

Effect of relaxation processes on Auger recombination in semiconductor quantum wells

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Abstract. In this paper we study the effect of carrier relaxation processes on Auger recombination in semiconductor quantum wells (QWs). It is shown that the calculation in the framework of the conventional perturbation theory is not applicable in the case of narrow wells and wires because of its divergence. Therefore a more rigid Green function techniques is used. The relaxation processes are shown to increase Auger recombination coefficient, however their influence becomes weaker with decrease of the QW width. The transition from the QW to the bulk case is explicitly carried out.

Introduction

It is several decades since Auger recombination (AR) was investigated in bulk semiconductors [1, 2]. It was shown that Auger process calculated in the first order of perturbation theory on Coulomb interaction has a threshold nature, i.e. its coefficient exponentially depends on temperature. In heterostructures, however, the transversal momentum component doesn't conserve thus allowing the thresholdless Auger process to appear [3, 4]. In our previous papers [5, 6] we showed that there are three different AR processes in quantum wells (QWs): (i) threshold, which is just a 2D analogue of the bulk process, (ii) quasithreshold arising from confinement of electrons and holes within the quantum well, and (iii) thresholdless which is caused by carrier scattering on the heteroboundaries. An explicit transition from the 2D to the 3D case for the CHCC Auger process carried out in [5, 6] showed that the quasithreshold and threshold mechanisms merge into the single bulk process when the QW width becomes considerably larger than the critical value given by:

$$a_c = \lambda_{Eg} \left(\frac{T}{E_{th}} \right)^{3/2} \exp \frac{E_{th}}{T}, \quad (1)$$

where $\lambda_{Eg} = 2\pi/k(Eg)$ is the wavelength of an electron having the band gap energy Eg , $E_{th} \approx \frac{2m_c}{m_h} Eg$ is the threshold energy in a homogeneous semiconductor, m_c and m_h are the electron and heavy hole masses, T is temperature in energy units. It is an easy matter to see that in semiconductors with the energy gap close to 1 eV the value of a_c can be as large as several thousands Angströms, which strongly exceeds the free path length in these semiconductors. Hence there is an obvious contradiction between this result and the common sense. The solution to this paradox is the direct taking into account of various scattering processes. Finally we note here that it is impossible to use conventional quantum mechanical perturbation analysis for this purpose. The reason is that the scattering mechanisms such as the electron(hole)-electron(hole) or electron(hole)-phonon processes become resonant and the corresponding expressions obtained in the second and higher orders of perturbation theory diverge [6].

1 Green function formalism for the calculation of Auger recombination processes

The temperature Green function formalism was firstly applied to AR processes in a homogeneous semiconductor in [7, 8]. However there was no investigation of Green function broadening due to relaxation processes on the value and temperature dependence of Auger coefficient. The author of those papers also used phenomenological expressions for the wave functions and overlap integrals rather than those obtained in the multi-band $\mathbf{k}\mathbf{p}$ -theory. Nevertheless, a convenient method for calculating the Auger rate in any order of interaction potential is suggested there.

The expression for the recombination rate obtained in the linear response theory on Coulomb interband scattering is as follows [7]:

$$\frac{\partial N_c}{\partial t} = \int_{-\infty}^{\infty} dt e^{i\mu_{\Delta}t} \sum_{\lambda_i, \xi_j} \int \dots \int d\mathbf{r}_1 \dots d\mathbf{r}_4 \Delta_{1,2,3,4} U(\mathbf{r}_1 - \mathbf{r}_2) U(\mathbf{r}_3 - \mathbf{r}_4) iG_4^R(t), \quad (2)$$

where

$$G_4^R(t) = \Theta(t) \sum_{i_1, j_1, \dots} \langle \hat{\Psi}_{\lambda_4, i_1}^{\alpha+}(\mathbf{r}_1, t) \hat{\Psi}_{\lambda_3, j_1}^{\beta+}(\mathbf{r}_2, t) \hat{\Psi}_{\lambda_2, j_2}^{\beta}(\mathbf{r}_2, t) \hat{\Psi}_{\lambda_1, i_2}^{\alpha}(\mathbf{r}_1, t) \\ \times \hat{\Psi}_{\xi_4, k_1}^{\gamma+}(\mathbf{r}_3, 0) \hat{\Psi}_{\xi_3, l_1}^{\delta+}(\mathbf{r}_4, 0) \hat{\Psi}_{\xi_2, l_2}^{\delta}(\mathbf{r}_4, 0) \hat{\Psi}_{\xi_1, k_2}^{\gamma}(\mathbf{r}_3, 0) \rangle \quad (3)$$

