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Effects of band structure on the energy exchange rate between quasithermal electron and hole distributions in semiconductors

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The rate at which energy is exchanged between Maxwellian distributions of electrons at temperature T_e and holes at temperature $T_h \neq T_e$ has been calculated using $\mathbf{K}\cdot\mathbf{P}$ theory to approximate the Bloch-function contribution to the Coulomb matrix element. Inter-valence-band scattering processes are found to contribute significantly to the net exchange rate, indicating that band structure must be included in a proper treatment of Coulomb scattering involving holes in semiconductors.

INTRODUCTION

The Coulomb interaction influences the dynamics of nonequilibrium or "hot-carrier" distributions in semiconductors in a number of ways. For instance, there have been many treatments of free-carrier screening of carrier-phonon interactions both in the context of laser annealing of Si,[1,2] and in the context of hot-electron cooling rates in GaAs and other III-V compound semiconductors.[3-5] More generally, in any kinetic equation analysis of hot-carrier dynamics, the role of carrier-carrier scattering must be considered at the outset. In the majority of cases, it has been assumed that Coulomb scattering is so much faster than either electron-phonon interactions or the influence of external perturbations, that quasiequilibrium free-carrier distributions can be adopted, albeit with effective temperatures which may be much different than that of the lattice.[3,4,6] This assumption removes the necessity of explicitly treating the Coulomb scattering process at all, and consequently simplifies the solution of the kinetic equations tremendously. Such an approach is justifiable if applied to the case of nanosecond or even some picosecond optical experiments, or to transport measurements in materials whose mobility is limited by impurities or phonons. However, recent advances in laser and material growth technologies have enabled the direct observation of phenomena which are governed by free-carrier Coulomb scattering. In particular, subpicosecond laser pulses have been used to probe the evolution of athermal free-carrier distributions on time scales comparable to that of the Coulomb thermalization process.[7-9] Combined optical-electrical measurements have also been performed on high-purity, two-dimensional semiconductor systems in which the mobility of the minority carriers is determined by interactions with the majority carriers.[10,11] Clearly, in order to model the results of these and future hot-carrier experiments, free-carrier interactions must be understood and treated on a microscopic, nonphenomenological level.

Recent attempts[3,4,12-14] to explicitly incorporate carrier scattering in kinetic and Monte Carlo models of hot-carrier dynamics have taken the Coulomb matrix element to be of the form $M(q)=4\pi e^2/(q^2+q_{\mathrm{TF}}^2)$ for a collision involving momentum exchange $\mathbf{q}$. It is generally acknowledged that the use of a single parameter $\mathbf{q}_{\mathrm{TF}}$ to account for static, small wave-vector screening is an approximation that simplifies the calculation but has yet to be quantitatively justified. Another approximation implicit in this form of $M(\mathbf{q})$ is the neglect of the Bloch nature of the single-particle states involved in the scattering. Although this point has been addressed in other contexts,[15-17] the implication of the approximation in the hot-carrier context seems not to be appreciated to the same extent as that of screening. However, in cw hot luminescence experiments, Zakharchenya[18] claims to observe effects due to the scattering of heavy holes into light-hole states via interactions with fast electrons. As pointed out by D'yakonov, Perel', and Yassievich[19] such processes can only be treated by including Bloch state overlap integrals in the Coulomb matrix element. Thus, in this paper, we present the results of electron-hole scattering calculations which explicitly include the effects of band structure for zinc-blende semiconductors. It is shown that even over a restricted range of densities and effective temperatures, not only the rate, but also the nature of the Coulomb mediated energy transfer between electrons and holes can be significantly influenced by the band structure.

