Electron-electron relaxation effect on Auger recombination in direct-band semiconductors

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Influence of electron-electron relaxation processes on Auger recombination rate in direct band semiconductors is investigated. Comparison between carrier-carrier and carrier-phonon relaxation processes is provided. It is shown that relaxation processes are essential if the free path length of carriers does not exceed a certain critical value, which exponentially increases with temperature. For illustration of obtained results a typical InGaAsP compound is used.

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It is well known that the intraband relaxation of carriers plays an important role in recombination processes.[1,2] In particular, relaxation was shown to cause broadening of gain and emission spectra in semiconductor lasers.[1] Influence of relaxation processes on Auger recombination (AR) in bulk semiconductors is more fundamental. Both for the CHCC and for the CHHS processes AR coefficient calculated in the first order of perturbation theory in electron-electron interaction is of the threshold type, being an exponential function of temperature.[3,4] Relaxation eliminates the threshold conditions enhancing AR. Phonon and impurity assisted Auger processes in $A_{III}B_V$ homogeneous semiconductors were studied in Refs. 5–7, As shown in Ref. 1 it is the electron (hole)-electron (hole) relaxation mechanism which gives the main contribution to broadening of the light emission spectra in semiconductors with high carrier density. However, influence of this relaxation mechanism on AR has not been studied yet. Since AR dominates over other recombination processes at high densities of electrons and holes and the role of the carrier-carrier scattering also increases with carrier concentration, the corresponding mechanism of relaxation might be expected to be of primary importance in calculating AR rate.

In this paper we study temperature and carrier-density dependences of Auger coefficient with and without regard to electron (hole)-electron (hole) relaxation processes. General Green function approach is used for calculation of AR coefficient. Wave functions and energy spectra of electrons and holes are found from the conventional $8\times8\,\mathbf{k}\cdot\mathbf{p}$ model. Comparison of the direct AR, phonon-assisted AR, and AR with carrier-carrier relaxation is provided both for the CHCC and CHHS processes.

Finite temperature Green function techniques for calculating AR rate was developed in Refs. 5,6. The formalism used in those papers is based on linear response and mean-field approximations. It was shown that the relaxation processes eliminate the threshold appearing in the first order of perturbation theory on Coulomb interaction and enhance AR rate. In Refs. 5,6, there were studied Auger processes with relaxation on phonons and impurities. However, wave functions and overlap integrals were phenomenologically assumed than calculated, which drastically affected the results. The most accurate calculation of the phonon-assisted AR was performed in Ref. 7. But the heavy hole wave functions were not derived there consistently with those of electrons.

In direct band $A_{III}B_V$ semiconductors the electron effective mass is usually much less than that of heavy holes.[2] This allows us to neglect by electron scattering processes, compared with those of holes,[1] and to use the free particle propagators for the former. By the same reason we also neglect by the momenta and energies of the electrons in the initial state.[4]

Following the approach developed in (Ref. 5,6) and using wave functions derived in 8×8 model[8] we obtain Auger coefficient for the CHCC process

$$C\approx\frac{32\sqrt{2\pi^5}e^4\hbar^2\langle E_c\rangle}{9m_h^{3/2}T^{3/2}E_g\epsilon_\infty^2}\,\frac{3E_g+2\Delta_{SO}}{E_g+\Delta_{SO}}\int_{-\infty}^{\infty}\frac{d\mathcal{E}}{k_c^2(\mathcal{E}+E_g)}\,\frac{dk_c}{d\mathcal{E}}\times\exp\left(-\frac{\mathcal{E}}{T}\right)D[k_c(\mathcal{E}+E_g),\mathcal{E}]. \quad (1)$$

Here $\langle E_c\rangle$ is the mean electron energy equal to $\frac{3}{2}T$ if they have Boltzmann distribution, m_h is the heavy-hole effective mass, T is the temperature in energy units, E_g and Δ_{SO} are the band gap and spin-orbital splitting respectively, $k_c(E)$ is the wave vector versus energy in the conduction band, $E_h(k)$ is the dispersion of the heavy holes, $D(k,E)$ is the spectral function related to the imaginary part of the heavy-hole proper self-energy $\Gamma(k,E)$ by

$$D(k,E)=\frac{1}{\pi}\,\frac{\Gamma(k,E)}{[\Gamma(k,E)]^2+[E-E_h(k)]^2}. \quad (2)$$

