ACOUSTIC PHONON CONTROLLED TRANSPORT IN LOW DIMENSIONAL STRUCTURES

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Abstract

The rates of electron scattering by acoustic phonons in low dimensional structures are calculated. It is shown that due to uncertainty of momentum conservation in low dimensional systems the acoustic phonon scattering becomes essentially inelastic in contrast to that in bulk materials. We propose simple procedure for incorporation of inelastic acoustic phonon scattering into a Monte Carlo technique. It is demonstrated that electron low-field mobility at temperatures less that 100 K calculated within elastic approximation is greatly underestimated. We have also demonstrated that velocity-field dependence in QWIs has a superlinear region. This superlinear region is associated with decline in acoustic phonon scattering efficiency as the electrons get heated.

I. Introduction

Low dimensional (LD) semiconductor structures are now widely recognized as a very promising basis for future technological applications. The electron transport in LD structures at low temperatures is controlled by acoustic phonon scattering. However, so far there is a considerable gap in understanding of some essential aspects of LD electron scattering by acoustic phonons. The elasticity of electron-acoustic phonon scattering is a commonly used approximation [1-4]. A closer look at this mechanism shows that electron scattering by acoustic phonons in quantum structures becomes essentially inelastic and becomes effective mechanism of energy dissipation [5]. This is due to the fact that the momentum conservation in LD structures for electron-acoustic phonon systems is not preserved.

We present results of calculations of electron scattering by acoustic phonons in 1D quantum wires (QWIs) and 2D quantum wells (QWs), where we consider inelasticity of this scattering in full detail. We develop procedure for inclusion of this inelasticity into a Monte Carlo technique. Monte Carlo simulation results are obtained for GaAs QWIs.

II. Scattering Rates

The rate of electron scattering from the state $\mathbf{k}$ to the state $\mathbf{k}'$ with the assistance of deformation acoustic phonon with wave-vector $\mathbf{q}$ is given by

$$W(\mathbf{k},\mathbf{k}',\mathbf{q}) = \frac{\pi E_a^2 q^2}{\rho V \omega_q}\left(N_q + \frac{1}{2} \pm \frac{1}{2}\right)\delta(\epsilon_k - \epsilon_{k'} - \Delta\epsilon \mp \hbar\omega_q), \qquad (1)$$

where V is the principal volume of the crystal, E_a is the deformation acoustic potential, ρ is the density of the material, $\omega_q = uq$ is the long wave approximation of acoustic phonon dispersion, where u is a sound velocity in the material, and $\Delta\epsilon$ is the energy separation

between initial and final subbands. Here and everywhere below upper sign corresponds to emission and lower sign to absorption of acoustic phonon. We will consider a rectangular quantum structure with infinitely deep potential well embedded into another material with similar elastic properties so that acoustic phonons can penetrate through the interface between these materials. The major difference between bulk and LD electron scattering comes from the overlap integral $I = \langle\psi_{k'}|e^{i\mathbf{qr}}|\psi_k\rangle$. Integrating over the volume of the quantum structure and neglecting umklapp processes we get

$$|I_{2D}|^2 = G_{n,n',q_z}\,\delta_{\mathbf{k}_\parallel \mp \mathbf{q}_\parallel, \mathbf{k}'_\parallel},$$

$$|I_{1D}|^2 = G_{j,j',q_y}\,G_{l,l',q_z}\,\delta_{k_x \mp q_x, k'_x}, \tag{2}$$

$$G_{l,l',q_z} = \frac{2\left[(2\pi)^2 q_z L_z l l'\right]^2\left[1-(-1)^{l+l'}\cos(q_z L_z)\right]}{\left[(q_z L_z)^4 - 2\pi^2(q_z L_z)^2(l^2+l'^2)+\pi^4(l^2-l'^2)^2\right]^2}\,. \tag{3}$$

where n is subband index for a QW; j and l are subband indices for a QWI due to size quantization in y and z directions, respectively. Primed indices denote the subband of the final state. The Kroenecker delta-function reflects momentum conservation in unquantized direction(s). The form-factor G is responsible for the uncertainty of momentum conservation in perpendicular to the quantum structure direction(s).

The total scattering rate from the state $\mathbf{k}$ of the initial subband to any state of the final subband,

$$\lambda(\mathbf{k}) = \frac{V}{(2\pi)^3}\sum_{\mathbf{k}'}\int d\mathbf{q}\; W(\mathbf{k},\mathbf{k}',\mathbf{q}). \tag{4}$$

The complexity of the form-factor does not allow one to get analytical results without certain simplifications. Let us consider now separately QWs and QWIs. For numerical estimates we use parameters of GaAs quantum structure embedded in AlAs at T=30 K.

