior is clearly evident in Tiersten's work in which he treats the valence bands of Ge as purely parabolic; consequently, he displays singlevalued transition rates for all sets of directions.

On the other hand, the light-hole (LH) band for the $\langle 100 \rangle$ set exhibits a very slight nonparabolicity over a broad range of energies. For very small \vec{k} or very large \vec{k} the LH band approaches the parabolic limit, which is reflected in the $L \rightarrow L$ scattering of Fig. 1(a). At the lower energies the curve tends to flatten out indicating parabolicity. As we go out to larger energies the plot rises gently, curving upwards owing to the slight nonparabolicity at



FIG. 1. Normalized transition probabilities per unit time versus energy. Scattering occurs between the directions as indicated. The first direction is the incident direction. H, L, and S stand for heavy, light, and spin-orbit band sets. Then $L \rightarrow H$, for example, implies scattering from the light- to the heavy-hole band set.







FIG. 2. Energy versus wave vector squared. Valence and spin-orbit band energies are given for the symmetry directions shown. HH, LH, and SO stand for heavy-hole, light-hole, and spin-orbit bands, respectively.

these energies. Further out in energy, not shown on the plot, the transition probability will bend and tend to be flat as parabolicity becomes stronger.

The effects of nonparabolicity are most pronounced in Fig. 1(b). Here the scattering occurs between the [110] and [110] directions in which both the HH and LH bands exhibit regions of nonparabolicity. It is quite clear that the HH band has a sharp nonparabolic structure at the lower energies then quickly becomes parabolic. Concurrently the transition rate for $H \rightarrow H$ scattering responds in a fashion reflecting the sharp nonparabolicity and the quick transition to a region of parabolicity.

However, the LH band does not behave in such an abrupt manner. As with the $\langle 100 \rangle$ set, it is slightly nonparabolic over a broad energy range. The contrast between the LH and HH bands in the $\langle 110 \rangle$ directions is brought out in the $L \rightarrow H$ scattering in Fig. 1(b). In the lower-energy range, the strong nonparabolic nature of the HH band is dominant causing the curve to bend sharply. At slightly higher energies the HH nonparabolicity attenuates while that of the LH band grows. The result is a weak bending of the curve. Eventually, at the higher energies, the LH band becomes more parabolic and the $L \rightarrow H$ transition rate begins to flatten out.

In Fig. 1(c), we show interstar transition rates for scattering between the $[001] \rightarrow [111]$ and $[111] \rightarrow [110]$ directions. These may be analyzed in a similar manner to that of Figs. 1(a) and 1 (b) with reference to the band diagram. It should be mentioned that not all the transition rates involving the spin-orbit band can be found on the plots given. This is simply due to the fact that the $S \rightarrow L$ transition probabilities are of larger magnitude than the scale plotted, and the $S \rightarrow S$ transitions are of smaller magnitude. Also, for the sake of completeness, we have included Fig. 3. It shows the contributions of the longitudinal modes, () L, and transverse modes (both branches), () T, to the scattering for the $[110] \rightarrow [1\overline{10}]$ set given in Fig. 1(b).

In our second set of plots, Figs. 4, -6, we illustrate the anisotropy of the transition rates as a function of direction in the Brillouin zone as well as energy. Each plot has reflection symmetry about an axis parallel to the forward scattering direction. We have concluded, as did Tiersten, for the $\langle 100 \rangle$ and $\langle 111 \rangle$ intraband scattering that LH's scatter much more strongly in the forward direction than in the backward direction, and HH's scatter much more strongly in the backward direction than in the forward direction. This can clearly be seen in Fig. 4. Note also that the bulk of the



FIG. 3. These plots show the contributions of the longitudinal modes, () L, and the transverse (both branches) modes, () T, to the transition rates displayed in Fig. 1(b).



FIG. 4. Normalized intraband transition probabilities per unit time versus scattering angle. This figure shows the evolution of transition rates as a function of energy and scattering angle with respect to the forward direction. Each contour in (a) and (b) has reflection symmetry about an axis parallel to the forward direction.



FIG. 5. Normalized intraband transition probabilities per unit time versus scattering angle (see Fig. 4 caption).