In Eq. (1) we used Boltzmann distribution of heavy holes, which is usually the case due to large value of their effective mass. Generalization of this expression to the case of Fermi statistics is straightforward. The high frequency dielectric constant ϵ_∞ is taken away from the integrand because the free-carrier screening effects are weak and unimportant for Auger process.[9] We neglected by the real part of the proper self energy in Eq. (2), since its only effect is the slight renormalization of the heavy hole mass. It should be noted, that Γ

strongly damps in the band gap $\mathcal{E}<0$ and the main contribution to the integral comes from the positive values of the hole energy.

Neglecting by relaxation processes leads to a well known expression for the Auger coefficient[4,9]

$$C\approx\frac{8\sqrt{2\pi^5}e^4\hbar^3\langle E_c\rangle}{3m_h^{3/2}m_c^{1/2}T^{3/2}E_g^{5/2}\epsilon_\infty^2}\exp\left(-\frac{E_{\rm th}}{T}\right)F\left(\frac{\Delta_{\rm SO}}{E_g}\right),\qquad(3)$$

where $F(x)$ is a multiplier of the order of 1:[4]

$$F(\alpha)=\left(\frac{1+\alpha}{1+2\alpha/3}\right)^{3/2}\left(\frac{1+\alpha/3}{1+\alpha/2}\right)^{1/2},$$

$E_{\rm th}\approx 2m_c/m_hE_g$ is the threshold energy.

Similarly can be obtained the expression for the CHHS Auger process

$$C=\frac{16\pi^2e^4\hbar^5}{3\epsilon_\infty^2m_h^3T^3}\frac{\langle E_c\rangle}{E_g}\frac{3E_g+2\Delta_{\rm SO}}{3(E_g+\Delta_{\rm SO})}\int_0^\infty\int_0^\infty dk_1dk_2\int_{-1}^1 d\cos\vartheta\frac{(1+\lambda_{\rm SO})^2}{1+2\lambda_{\rm SO}^2+\dfrac{\Delta_{\rm SO}}{E_g-E_{\rm SO}}\dfrac{2\lambda_{\rm SO}^2+\lambda_{\rm SO}-1}{3\lambda_{\rm SO}}}\frac{\cos^2(\vartheta)k_1^2}{(\mathbf{k}_1+\mathbf{k}_2)^2}\left[1+\frac{k_2}{2k_1}\sin\vartheta\right]$$
$$\times\int_{-\infty}^\infty dED(k_1,E)D(k_2,E_{\rm SO}-E_g-E)\exp\left(\frac{Eg-E_{\rm SO}}{T}\right),\qquad(4)$$

where $E_{\rm SO}\equiv E_{\rm SO}(|\mathbf{k}_1+\mathbf{k}_2|)$ is the energy of the split-off hole, ϑ is the angle between the wave vectors $\mathbf{k}_1$ and $\mathbf{k}_2$,

$$\lambda_{\rm SO}=\frac{\Delta_{\rm SO}}{3\left(E_{\rm SO}+4/3\,\Delta_{\rm SO}+\dfrac{\hbar^2k_{\rm SO}^2(E_{\rm SO})}{2m_h}\right)}.$$

The presence of the multiplier $(1+\lambda_{\rm SO})^2$ in the integrand ensures that near the Γ point (at the center of Brillouin zone), where $E_{\rm SO}\approx-\Delta_{\rm SO}$ and $\lambda_{\rm SO}\approx-1$, the overlapping between heavy holes and split-off holes vanishes.[10] Note that the exchange interaction does not vanish for the CHHS process as it does in the case of the CHCC one. Namely, this interaction is responsible for the second term in the square brackets in the integrand of Eq. (4). If the spectral functions are substituted by δ functions, Eq. (4) turns to the expression derived by Ge'lmont *et al.*[10]