THEORY

We restrict the analysis to direct band-gap zinc-blende semiconductors and consider the Coulomb interactions between free electrons in the conduction band and free holes in the spin-$\frac{3}{2}$-like valence bands (those degenerate at the zone center). An electron initially in a conduction-band state $\mathbf{K}_e$, can scatter into an empty conduction-band state $\mathbf{K}_e'$, via interactions in which (i) heavy holes scatter into heavy-hole states, (ii) light holes scatter into light-hole states, (iii) heavy holes scatter into light-hole states, and (iv) light holes scatter into heavy-hole states. Following the general development due to Landsberg,[20] the matrix element for any of these processes can be expressed as

$$|M^{i,j}(\mathbf{K}_e,\mathbf{K}_e';\mathbf{K}_h,\mathbf{K}_h')|^2=2\left(\frac{4\pi e^2}{\epsilon}\right)^2\left\{\frac{|\langle U^c_{\mathbf{K}_e'}|U^c_{\mathbf{K}_e}\rangle\langle U^{v_i}_{\mathbf{K}_h}|U^{v_j}_{\mathbf{K}_h'}\rangle|^2}{(|\mathbf{K}_e-\mathbf{K}_e'|^2+q_{\mathrm{TF}}^2)^2}+\frac{|\langle U^c_{\mathbf{K}_e'}|U^{v_j}_{\mathbf{K}_h'}\rangle\langle U^{v_i}_{\mathbf{K}_h}|U^c_{\mathbf{K}_e}\rangle|^2}{(|\mathbf{K}_e-\mathbf{K}_h|^2+q_{\mathrm{TF}}^2)^2}\right.$$
$$\left.+\left|\frac{\langle U^c_{\mathbf{K}_e'}|U^c_{\mathbf{K}_e}\rangle\langle U^{v_i}_{\mathbf{K}_h}|U^{v_j}_{\mathbf{K}_h'}\rangle}{(|\mathbf{K}_e-\mathbf{K}_e'|^2+q_{\mathrm{TF}}^2)}-\frac{\langle U^c_{\mathbf{K}_e'}|U^{v_j}_{\mathbf{K}_h'}\rangle\langle U^{v_i}_{\mathbf{K}_h}|U^c_{\mathbf{K}_e}\rangle}{(|\mathbf{K}_e-\mathbf{K}_h|^2+q_{\mathrm{TF}}^2)}\right|^2\right\}\delta(\mathbf{K}_e'+\mathbf{K}_h'-\mathbf{K}_h-\mathbf{K}_e)\ , \tag{1}$$

where ϵ is the background dielectric constant of the material, the $U^i_{\mathbf{K}}$ represent the periodic part of the electronic wave function of wave vector $\mathbf{K}$ in the ith band, $\mathbf{K}_h$ and $\mathbf{K}_h'$ represent the wave vectors of the initial and final hole states, and all spin states have been summed over. Umklapp-like processes have been ignored, as only scattering events near the zone center are considered.

The "exchange" terms involving overlap integrals between conduction- and valence-band states are expected to be small compared to those between light- and heavy-hole states. We have compared the magnitudes of the integrals for these two cases at selected points in the zone using a four-band $\mathbf{K}\cdot\mathbf{P}$ calculation. With a few exceptions, the intra- and inter-valence-band terms are in fact more than an order of magnitude larger, hence we neglect all terms involving overlap integrals between the conduction and valence bands. For simplicity we also restrict ourselves to relatively low densities and tempertures so that all three bands can be assumed to have parabolic dispersion. Then the overlap integrals between conduction-band states are well approximated by unity, and only intra- and inter-valence band overlap integrals are included.

Numerical calculations of the valence-band overlap integrals using three- and four-band $\mathbf{K}\cdot\mathbf{P}$ models show that there is relatively little error introduced by using the analytic expressions obtained by Wiley[21] from a simplified two band $\mathbf{K}\cdot\mathbf{P}$ model

$$|\langle U^i_{\mathbf{K}_1}|U^j_{\mathbf{K}_2}\rangle|^2=\begin{cases}\dfrac{1+3\cos^2\theta}{4}, & i=j\\ \dfrac{3\sin^2\theta}{4}, & i\neq j\ ,\end{cases} \tag{2}$$

where θ is the angle between $\mathbf{K}_1$ and $\mathbf{K}_2$. The total rate at which an electron, occupying a conduction-band state of wave vector $\mathbf{K}_e$, is scattered out of that state via Coulomb interactions with a distribution of holes in the valence bands, is given by

$$\Gamma(\mathbf{K}_e)=\frac{2\pi}{\hbar}\sum_{i,j=1}^{2}\int\frac{d\mathbf{K}_h}{(2\pi)^3}f^{v_i}(\mathbf{K}_h)\Gamma^{i,j}(\mathbf{K}_e,\mathbf{K}_h)\ ,$$

