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Electron high-field transport in multisubband quantum wire structures

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Abstract. The Monte Carlo simulation of electron transport in multisubband quasi-one-dimensional GaAs/AlAs quantum wires (QWIS) are presented. The electron intrasubband and intersubband scattering by surface-optical and confined longitudinal-optical phonons in QWIS has been included in the program. It is demonstrated that at room temperature the electron drift velocity in the QWI is suppressed by electron intersubband scattering and does not exceed the bulk material values. 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 thicknesses are calculated as well. The results show that even small variation in thickness leads to a significant broadening of the very first peaks and complete washing-out of the peak-like structure at higher energies.

1. Introduction

During the years following Sakaki's work [1], a number of papers on quantum wires (QWIS) appeared, dealing mainly with theoretical analyses of quantization, scattering mechanisms and linear transport in low electric fields (see e.g., [2] and papers in [3]). Most of the previous studies on nonlinear electron transport in QWIS have been limited to the case of scattering by bulk three-dimensional (3D) phonon modes [4]. However, experiments clearly demonstrate the importance of surface-optical (SO) modes [5] and phonon confinement [6] in QWIS. Moreover, most theoretical studies on QWIS deal with ideal 1D systems characterized by fixed subband energy positions. However, all current and foreseeable future technologies of fabricating QWIS do not assure the possibility to create ideal structures with constant thickness [7–10]. The variation of QWI thickness results in the variation of subband energy positions. 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 [8–10].

In the present paper we consider nonlinear (hot) electron transport in a rectangular GaAs QWI embedded in AlAs. Both the phonon confinement and multisubband structure are taken into account. We consider electron scattering in an ideal QWI with a constant thickness along the wire as well as in a real QWI with variable thickness. The Monte Carlo simulations are performed for the ideal QWI.

2. Scattering rates

The model of the QWI and the scattering rates is discussed in detail in [10, 11]. We consider ideal QWIS with constant thickness and real QWIS with a smooth variation of thickness along the structure so that the characteristic length of the fluctuations is much greater than the de Broglie wavelength Λ_B. Numerical calculations of the scattering rates have been performed for the GaAs QWI of dimensions $L_y = 150$ and $L_z = 250$ Å embedded in AlAs. We have considered 9 subbands. The scattering rates in real QWIS have been calculated assuming a thickness varying with the harmonic law. The variation amplitudes δL_y and δL_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: $L_z = L_{z0} + \delta L_z \cos(Kx)$, $L_z = L_{z0} + \delta L_z \sin(Kx)$ and $L_z = L_{z0} + \delta L_z \cos(2Kx)$ with $L_y = L_{y0} + \delta L_y \cos(Kx)$ 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 $K\Lambda_B \ll 1$. The calculated energy dependences of the total electron transition rate from the

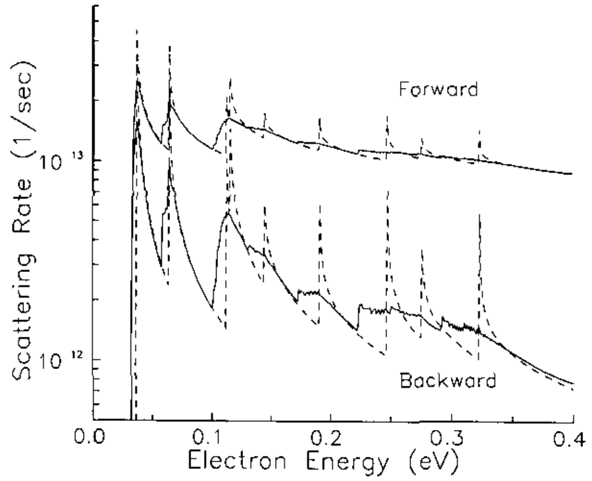

Figure 1. Electron scattering rate due to LO phonon emission in/from the first subband as a function of the electron kinetic energy. Broken curves are for the ideal QWI; solid curves for the real QWI with 5% thickness variation along the structure. Upper curves represent forward electron scattering (wavevector direction does not change); lower curves represent backward scattering (wavevector change its direction to opposite). $T = 300$ K.