(a) Quantum Wells

The scattering rate of 2D electrons by acoustic phonons obtained from (7) for electrons on subband n with wave vector $\mathbf{k}_{||}$ scattered to subband n' can be rewritten in the following form:

$$\lambda_{n,n'}(k_{||}) = \frac{E_a^2 m k_B T}{2L_z\rho\hbar^3 u^2}\,\mathcal{J}_{n,n'}(k_{||})\,, \tag{5}$$

where $\mathcal{J}_{n,n'}(k_{||})$ is a dimensionless function of the order of unity, given by

$$\mathcal{J}_{n,n'}(k_{||}) = \int_0^{+\infty}\frac{L_z\,dq_z}{\pi}\int_0^{\pi}\frac{d\varphi}{\pi}\,\mathcal{N}\left(\frac{\hbar u q}{k_B T}\right)G_{n',n,q_z}\times$$

$$\times\left|1\pm\frac{mu}{\hbar k'_{||}}\,\frac{k'_{||}-k_{||}cos(\varphi)}{\sqrt{k_{||}^2+{k'_{||}}^2-2k_{||}k'_{||}cos(\varphi)+{q_z}^2}}\right|^{-1}\theta(k_{||},\varphi,q_z,n,n')\,. \tag{6}$$

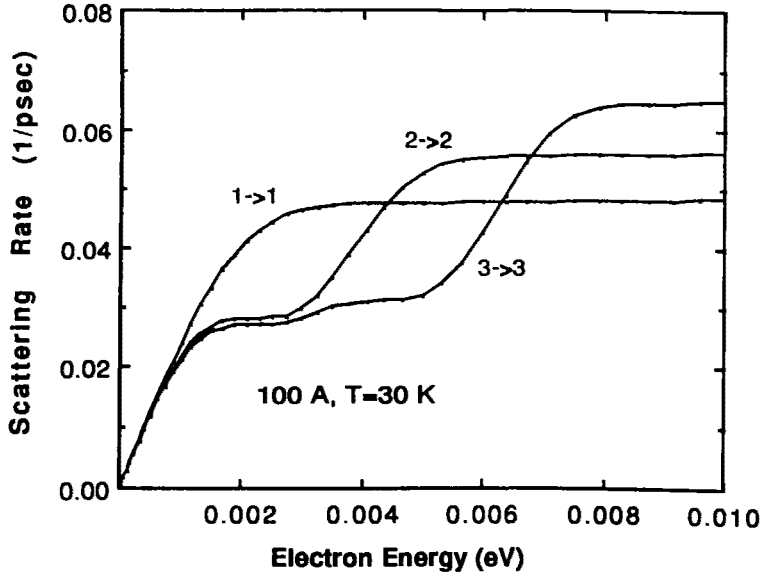
We use the following notation in formula (6) : φ is an angle between electron wave vector before scattering $\mathbf{k}_{||}$ and electron wave vector after scattering $\mathbf{k}'_{||}$. An absolute value of the in-plane electron wave vector after scattering, $k'_{||}$, is a solution of the energy conservation equation. The function $\mathcal{N}(x) = x/(e^x-1)+x/2\pm x/2$ in eq. (6) is a dimensionless

function associated with phonon occupation number, $\theta(k_{||}, \varphi, q_z, n, n')$ is an integer-value function which is equal to a number of the roots of the energy conservation equation.

For the elastic approximation $\hbar uq \to 0$ we obtain the following expression:

$$\mathcal{J}_{n,n'}(k_{||}) = (1 + \frac{1}{2}\delta_{n',n})\Theta(\epsilon_n - \epsilon_{n'} + \frac{\hbar^2 k_{||}^2}{2m}),$$

where $\Theta(x)$ is a unit step-function. The elastic approximation fails in the region of low electron energy which amount for $1 - 5$ meV for GaAs QWs. Mathematical complexity of the problem does not allow one to solve it analytically. Figure 1 demonstrates the energy dependence of the acoustic phonon emission rate in three lowest subbands (intrasubband transitions) of the 100$\AA$ thick QW for T=30 K, obtained by direct numerical solution of eqs. (5) and (6). Instead of single-step-wise function which follows from the elastic approximation, the emission rate is a smooth function of electron energy. The complex structure of the form-factor for transitions within upper subbands results in several plateau regions in the energy dependence of the emission rate.