with

$$\Gamma^{i,j}(\mathbf{K}_e,\mathbf{K}_h)=\int\frac{d\mathbf{K}_e'}{(2\pi)^3}\int\frac{d\mathbf{K}_h'}{(2\pi)^3}[1-f^c(\mathbf{K}_e')][1-f^{v_j}(\mathbf{K}_h')]$$
$$\times|M^{i,j}(\mathbf{K}_e,\mathbf{K}_e';\mathbf{K}_h,\mathbf{K}_h')|^2\delta\left(\frac{\hbar^2}{2}\left(\frac{K_e^2}{m_c}+\frac{K_h^2}{m_{v_i}}-\frac{K_e'^2}{m_c}-\frac{K_h'^2}{m_{v_j}}\right)\right)\ , \tag{3}$$

where the sums are over the two valence bands, the $f^{v_i}(\mathbf{K})$ are the occupation factors for the holes, and the delta function ensures conservation of energy in each collision. For a given set of distributions of the free carriers, the Thomas-Fermi screening wave vector $\mathbf{q}_{\mathrm{TF}}$ can be calculated by taking the appropriate limit of the free-carrier contribution to the system's dielectric function

$$q_{\mathrm{TF}}^2=q^2[(\lim_{\substack{\omega=0\\ q\to 0}}\epsilon^{fc}(\mathbf{q},\omega))^{-1}-1]\ . \tag{4}$$

We ignore, for the present, the errors introduced by adopting this simplified picture of screening.[22,23] The principal point of this paper is to demonstrate the relative importance of inter- and intra-valence-band Coulomb scattering. Although a more accurate account of screening may change the quantitative results, the qualitative conclusions should still apply.

If we restrict ourselves to Maxwellian distributions then the population of the final states can be neglected in Eq. (3). With the overlap integrals of Eq. (2) substituted in Eq. (3), the integrals over $\mathbf{K}_e'$ and $\mathbf{K}_h'$ can be done analytically. For the intraband terms the result is

$$\Gamma^{i,i}=\tfrac{1}{4}S\{\mu_i^{*2}Q_i'/[q_{\mathrm{TF}}^2(4\mu_i^{*2}Q_i'^2+q_{\mathrm{TF}}^2)]$$
$$+3R/(32\mu_i^{*2}Q_i'^3K_h^2)\}\ , \tag{5}$$

and for the inter-band terms it is

$$\Gamma^{i,j}=\tfrac{3}{4}S(\mu_j^{*2}Q_{i,j}''/\{q_{\mathrm{TF}}^2[2\mu_j^{*2}(Q_j'^2+Q_{i,j}''^2)+q_{\mathrm{TF}}^2]+\mu_j^{*4}(Q_j'^2-Q_{i,j}''^2)\}-R/(32\mu_j^{*2}Q_{i,j}''Q_j'^2K_h^2))\ , \tag{6}$$

with R defined by the function

$$R=[2C_1+2C_2D+2F(X-DY)/A']/(D^2-1)-C_2\ln\left[\frac{D+1}{D-1}\right]+[(F'B'/2A'-G')/\sqrt{A'}]$$

$$\times\ln\left[\frac{(D-1)[2\sqrt{A'}(X+Y)+D(B-2C)+(2A-B)]}{(D+1)[2\sqrt{A'}(X-Y)+D(B+2C)+(2A+B)]}\right]+(H'/\sqrt{C})\ln\left[\frac{2\sqrt{C}(X+Y)-(B-2C)}{2\sqrt{C}(X-Y)-(B+2C)}\right], \quad (7)$$

where

$$\mu_j^*=\left[\frac{1}{m_c}+\frac{1}{m_{v_j}}\right]^{-1},\ v_{i,j}=\left[\frac{1}{m_{v_j}}-\frac{1}{m_{v_i}}\right]^{-1},\ Q_j'=\left[\frac{K_e}{m_c}-\frac{K_h}{m_{v_j}}\right],\ Q_{i,j}''^2=Q_j'^2-v_{i,j}K_h^2/\mu_j^*,$$