is the four particle retarded Green function, $\Theta(t)$ is the step function, $U(\mathbf{r})$ is the interaction Coulomb potential screened by the host lattice, λ_i and $\xi_j = c, v$ numerate the conduction or the valence band, $i_1, j_1, \dots$ are the spin indices [6], $\alpha, \beta, \dots$ are the indices numerating the components of wave functions in 8×8 basis [6] ($\alpha = |s \uparrow\rangle, |s \downarrow\rangle, \dots$), $\Delta_{1,2,3,4} = \delta_{\lambda_2, c} + \delta_{\lambda_1, c} - \delta_{\lambda_3, c} - \delta_{\lambda_4, c}$ shows that only interband Auger transitions are responsible for the non-conservation of particles in the conduction (valence) band, $\mu_{\Delta} = (\mu_c - \mu_v) [\delta_{\lambda_4, c} + \delta_{\lambda_3, c} - \delta_{\lambda_2, c} - \delta_{\lambda_1, c}]$, $\hat{\Psi}(t)$ is the field operator in the modified Heisenberg picture where all terms leading to interband transition are excluded from the total Hamiltonian [7]. We note here that in a homogeneous semiconductor wave functions with different spins are orthogonal ($i_1 = i_2, j_1 = j_2, \dots$), however this is not the case for QWs. It was assumed that both electrons in the conduction band and holes in the valence band have Fermi-Dirac distribution with their own chemical potentials ($\mu_c \neq \mu_v$). This assertion is valid when the intraband relaxation times are much shorter than those of interband transitions.

Further simplifications come from using the mean field approximation for the four-particle Green function. In this case the function G_4^R splits into two different terms corresponding to the direct and exchange scattering processes. This approximation is justified at high temperatures when there are no coherent, e.g. excitonic, states and the vertex corrections are small. Because the relaxation time for holes is much shorter than that for electrons, we neglect by the electron scattering processes. For the sake of simplicity electrons in initial state are supposed to occupy only their ground state. However this assumption is not essential because the ground state energy can be substituted by the mean thermal one for sufficiently wide QWs. Then after some manipulations, for the recombination rate per unit square, we obtain:

$$\frac{1}{S} \frac{\partial N_c}{\partial t} \approx \frac{24\pi^3 e^4 \hbar n_c^2}{m_c E_g^2 \kappa_0^2} \sum_{nj, mi} \int_{-\infty}^{\infty} dE \int_0^{\infty} \frac{dq}{k_4} f_h(E) D_{nj, mi}(q, E)$$

$$\times \langle 2M_I^{nj}(q, k_4)M_I^{mi*}(q, k_4) - M_I^{n,j}(q, k_4)M_{II}^{mi*}(q, k_4) \rangle, \quad (4)$$

where

$$M_I^{nj}(q, k_4) = \int_{-a/2}^{a/2} \psi_f^{s*}(x, q, k_4) \psi_{c1}^s(x) \psi_{c2}^\beta(x) \psi_{hnj}^{\beta*}(x, q) dx,$$

a is the QW width, M_{II} can be obtained from M_I by interchanging indices c_1 and c_2 , $n_c = N_c/S$ is the 2D electron density, nj and mi numerate the energy levels and spin states of a heavy hole, $f_h(E) = \exp[(\mu_h - E)/T]$ is the hole distribution function, which are supposed to be non-degenerated for the case of simplicity, $D_{nj, mi}(q, E)$ is the spectral function, obtained from the imaginary part of a heavy hole Green function, angular brackets in (4) denote averaging over the states of localized electrons. It is to be noted that only the quasithreshold AR mechanism was taken into account in (4), because it was shown to prevail in QWs at high temperatures [6]. In general the Green function in a QW is not diagonal and the spectral function D cannot be written in a simple Lorentzian form. However, in two limiting cases of wide and narrow wells D becomes diagonal. Thus in narrow QWs there is only one energy level in the well and in wide QWs Green function becomes diagonal because of the spatial homogeneity. Therefore if instead of $D_{nj, mi}$ an expression having Lorentz form multiplied by $\delta_{n,m} \delta_{j,i}$ were used the obtained results would be accurate in both limits of narrow and wide QWs and could be considered as interpolate ones for intermediate widths. In this case it is easy to verify that the Auger coefficient is the squared matrix element of Auger transition averaged over the initial states and summed over the final states, but where instead of the δ -function representing the energy conservation law there is a spectral function. In the limit $\Gamma \rightarrow 0$ (4) turns to the coefficient obtained in the first order of perturbation theory. The expression for the quasithreshold Auger coefficient obtained in [6] can be easily generalized yielding