first subband to elsewhere due to emission of longitudinal optical (LO) phonon for ideal and real QWIs are presented in figure 1. The forward and backward scatterings are plotted as separate scattering mechanisms in order to reveal the polar character of electron–phonon interaction. Our calculations demonstrate that electron forward scattering is dominant for both LO and SO phonons. The electron–SO–phonon scattering rates are more than an order of magnitude lower and are presented in [10]. A unique feature of ideal QWIs is the well pronounced resonant nature of electron scattering as a result of multiple sharp peaks (diverging to infinity). For the real QWI, the typical results shown in figure 1 are obtained for the first of the above-mentioned cases with a reasonable 5% variation amplitude ($\delta L_y/L_{y0} = \delta L_z/L_{z0} = 0.05$). One can see that such a variation yields 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 a dramatic smearing out of the peak-like structure on the curves discussed.

3. Monte Carlo simulation

The calculated scattering rates for the ideal QWI have been included in the Monte Carlo program which permits consideration of up to 9 subbands. The relaxation of the electron distribution function at low electric fields and high-field electron transport have been simulated at lattice temperatures of 300 and 77 K. The aim of these simulations is to reveal the role of electron intersubband scattering due to LO and SO phonons in electron transport phenomena in QWIs. Under the conditions of intensive intersubband scattering at 300 K electrons do not exhibit the expected high mobilities, as one can see from figure 2, where velocity-field dependences for the QWI and bulk undoped GaAs are plotted for comparison. At 300 K electron scattering by LO phonons determines electron low-field mobility. The role of acoustic and impurity scattering as well as scattering by SO phonons is negligible. Electron mobility enhancement in ideal QWIs is seen in figure 2 at 77 K and low electric fields; in that case electrons do not undergo effective scattering in the 'passive' region below the optical phonon energy. However, at 77 K the probability of absorption of LO phonons is of the same order as that of acoustic scattering and the electron mobility is controlled not only by the electron–LO-phonon scattering but also by the acoustic phonon scattering which is not considered in the present work. Therefore, we observe mobility higher than it should be. If the concentration of impurities is low so that the rate of impurity scattering is below $10^{10}\,\mathrm{s}^{-1}$, the effects of impurity scattering can be neglected since LO phonon absorption rates are close to $10^{11}\,\mathrm{s}^{-1}$. At 77 K and higher electric fields, electron transport is determined by the almost ideal streaming condition [12] due to the low scattering rates in the 'passive' region and high probability of phonon emission. That is why we observe *drift velocity saturation at higher fields at 77 K*. In order to calculate correctly electron transport at fields higher than about $3\,\mathrm{kV\,cm}^{-1}$, one must consider electron intervalley scattering. It must be noted that electron scattering by SO phonons does not influence considerably electron steady-state high-field transport. However, SO phonons having energies different from those of LO phonons yield very fast energy dissipation and relaxation of the electron distribution function at low electric fields. In the case

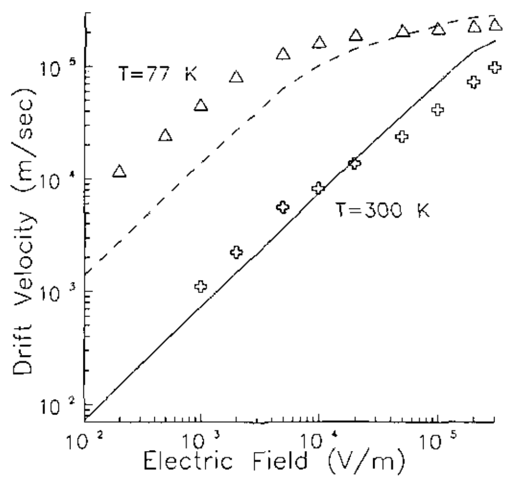

Figure 2. Electron drift velocity dependence on electric field. Symbols represent results obtained for the QWI and curves represent dependences for pure bulk GaAs. Triangles and broken curve are for $T = 77$ K and the crosses and full curve are for $T = 300$ K.

when SO phonon scattering is not considered, the injected electron distribution function exhibits sharp peaks at energies which are multiples of the LO phonon energy and does not relax to the equilibrium distribution function in the absence of an electric field. It must be stressed that at room temperature the role of SO phonons in energy dissipation is more important than that of inelastic acoustic phonons because the rate of electron scattering by SO phonons is essentially higher than that by acoustic phonons in QWIs of dimensions equal to or smaller than those considered in this work.

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