# ELECTRON INTERSUBBAND SCATTERING IN REAL QUANTUM WIRES

R. Mickevicius and V. V. Mitin
Department of Electrical & Computer Engineering,
Wayne State University, Detroit, Michigan 48202

K. W. Kim
Department of Electrical & Computer Engineering,
North Carolina State University, Raleigh, NC 27695

Michael A. Stroscio
U.S. Army Research Office, P.O.Box 12211,
Research Triangle Park, NC 27709

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The rates of electron intra- and intersubband scattering by surface optical (SO) and confined longitudinal optical (LO) phonons in quasi-one-dimensional GaAs/AlAs quantum wires (QWIs) are calculated. It is shown that electron-SO-phonon intersubband scattering can be resonant, so that the scattering rate tends to infinity when intersubband energy separation approaches SO phonon energy. The energy dependence of the total scattering rate in ideal QWIs exhibits multiple sharp peaks related to intersubband transitions. The scattering rates in the real QWIs with variable thickness are calculated. The results show that even small variation in thickness leads to the significant broadening of the very first peaks and complete washing-out of the peak-like structure at higher energies. Monte Carlo simulations of electron transport in the QWI have been performed. It is demonstrated that electron drift velocity in the QWI is considerably suppressed by electron intersubband scattering and is considerably lower than the bulk material values. The role of SO phonons in electron energy dissipation is discussed.

## I. Introduction

Despite rapidly growing number of publications on quantum wires (QWIs), the theoretical investigations are limited either to the case of extreme quantum limit (EQL) wherein only one subband is considered [1,2] or (and) to the case of scattering by bulk three-dimensional (3-D) phonon modes [3]. However, it is difficult to meet these limitations because electrons can populate upper subbands at higher temperatures or in the hot-electron regime [4] and experiments evidently demonstrate importance of surface-optical (SO) modes [5] and phonon confinement [6] in QWIs. Moreover, most theoretical studies on QWIs deal with ideal 1-D systems characterized by fixed subband energetic positions. The unique feature of ideal QWIs is the well-pronounced resonant nature of electron scattering as a result of multiple sharp peaks (diverging to infinity) on energy dependence of the total electron scattering rate. However, all current and foreseeable future technologies of fabricating QWIs do not assure the possibility to create ideal structures with constant thickness [4,7]. The variation of QWI thickness results in the variation of subband energetic position. Consequently, electron scattering is no longer energetically coherent in different parts of a QWI and this should lead to the broadening or even complete washing-out of the resonant peaks [8,9].

The aim of the present paper is to investigate both the phonon confinement and multi-subband structure in a rectangular QWI of polar semiconductor embedded in another polar semiconductor. We consider an ideal QWI with thickness constant along the wire (Section II) and a real QWI with variable thickness (Section III). In Section IV some preliminary results of Monte Carlo simulation are discussed.

## II. Ideal QWI

The 1-D electron energy in a rectangular QWI is of well-known form

$$E(q_x,j,l) = E_x(q_x) + E_{jl}\,,$$

$$E_x(q_x) = \frac{\hbar^2 q_x^2}{2m^*}\,,$$

$$E_{jl} = \frac{\hbar^2}{2m^*}\left[\left(\frac{\pi j}{L_y}\right)^2 + \left(\frac{\pi l}{L_z}\right)^2\right]\,, \qquad (1)$$

where $E_x$ is the electron kinetic energy, $q_x$ being the electron wave-number in x-direction, and $E_{jl}$ is the subband {j,l} energetic position with respect to the bulk ground level. It is seen from Eq.(1) that subband energetic positions depend on the structure thickness $L_y$ and $L_z$. In this Section we will consider an ideal QWI with constant thickness along the wire, so that $E_{jl}$ is independent of x.

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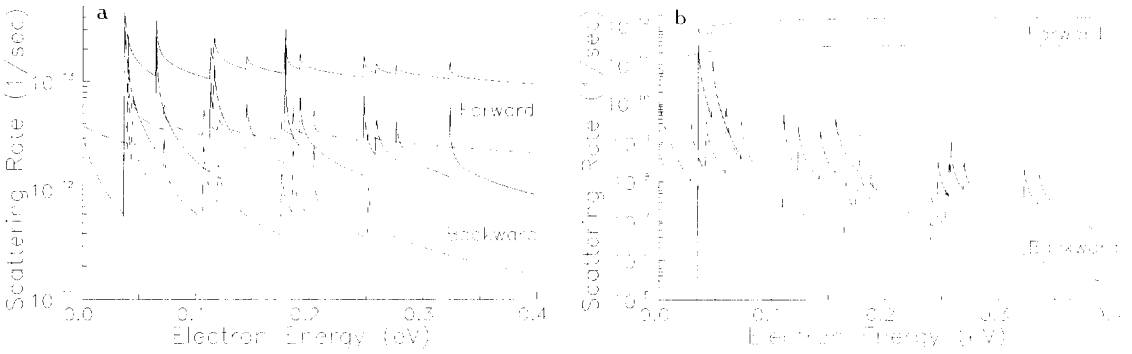