$$C \approx \frac{\pi^2 e^4}{\kappa_0^2} \frac{\hbar^3 \gamma^4}{E_g^5} \frac{F(\Delta_{so}/Eg)}{a(a+2/\kappa_c)^2} \frac{1}{Z} \sum_n \int_0^\infty dq \int_0^\infty dE \frac{q}{q^2 + k_{hn}^2} \frac{q_c^2 k_{hn}^2 + q_h^2 (k_c^2 + \frac{1}{2} q_c^2)}{k_4} \times (G_{-1} + 2G_0 + G_1) \frac{1}{\pi} \frac{\Gamma_n(q, E)}{\Gamma_n(q, E)^2 + (E - E_{hn}(q))^2}, \quad (5)$$

where

$$G_\lambda = \frac{1 - \cos(k_4 - k_{hn} - 2\lambda k_c)a}{k_4 - k_{hn} - 2\lambda k_c}, \quad Z = \sum_n \int_0^\infty q dq \exp\left(-\frac{E_{hn}(q^2)}{T}\right),$$

k_{hn} and E_{hn} are the wave vector and the energy of a hole at the n th level, q_c is the average longitudinal momentum of the localized electrons, $F(\Delta_{so}/Eg)$ is the multiplier close to unity introduced in [6], k_c and κ_c are the absolute values of electron transversal wavevectors in a quantum well and barrier region respectively, γ is Kane's parameter, k_4 can be determined from the following equation:

$$E_f(k_4^2 + q^2) - Eg - 2Ec = E,$$

where $E_f(k)$ is the energy of a conduction band electron. Obviously both G_λ and D in fact eliminate threshold conditions. Thus G_λ allows non-conservation of the momentum

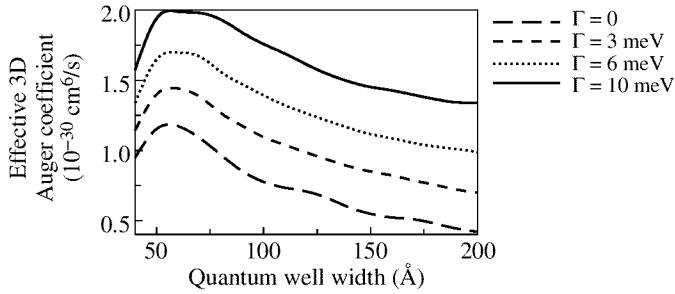


Fig. 1.

and D violates the energy conservation law. The critical quantum well thickness at which the 2D–3D transition occurs can be determined now by comparing widths of G and D . Another important feature arises from the analysis of (5). Namely, the calculations made in the framework of conventional perturbation theory wouldn't give the term Γ^2 in the denominator of the spectral function D . Because there is no threshold in sufficiently narrow wells and all values of the hole momentum q are allowed, this expression would diverge at the resonance where the denominator becomes zero. Therefore the approach based on the conventional perturbation theory is not applicable in the case of QWs.

2 Discussion

Certainly the calculation of Γ , or to be more precise of the imaginary part of the Green function, is quite a separate problem which is to be discussed elsewhere. The value of Γ obviously depends on carrier density, QW width, etc. However to illustrate the effect of relaxation processes in the QWs we consider Γ to be an external parameter and compare dependences of AR coefficient, multiplied by the squared QW width, on QW width at different Γ values (Fig. 1).

The analysis of this figure shows that in narrow QWs the finite lifetime of carriers is not very important factor and AR can be calculated in the first order of the perturbation theory, while in wide QWs Γ plays a crucial role and the more its value the less width where the 2D–3D transition occur.

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