$$Q_{i,j}^{*2}=Q_j'^2+Q_{i,j}''^2,\ D=1+[\mu_j^{*2}(Q_j'-Q_{i,j}'')^2+q_{\mathrm{TF}}^2]/2\mu_j^{*2}Q_j'Q_{i,j}'',$$

$$C_1=3K_h^2+2\mu_j^*K_hQ_j'\cos\gamma-\mu_j^{*2}Q_{i,j}^{*2},\ C_2=-2\mu_j^*Q_{i,j}''(K_h\cos\gamma-\mu_j^*Q_j'),$$

$$A=[\mu_j^{*2}Q_{i,j}^{*2}+K_h(K_h+2\mu_j^*Q_j'\cos\gamma)]^2-4\mu_j^{*2}Q_{i,j}''^2K_h^2\sin^2\gamma,$$

$$B=-4\mu_j^*Q_{i,j}''(\mu_j^*Q_j'+K_h\cos\gamma)[\mu_j^{*2}Q_{i,j}^{*2}+K_h(K_h+2\mu_j^*Q_j'\cos\gamma)],$$

$$C=4\mu_j^{*2}Q_{i,j}''^2(\mu_j^{*2}Q_j'^2+2\mu_j^*Q_j'K_h\cos\gamma+K_h^2),$$

$$F=(K_h^2-\mu_j^{*2}Q_{i,j}^{*2})^2,\ G=4\mu_j^{*2}Q_j'Q_{i,j}''(K_h^2-\mu_j^{*2}Q_{i,j}^{*2}),$$

$$H=4\mu_j^{*2}Q_j'^2Q_{i,j}''^2,\ F'=F+DG+D^2H,\ G'=-(G+2DH),$$

$$H'=H,\ A'=A+DB+D^2C,\ B'=-(B+2DC),\ C'=C,$$

$$X-Y=(A+B+C)^{1/2},\ X+Y=(A-B+C)^{1/2},\ S=64\pi e^4/\hbar^3\epsilon^2,$$

and γ is the angle between $\mathbf{K}_e$ and $\mathbf{K}_h$. We give this result because it should be useful for incorporation of interband scattering in Monte Carlo simulations of hot-carrier dynamics. Of more direct relevance to the question of hot-carrier cooling rates is the rate at which a hot-electron distribution exchanges energy with a cooler distribution of holes.

We consider a quasithermal system consisting of Maxwellian distributions of N electrons in the conduction band with effective temperature T_e, and N holes thermally distributed between the heavy- and light-hole bands at an assumed temperature $T_h \neq T_e$. The average scattering and energy-loss rates, per electron, with the system of free holes is then a function only of the density and of the two temperatures. The energy-loss rates were found by numerically integrating Eq. (3), with an additional term $\hbar^2(K_e^2-K_e'^2)/2m_c$ included in the integrand, over the electron distribution.

Figure 1 shows a plot of the average energy-loss rate

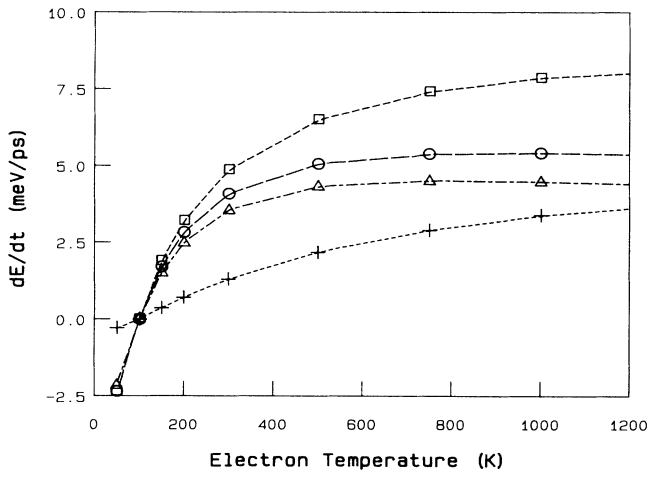

FIG. 1. Average rate of energy loss per electron to a system of holes at $T_h=100$ K. The density of electrons and the total density of light and heavy holes equals 2.5×10^{16} cm^{-3}. The curves represent calculations including intralight- and heavy-hole processes with (△) and without overlap integrals (○), interband processes (+), and the sum of inter- and intraband processes including overlap integrals (□).