(b) Quantum Wires

Let us assume that $q_x \ll q_T$, where $q_T = \sqrt{q_y^2 + q_z^2}$ is a transverse component of phonon wavevector and that $\hbar uq \ll k_B T$. To meet both above assumptions it is required that $\hbar u q_{Tmax} \ll k_B T$, where $q_{Tmax} = \pi\sqrt{(j+j')^2/L_y^2 + (l+l')^2/L_z^2}$ is roughly the maximum transverse component of phonon wavevector where the form-factor is non-zero. Then after summation of eq. (7) over k' and integration over q_x we get

$$\lambda(\epsilon) = \frac{{E_a}^2 k_B T}{4\pi^2 \rho u^2 \hbar^2}\sqrt{\frac{m^*}{2}}\int \frac{dq_y dq_z\, G}{\sqrt{\epsilon \mp \hbar u q_T - \Delta\epsilon}} \ . \tag{7}$$

Here G stands for $G_{j,j',q_y}\, G_{l,l',q_z}$. The integration limits for absorption rate are imposed by the form-factor which tends to zero above q_{Tmax}. The uncertainty of momentum conservation is roughly defined by $\hbar q_{Tmax}$, i.e., it increases with decreasing the transverse dimensions of the QWI. As the electron energy tends to zero the absorption rate saturates since q_{Tmax} is not equal to zero.

Let us consider the asymptote of very large electron energies $\epsilon - \Delta\epsilon \gg \hbar u q_{Tmax}$. In this case we may neglect phonon energy (elastic approximation). Note that for this asymptote emission and absorption rates are equal. Then (7) turns into:

$$\lambda(\epsilon) = \frac{{E_a}^2 k_B T}{\rho u^2 \hbar^2 L_y L_z}\sqrt{\frac{m^*}{2(\epsilon - \Delta\epsilon)}}\,(1 + \frac{1}{2}\delta_{j,j'})(1 + \frac{1}{2}\delta_{l,l'}) \ . \tag{8}$$

Thus the large energy asymptote diverges as $\epsilon^{-1/2}$ function of electron kinetic energy after scattering, the same as 1D density of states function. The large energy asymptote is extended to low energy region in [1-4] to evaluate electron mobility. The scattering rate within this elastic approximation is inversely proportional to a QWI cross section $L_y \times L_z$.

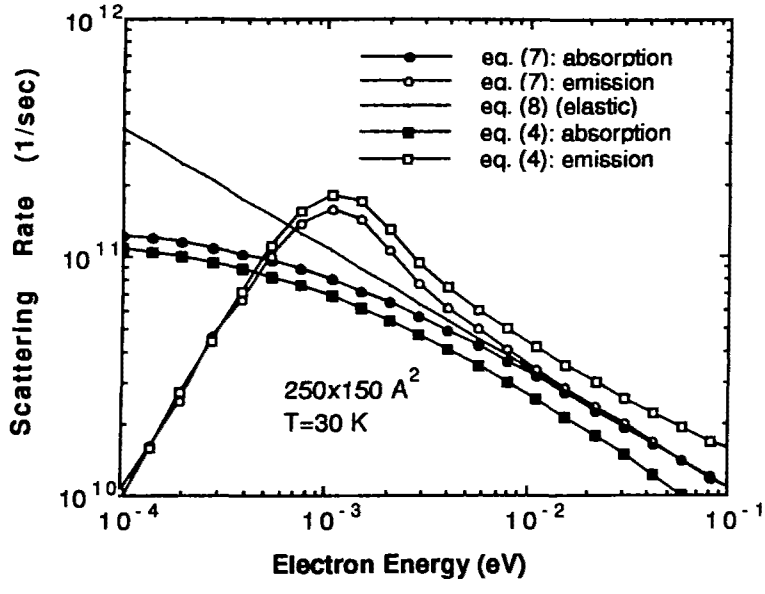


Figure 2 demonstrates the differencies between the scattering rate dependencies on electron energy calculated for QWI with cross section $250 \times 150\mathring{A}^2$ within three different approaches: elastic approximation of eq. (8), the approach of eq. (7), and the direct numerical integration of eq. (4) without any simplifications. The correct inelastic treatment of acoustic phonon scattering yields qualitatively different scattering rates. Emission and absorption rates within the inelastic approach are considerably different at low energies.