Let us now consider the relaxation processes in detail. In this paper we will study two basic scattering mechanisms in undoped semiconductors: (i) on polar optical phonons and (ii) on electron hole plasma. The imaginary part of the proper self-energy for the first mechanism with account of the complex valence band structure is as follows:

$$\Gamma_{ph}(k,E)=\frac{m_he^2\omega_{lo}}{4\hbar\bar{\epsilon}k}\left[\frac{1}{\exp\dfrac{\hbar\omega_{lo}}{T}-1}\int_{(1-\Delta_1)^2}^{(1+\Delta_1)^2}\frac{3(\Delta_1^2+1-\xi)^2+4\Delta_1^2}{16\Delta_1^2\xi}d\xi+\frac{\exp\dfrac{\hbar\omega_{lo}}{T}}{\exp\dfrac{\hbar\omega_{lo}}{T}-1}\int_{(1-\Delta_2)^2}^{(1+\Delta_2)^2}\frac{3(\Delta_2^2+1-\xi)^2+4\Delta_2^2}{16\Delta_2^2\xi}d\xi\right],\qquad(5)$$

ω_{lo} is the phonon frequency assumed to be independent of the wave vector,

$$\Delta_{1,2}\equiv\Delta_{1,2}(k,E)=\begin{cases}\sqrt{\dfrac{2m_h(E\mp\hbar\omega_{lo})}{\hbar^2k^2}} & \text{if } E>\pm\hbar\omega_{lo},\\ 0, & \text{otherwise},\end{cases}$$

with indices 1,2 corresponding to upper, lower sign, respectively,

$$\frac{1}{\bar{\epsilon}}=\frac{1}{\epsilon_\infty}-\frac{1}{\epsilon_0},$$

ϵ_0 is the low-frequency dielectric constant. The first and the second terms in Eq. (5) correspond to phonon absorption and phonon emission, respectively. If screening effects are taken into account than in both terms of Eq. (5) ξ^{-1} should be substituted by $\xi/(\xi+\lambda_{\rm TF}^2/k^2)^2$ with $\lambda_{\rm TF}$ being Thomas-Fermi screening momentum. Integration in Eq. (5) can be conducted explicitly however, the resulting expression is quite cumbersome. A formula similar to Eq. (5) was derived in Ref. 7, but there is some discrepancy due to more accurate consideration of the heavy-hole spectrum in this paper.

Let us consider the relaxation due to hole scattering on equilibrium electron-hole plasma. Using the RPA approach for calculating the imaginary part of the self-energy Γ_e due to carrier-carrier scattering[11] we obtain

$$\Gamma_e(k,E) = -\frac{me^2}{\epsilon_0 \pi k}\int_0^\infty d\mathcal{E}\int_{q_{\min}}^{q_{\max}}\frac{dq}{q}\left(\frac{1}{\exp\left(\frac{\mathcal{E}-\mu_v}{T}\right)+1} + \frac{1}{\exp\left(\frac{\mathcal{E}-E}{T}\right)-1}\right) \times \frac{\delta\epsilon''(q,E-\mathcal{E})}{[1+\delta\epsilon'(q,E-\mathcal{E})]^2+[\delta\epsilon''(q,E-\mathcal{E})]^2} \times \left[1-\frac{3}{4}\frac{[E_h(q)-E_h(q_{\min})][E_h(q_{\max})-E]}{4E_h(k)\mathcal{E}}\right], \tag{6}$$

$$q_{\min} = \left|\sqrt{\frac{2m_h\mathcal{E}}{\hbar^2}}-k\right|, \quad q_{\max} = \sqrt{\frac{2m_h\mathcal{E}}{\hbar^2}}+k.$$

Here $\delta\epsilon$ is the contribution to the dielectric constant from free carriers, a double prime refers to the imaginary part and single prime does to the real part of $\delta\epsilon$. The last multiplier in Eq. (6) comes from the complex structure of the valence band. Explicitly

$$\delta\epsilon''(k,E) = -\frac{2m_h^2 e^2}{\epsilon_0^2 k^3}\int_{(E_h(k)-E)^2/4E_h(k)}^\infty dE_q [f_h(E_q)-f_h \times (E_q+E)]\left[1-\frac{3E_h(k)}{4E_q}\frac{E_q-\frac{[E_h(k)-E]^2}{4E_h(k)}}{E_q+E}\right], \tag{7}$$

where

$$f_h(E) = \frac{1}{\exp\left(\frac{E-\mu_h}{T}\right)+1}$$

is the heavy hole distribution function. The expression for the real part of $\delta\epsilon$ is quite complicated.[9] However, as numerical computation shows, Thomas-Fermi approximation gives very reasonable results. So $\delta\epsilon''$ in denominator of Eq. (6) can be set zero and