FIG. 6. Normalized interband transition probabilities per unit time versus scattering angle (see Fig. 4 caption).

scattering of HH's is in the backward directions, while the bulk of the scattering of the light holes is in the forward directions. This trend maintains itself as energy is increased, and is found to be true for all forward directions of the $\langle 100 \rangle$ and $\langle 111 \rangle$ sets.

But, unlike Tiersten, we have also considered the $\langle 110 \rangle$ set of directions. We have found that only at the lower energies do the intraband scattering probabilities of light and heavy holes respond in the same fashion as described above for the $\langle 100 \rangle$ and $\langle 111 \rangle$ directions. As can be seen in Fig. 5(a), as the transition rates evolve in energy the predominance of backward scattering for HH's is reduced relative to the forward scattering. Also note that, in general, as energy is increased there arises a preponderance of scattering in the forward directions. The LH's on the other hand, Fig. 5(b), reverse the trend almost immediately. With small increments in energy the LH's then scatter more strongly in the backward direction, but there still appears to be a tendency for the bulk of the scattering to be in the forward directions. Only at the higher energies ($\sim \Delta$) do we see the backward directions becoming more dominant.

Figure 6 shows interband scattering between

light- and heavy-hole bands for the indicated directions. Forward and backward scattering rates are equal in both 6(a) and 6(b). As energy is increased they stay equal but reduced in magnitude. There is no overall preponderance of scattering in the forward or backward directions in either (a) or (b). However, at higher energies the curves do become slightly skewed, favoring the forward scattering directions.

Finally, as a check on the accuracy of our computational procedure we have calculated the transition rates for Ge and compared our results with those of Tiersten. Both sets of results are listed in Table I. Two comments are, however, in order.

Firstly, unlike Tiersten we did not assume Ge to be purely parabolic. We included the coupling between the SO, LH, and HH bands. Formally this manifests itself in Eq. (2.15). The sum over n' is taken over the three doubly degenerate bands instead of the two doubly degenerate valence bands. As a result our transition probabilities reflect whatever nonparabolicity that may be present in the band structure of Ge. In order to compare our results with those of Tiersten we chose values calculated at E = 0.0045 eV which should be in the parabolic limit.

$N \rightarrow M$	$H {\rightarrow} H$	$L \rightarrow L$	$L \rightarrow H$
Scattering directions	(heavy-hole band)	(light-hole band)	(interband)
[100]→[100]	0.25	2.56	14.29
	0.24	2.40	16.84
[100]→[100]	5.15	0.003	14.29
	4.40	0.000 65	16.84
[100]→[001]	8.74	7.68	7.52
	9.89	8.84	7.09
[001]→[111]	6.74	5.80	9.85
	6.76	5.56	9.23
[001]→[ĪĪĪ]	8.65	4.49	9.73
	9.00	4.97	9.57
[111]→[111]	0.0001	4.06	10.04
	0.0001	4.15	8.66
[111]→[111]]	8.71	0.99	10.04
	9.55	0.97	8.66
[111]→[111]	6.07	6.07	9.34
	6.80	6.92	9.86
[111]→[Ī1Ī]	7.82	3.73	9.38
	7.40	3.15	10.11
[111]→[001]			9.15
			10.13
[111]→[001]			10.09
			12.01

TABLE I. $W_{NM}(\vec{k}, \vec{k}') 2V\hbar/\pi k_B T$ (units of $10^{11} \text{ eV}^2 \text{ cm}^3/\text{erg}$) for Ge: a comparison of Tiersten's results with our results. The top set of values are those of Tiersten. The bottom set of values are ours calculated at E = 0.0045 eV.

Secondly, Tiersten did not assume, as we have, the phonon spectrum to be elastically isotropic. Instead, he obtained his polarization vectors and sound velocities exactly from the secular equation for elastic waves. Therefore any variation between the two sets of values can more than likely be attributed to the two differences mentioned above. Nevertheless, the two sets of calculations are in good agreement.

ACKNOWLEDGMENTS

We would like to thank Dr. P. Hemenger of the Materials Laboratory at Wright-Patterson AFB, without whose efforts this research would not have been possible. The work of one of us (F. S.) was performed under Air Force Contract No. F33615-78-C-5064 at the Wright-Patterson Materials Laboratory, Ohio.

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 - 3 and the notation of the first entry of Ref. 4.