Fig.1. Electron-LO-phonon (a) and electron-SO-phonon (b) scattering rates in/from the first subband as a function of electron kinetic energy. Solid curves represent emission, dashed absorption. Upper curves represent forward electron scattering (wave-vector direction does not change), lower curves backward scattering (wave-vector change its direction to opposite). T=300 K.

Numerical calculations of the scattering rates have been performed for the GaAs QWI of dimensions $L_y$ = 150 Å and $L_z$ = 250 Å embedded in AlAs. We have considered 11 subbands (choosing subband indices j=1,2,3 and l=1,2,3,4). The calculated energy dependencies of the total electron-LO-phonon and electron-SO-phonon scattering rate from the first subband to elsewhere for the case of ideal QWIs is presented in Fig.1. The forward and backward scatterings are plotted as separate scattering mechanisms in order to reveal the polar character of electron interaction with LO and SO modes. Indeed electron forward scattering is dominant both for LO and SO phonons. The multiple sharp peaks on the "backward" curves of Fig.1b are almost unnoticeable on the "forward curves". This is because forward intrasubband scattering by SO phonons is several orders of magnitude higher than forward intersubband scattering responsible for the peaks. The strength of backward intrasubband scattering is more than three orders of magnitude lower and is comparable with the strength of backward intersubband scattering. As a result, intersubband transition peaks are well pronounced. Comparing Figs.1a and 1b, one can see that each peak in Fig.1a is doubled in Fig.1b. This is due to the fact that SO phonon modes in GaAs/AlAs QWIs split into two branches one being related to GaAs and the other to AlAs. Fig.1 clearly demonstrate that electron scattering by LO phonons dominate over scattering by SO phonons in the given structure.

When intersubband energy is close to that of SO phonon (GaAs- or AlAs-like), the phonon wave-number $k_x$ is close to zero. This is the so called resonant intersubband electron-SO-phonon scattering condition which has been discussed in Ref.3 for 3-D LO phonons in QWIs. The electron-SO-phonon scattering rate is inversely proportional to the fourth power of phonon wave-number $k_x$ [2] and tends to infinity for any electron energy when intersubband energy approaches that of SO phonon. In our particular structure the energy separations between the 2nd and 3rd, the 5th and 6th, and the 8th and 9th subbands are transitions between these subbands are forbidden by selection rules [4]. Nevertheless, it is possible to create QWIs with subbands in resonance where resonant intersubband transitions are allowed. In order to verify this statement we have additionally considered a model structure with allowed transitions between subbands in resonance. The transition rates between these subbands exceed all other scattering rates by SO phonons and are comparable or even higher than electron-LO-phonon scattering rates. The electron-confined-LO-phonon scattering is not so influenced by the resonant intersubband scattering condition [4].

## III. Real QWI

Let us consider now a real QWI with variable thickness. It is evident from Eq.(1) that the variation of a structure thickness causes the variation of subband energetic positions $E_{jl}(x)$. We restrict ourselves by the smooth variation of thickness along x so that the characteristic length of the fluctuations is much greater than the de Broglie wave-length $\Lambda_B$. Since the total electron energy does not depend on the QWI thickness the variation of $E_{jl}$ with x results in the variation of electron kinetic energy $E_x$. Let us consider the simple case of the random thickness fluctuations which cause random fluctuations of final electron kinetic energy after scattering within the interval $(E_o - \Delta E, E_o + \Delta E)$. Then the average over the structure length rate of one particular transition can be calculated analytically [4]:

$$\lambda(E_0) = \frac{P(E_0)}{\Delta E}[\theta(E_0 + \Delta E)\,(E_0 + \Delta E)^{1/2} - \theta(E_0 - \Delta E)\,(E_0 - \Delta E)^{1/2}], \quad (2)$$

where $P(E_0)$ represent the non-diverging part of the scattering rate, $\theta$ is the step function. When $E_0$ = 0,

$$\lambda(0) = \frac{P(0)}{\sqrt{\Delta E}}, \qquad (3)$$

i.e., the scattering rate is no longer diverging.