$$\delta\epsilon' = \lambda_{TF}^2/q^2, \tag{8}$$

where λ_{TF} is the inverse Thomas-Fermi screening length:[5]

$$\lambda_{TF} = \sqrt{\frac{4\sqrt{2}e^2\sqrt{T}}{\pi\hbar^3\epsilon_0}[m_h^{3/2}S(\mu_h/T)+m_c^{3/2}S(\mu_c/T)]}, \tag{9}$$

where

$$S(x) = \int_0^\infty dy \frac{1}{\exp(y^2-x)+1}.$$

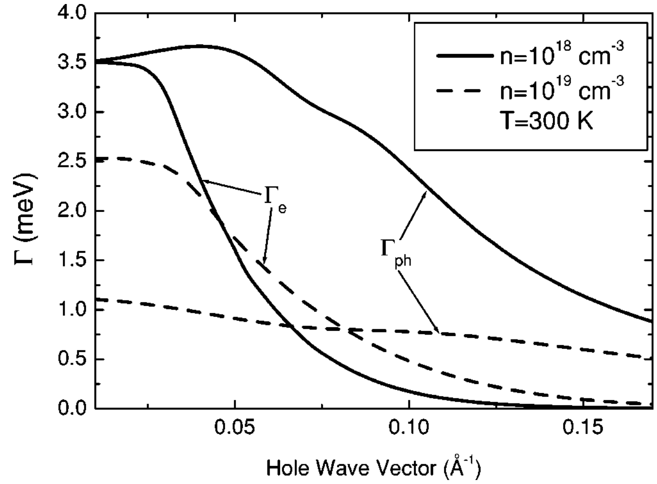

FIG. 1. Imaginary part of the proper self energy for scattering of a heavy hole on the electron-hole plasma (Γ_e) and on the longitudinal polar optical phonos ($\Gamma_{\rm ph}$) as a function of the heavy hole momentum (k) at ($E=0$).

Substituting Eqs. (7) and (8) into Eq. (6) gives the final expression for the lifetime of holes in the case of carrier-carrier scattering.

The imaginary part of the proper self energy $\Gamma_e(k,E)$ strongly depends on both arguments having a steep maximum at $E_h(k)=E$ and rapidly decreasing when the latter inequality is broken. There are two main reasons for reducing Γ_e when $E_h(k)\neq E$: (i) Coulomb interaction is relatively weak at large transferred momenta, (ii) there is an exponentially small number of carriers with large momenta in equilibrium electron-hole plasma. On the other hand, scattering on phonons is almost independent of the transferred momentum and therefore Γ_{ph} is a smooth function of its arguments. Figure 1 shows dependences $\Gamma_e(k)$ and $\Gamma_{ph}(k)$ at a fixed value of $E=0$. While the value Γ_e is larger then that of Γ_{ph} at small values of k and relatively high carrier densities, the inverse relation could be observed at large k or small densi-

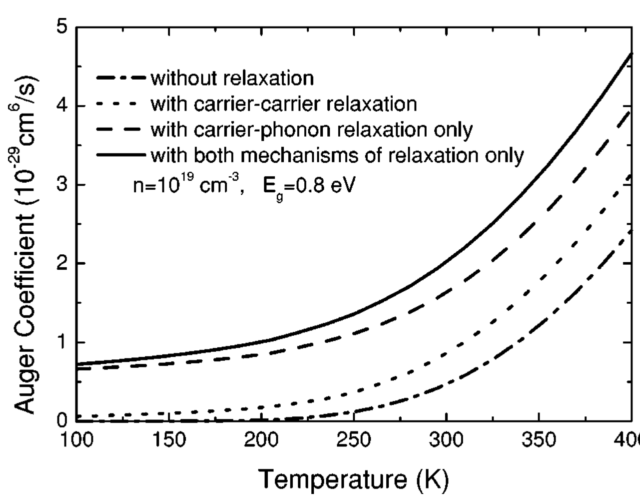

FIG. 2. CHCC Auger coefficient versus temperature with regard to different relaxation processes. Parameters of an InGaAsP compound lattice matched to InP were used in calculations.