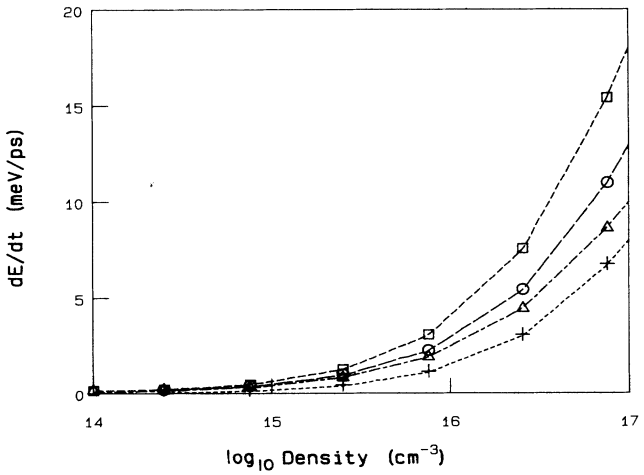

FIG. 2. Average rate of energy loss per electron to a system of holes at $T_h=100$ K, with $T_e=1000$ K. The curves represent calculations including different scattering mechanisms and approximation as described in Fig. 1.

per electron to the system of holes as a function of the electron temperature for $N=2.5\times10^{16}$ cm^{-3} and $T_h=100$ K. The effective masses of the electrons, heavy holes, and light holes were taken to be $m_c=0.08$, $m_{v_1}=0.45$, and $m_{v_2}=0.08$, respectively, to represent GaAs. The contributions from intra- and inter-valence-band processes are shown separately along with the result obtained without including the Bloch-function overlap integrals. A plot of the average energy-loss rate as a function of density for fixed temperatures of $T_e=1000$ K and $T_h=100$ K is shown in Fig. 2. Again the various contributing terms are shown separately. Similar results, not shown, were obtained for mass parameters appropriate to InP.

DISCUSSION

There are two separate effects attributable to the inclusion of overlap integrals in the Coulomb matrix element. First, there is a correction to the intra-valence-band scattering terms, which always tends to reduce their contribution to the overall scattering rate. Second, there is the contribution from inter-valence-band processes, which is zero when overlap integrals are not included. In terms of the net energy-exchange rate the two effects tend to cancel; nevertheless, for $T_e-T_h=900$ K at $N=2.5\times10^{16}$ cm^{-3}, the total energy exchange rate is $\sim50\%$ higher than that obtained with the simple model. More important to note is the fact that under these same conditions, inter-valence-band processes contribute $\sim40\%$ to the overall interaction of electrons and holes. As our calculations assume quasithermal distributions of holes between the two valence bands, they only correspond to the *initial* states of hot-carrier relaxation. The relatively large contribution of inter-valence-band transitions implies that a full kinetic analysis should include independent temperatures and *densities* for all three bands.

As can be seen from Figs. 1 and 2, the importance of band structure increases with temperature difference and with density. The upper range of our density was restricted by the assumption of Maxwellian distributions. This suggests that these effects might become even more important under conditions of partial or strong degeneracy. The upper bound on the temperatures was imposed by our restriction to scattering events closed to the zone center. To go to higher temperatures, the proper dispersion, as self-consistently calculated within a three- or four-band $\mathbf{K}\cdot\mathbf{P}$ model, would have to be included in the energy-conserving delta function of Eq. (3). This of course complicates the calculation; however, the main effect will be to significantly increase the density of states in the light-hole band at larger wave vectors. We, therefore, expect that proper inclusion of dispersion will increase the effects due to interband processes over those which we demonstrate here.

Finally, we note that the average energy exchange per collision is significantly larger for the interband as compared to the intraband processes. As the mass of the heavy holes is so much larger than that of the electrons in GaAs, it is sometimes said that electron-hole scattering can be conceptually thought of as being similar to elastic scattering from ionized impurities. This is clearly based on a classical view of the scattering process and it is not applicable when inter-valence-band transitions are included.

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