There is no divergency of the scattering rates within inelastic approach. The energy $\hbar u q_{T max}$ given by uncertainty of momentum conservation defines the position of the maximum on emission curve and coincides with the characteristic energy of acoustic phonon interacting with electrons.

III. Results of the Monte Carlo Simulation

The necessity to allow for inelasticity of acoustic phonon scattering in Monte Carlo simulations complicates the procedure of choice of the final states for scattered electron. We have developed very efficient procedure for random selection of acoustic phonon energy involved in the scattering. The essence of this procedure is that we first numerically perform von Neumann procedure for a set of random numbers and tabulate the phonon energy as a function of a random number. For a QWI we have solved the following equation:

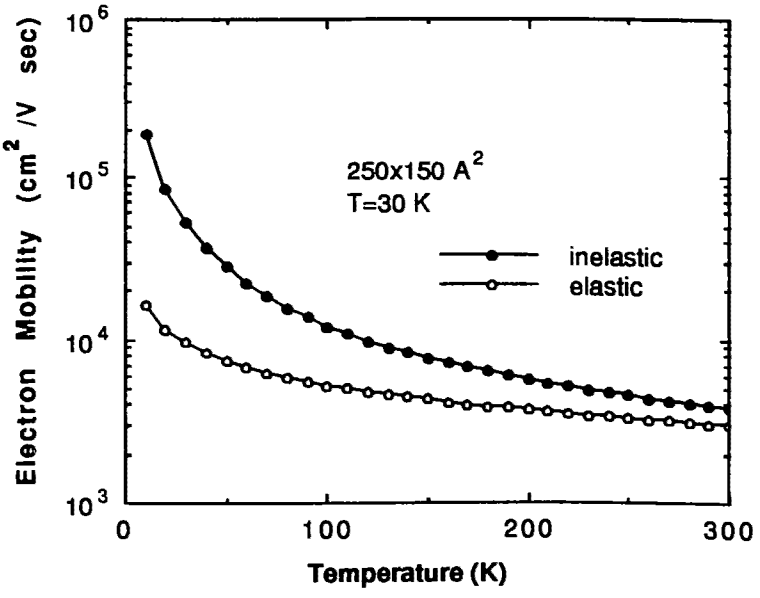
$$r \int_0^{q_{T max}} dq_T F(q_T) \; = \; \int_0^{q_T^*} dq_T F(q_T) \; , \tag{9}$$

with respect to q_T^* for a set of 100 random values of r ranging from 0 to 1. Here the function $F(q_T)$ is an integrand of eq. (7) and represents the scattering probability dependence on the transverse components of the phonon wavevector. Since q_T is directly related to the phonon energy within approximation $q_x \ll q_T$[1], one can find the desired phonon energy for each value of r. A table of such values has been calculated for a set of electron energies

[1]Within more accurate approach where q_x is not neglected, the acoustic phonon energy is uniquely related to q_x, so that this dependence can be used to generate the acoustic phonon energy [5].

for emission and absorption of acoustic phonon separately. Then the choice of phonon energy involved into a scattering event is just the generation of random number r and the selection of the corresponding phonon energy value from the appropriate table. This procedure essentially speeds up the Monte Carlo simulation.

To test the scattering rates and the Monte Carlo procedure we have simulated the electron transport at low lattice temperatures. Monte Carlo simulations yield very accurate thermal equilibrium energy and distribution function for electron system indicating that acoustic phonon scattering is treated correctly. The elastic scattering model fails to yield good equilibrium energy and distribution function. Figure 3 demonstrates low field electron mobility in the QWI with cross section $40 \times 40\mathring{A}^2$ as a function of lattice temperature. One can see that electron mobility calculated within elastic approach is significantly underestimated in the low temperature region. The reason for this is obvious: an overestimation of acoustic phonon scattering rate (especially emission rate) at low energy region. It must be noted that in thicker QWIs the discrepancy between low field electron mobilities obtained within elastic and inelastic models is less pronounced because inelasticity of acoustic phonon scatering is weaker in thick QWIs.



We have also observed superlinear region on velocity-field dependence associated with reduction of acoustic phonon scattering efficiency as the electron system gets heated. This superlinear region appears only for rather thick QWI. In thin QWIs (cross section of the order of $40 \times 40\mathring{A}^2$) the acoustic phonon scattering is so strong and inelastic that it prevents electron heating up to very high electric fields. The superlinearity on velocity-field dependence is greatly overestimated within elastic approximation since elastic scattering does not prevent electron runaway from the low energy region. As a result, the velocity-field dependences calculated within elastic and inelastic approaches are considerably different.

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