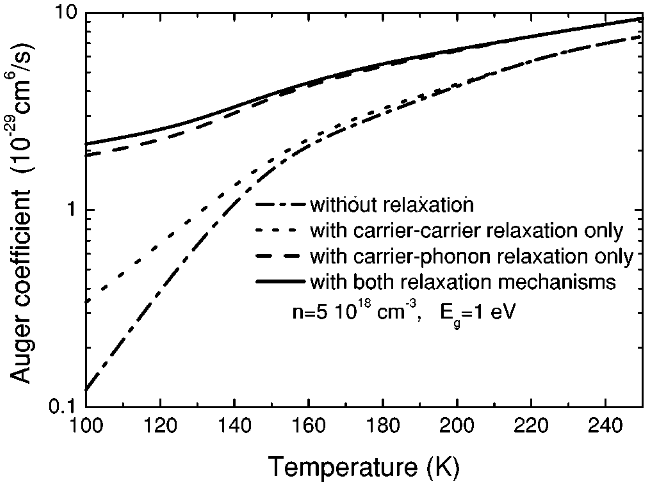

FIG. 3. CHHS Auger coefficient versus temperature with regard to different relaxation processes.

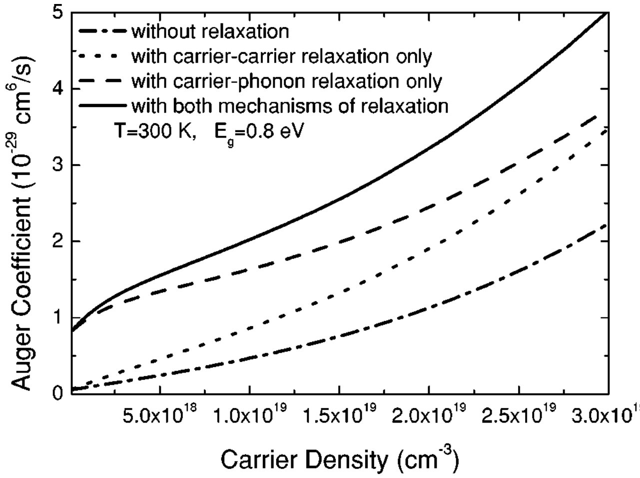

FIG. 4. Dependence of CHCC Auger coefficient on carrier density with and without account of various scattering processes.

ties. The role of carrier-carrier scattering obviously increases with carrier density and temperature. In AR, large transferred momenta play a crucial role.[4,9] Therefore the carrier-carrier scattering mechanism is less important here than in radiative recombination. Nevertheless this relaxation process remains effective at high temperatures and carrier densities (Figs. 2–4). Parameters of a typical InGaAsP compound lattice matched to InP were used for the illustration of obtained results.

The threshold energy for the CHCC AR is considerably larger than that for the CHHS process, therefore relaxation processes are important for the former up to very high temperature (Fig. 2), while for the latter they usually give a considerable effect only when T is small (Fig. 3). At T close to zero phonon-assisted AR predominates, while the role pf AR with carrier-carrier relaxation increases at higher T (Fig. 2). The carrier-carrier relaxation mechanism is also responsible for a stronger dependence of AR coefficient on the carrier density (Fig. 4).

In conclusion we note that owing to relaxation processes AR becomes thresholdless, because the restrictions imposed by the energy-momentum conservation are lifted. From Eq. (1) we can estimate the characteristic scattering length a_c for the CHCC process

$$a_c = \lambda_{Eg}\left(\frac{T}{E_{th}}\right)\exp\left(\frac{E_{th}}{T}\right), \qquad (10)$$

where $\lambda_{E_g} = 2\pi/k_c(E_g)$. If the free path length λ exceeds a_c the relaxation is not important, otherwise it should be taken into account. Note that the similar result was derived in Ref. 8 for the case of a quantum well. The role of the momentum relaxation mechanism there was played by scattering on heterobarriers. The characteristic quantum well width above which the bulk approximation for the AR is valid was found to be

$$\tilde{a}_c = \lambda_{Eg}\left(\frac{T}{E_{th}}\right)^{3/2}\exp\left(\frac{E_{th}}{T}\right), \qquad (11)$$

that is close to Eq. (10). The unessential difference in the exponent of T/E_{th} is attributed to 1D scattering in the case of a quantum well.

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