The numerical calculations of the scattering rates in real QWIs have been performed with the same model of scattering processes as in ideal QWIs but with variable thickness $L_y$ and $L_z$. We have assumed the thickness varying with the harmonic law. The variation amplitudes $\Delta L_y$ and $\Delta L_z$ have been chosen from 0.01 to 0.1 fraction of the corresponding thicknesses $L_y$ and $L_z$. We have considered three cases with different mutual phases of the variation of $L_y$ and $L_z$: $L_z = L_{zo} + \Delta L_z \cos(Kx)$, $L_z = L_{zo} + \Delta L_z \sin(Kx)$, and $L_z = L_{zo} + \Delta L_z \cos(2Kx)$ with $L_y = L_{yo} + \Delta L_y \cos(Kx)$ in all cases. It has been found that the results do not show significant difference between these models as long as we are in the limit of smooth fluctuations $K\Lambda_B << 1$. Fig.2 demonstrates the typical results obtained for the first case with the reasonable 5% variation amplitude ( $\Delta L_y/L_{yo} = \Delta L_z/L_{zo} = 0.05$). One can see that such variation yield considerable broadening and reduction of the very first scattering peaks and complete disappearance of the peaks at higher energies. Similar curves with a different degree of broadening are obtained for other variation amplitudes. Even a variation in amplitude as small as 1% leads to the disappearance of the divergence at the resonant energies and essential smearing out of the peak-like structure on the curves discussed. Similar results are provided by the simplified model of Eq.(2).

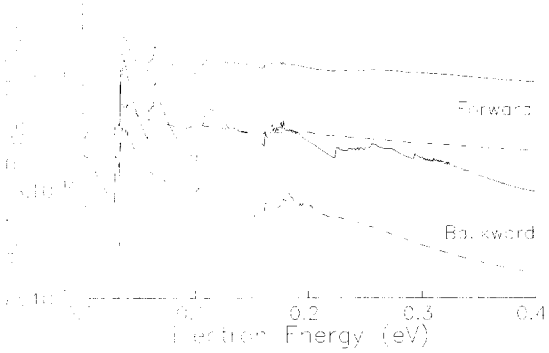


Fig.2. Electron-LO-phonon scattering rates in/from the first subband when the variable thickness is included. The notation is the same as in Fig.1.

## IV. Monte Carlo Simulations

The calculated scattering rates for the ideal QWI have been included into the Monte Carlo program which

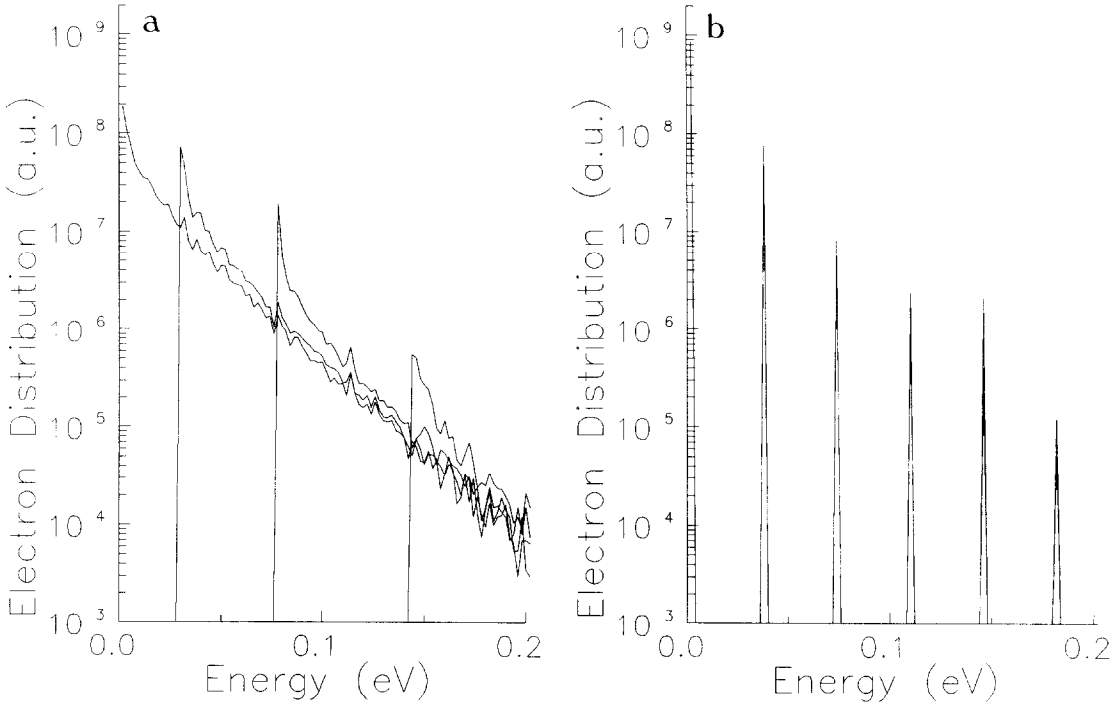


Fig.3. The steady-state distribution function of cold injected electrons when SO phonons are included (a) and ignored (b). T=300 K, no electric field is applied.

permits consideration of up to 11 subbands. The electron distribution function relaxation at low electric fields and high-field electron transport have been simulated at lattice temperature 300 K. The aim of these preliminary simulations is to reveal the role of electron intersubband scattering and SO phonons in electron transport phenomena in QWIs. Under the conditions of intensive intersubband scattering at 300 K electrons do not exhibit expected high mobilities. Thus, at 0.1, 0.5, 1, and 2 kV/cm electron drift velocity in the QWI is 0.87, 2.4, 4.4, and $7.7\times10^6$ cm/sec, respectively. The undoped bulk GaAs values are about 0.8, 4, 7, and $13\times10^6$ cm/sec, respectively. Electron mobility enhancement in ideal QWIs is expected at low temperatures and low electric fields because in that case electrons do not undergo effective scattering in the "passive" region below optical phonon energy. It must be noted that electron scattering by SO phonons does not influence considerably electron steady-state transport even if the resonant scattering between 2nd and 3rd, 5th and 6th, and 8th and 9th subbands is allowed, because electron resonant intersubband scattering by SO phonons does not change neither electron momentum nor kinetic energy. That is why electron resonant transitions between equivalent subbands are similar to fictitious self-scattering. On the other hand, if subbands are not equivalent or optical transitions between some subbands are possible the resonant scattering by SO phonons might play an important part. However, SO phonons play decisive role in electron energy dissipation and distribution function relaxation. SO phonons having energies different from that of LO phonons yield very fast energy dissipation and relaxation of electron distribution function even in the absence of nonelastic acoustic scattering as it is demonstrated in Fig.3a. In the case when SO phonon scattering is not considered the injected electron distribution function exhibits sharp peaks at energies multiple to LO phonon energy (Fig.3b) and is not relaxing to equilibrium distribution function. It must be stressed that at room temperature the role of SO phonons in energy dissipation is more important than that of nonelastic acoustic phonons because the rate of electron scattering by SO phonons is essentially higher than that by acoustic phonons in QWIs of dimensions which we consider or smaller. It is seen from Fig.3b that the 5th peak of the distribution function is higher than the 4th one. This result is similar to the result obtained by Leburton et al [3] and is related to the resonant intersubband transitions to the bottom of corresponding subband. Indeed, from comparison of Figs.3a and 3b it is seen that the 5th peak is located exactly at the energy corresponding to the bottom of the 6th subband. It is evident from Fig.1 that transitions to the bottom of each subband are highly probable. More detailed study of electron transport in QWIs will be presented elsewhere.

## References


1. M. A. Stroscio, Physical Review **B40**, 6428 (1989).
2. K. W. Kim, M. A. Stroscio, A. Bhatt, R. Mickevicius, and V. V. Mitin, Journal of Applied Physics **70**, 319 (1991).
3. S. Briggs, D. Jovanovic, and J. P. Leburton, Applied Physics Letters **54**, 2012 (1989).
4. R. Mickevicius, V. V. Mitin, K. W. Kim, M. A. Stroscio, and G. J. Iafrate, submitted to Journal of Physics: Condensed Matter.
5. M. Watt, C. M. Sotomayor-Torres, H. E. G. Arnot, and S. P. Beaumont, Semiconductor Science and Technology **5**, 285 (1990).
6. G. Fasol, M. Tanaka, H. Sakaki, and Y. Horikosh, Physical Review **B38**, 6056 (1988).
7. H.I. Smith, K. Ismail, W. Chu, A. Yen, Y.C. Ku, M.L. Schattenberg, and D. A. Antoniadis, In: Nanostructure Physics and Fabrication, Ed. by M. A. Reed and P. Kirk, Academic Press, Boston, 1989, p. 57.
8. P. F. Bagwell, D. A. Antoniadis, and T. P. Orlando, In: VLSI Electronics Microstructure Science, Vol.18: Advanced MOS Device Physics, Ed. by N. G. Einspruch and G. Gildenblat, Academic Press, NY, 1989, pp. 305-355.
9. V.V.Mitin, Superlattices and Microstructures **8**, 413 (1990).