ELECTRON MOBILITY IN QUANTUM WIRES LIMITED BY OPTICAL-PHONON SCATTERING

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Abstract

Electron mobility in a quantum wire of GaAs/AlGaAs heterostructure is calculated by using the Boltzmann transport equation and detailed balance equation, where the results of self-consistent calculations for the eigen states and energies of electrons in the quantum wire system are used to evaluate the conductivity. Resonant behavior of the conductivity is expected due to the resonant scattering of electrons between the subbands induced by longitudinal optical phonon scattering. The resonance is shown to depend on the magnitude of one-dimensional form factors which are proportional to the transition probability of electrons in quasi-one dimensional system.

1. INTRODUCTION

It has been pointed out that the suppression of small angle scattering in quasi-one dimensional structures results in an enhancement of electron mobility at low temperatures [1]. At high temperatures, however, electron-longitudinal optical (LO) phonon scattering will play an important role in quantum wires (QWs) of GaAs/AlGaAs. In QWs fabricated on GaAs/AlGaAs heterostructures, electrons are confined just below the hetero-interface and the gate electrodes fabricated on the surface form quasi-one dimensional electron gas (Q1DEG), where the electron density in channel area can be controlled by gate voltage. In other words, electronic states may be changed by the gate voltage, and thus we can tune the inter-subband energy to the optical phonon energy. Since the electron mobility in QWs at high temperatures is limited by the optical phonon scattering, an oscillatory behavior of electron mobility is expected when the gate voltage is changed [2,3] or when a high magnetic field is applied [4, 5]. In the present work, we calculate the conductivity in a typical gated QW structure and show that the resonant behavior similar to magnetophonon resonance appears by changing the gate voltage without the presence of magnetic field. For this purpose we solve the Poisson and Schrödinger equations self-consistently and obtain one dimensional eigen states and then calculate electron mobility in a QW at high temperatures. The magnitude of the resonance depends strongly on the parity of the wave functions in the direction perpendicular to the heterointerface.

2. SELF-CONSISTENT CALCULATION

We consider a mesa etched quantum wire structure [6] shown in Fig 1. As shown in Fig 1, we choose y and z directions as parallel and normal to the interface, respectively, and the motion of electrons is quantized in these two directions. Up to 20 subbands are calculated self-consistently including different confinement in z direction, where we solved the Poisson and Schrödinger equations numerically by discretizing the structure in a nonuniform rectangular mesh. In Fig 2, we present calculated results of subband energies as a function of gate voltage. The subband index (n, m) is used in Fig 2, which represents node number n of the wave function in the y and node number m in the z directions. For example, eigen state (0, 1) indicates the first quantization state in y direction



Figure 1: Cross-section of a mesa etched Al-gated QW structure used for the present calculations. The device consists of an unintentionally p-doped GaAs substrate ($N_A < 10^{14} \text{ cm}^{-3}$), followed by an undoped AlGaAs spacer layer and an ndoped AlGaAs cap layer ($N_D = 1.5 \times 10^{18} \text{ cm}^{-3}$).

Figure 2: The electron eigen energies in the QW shown in Fig 1 at T = 150 K. The dotted lines represent the eigen states (n,0) and the dashed lines represent the eigen states (n, 1). The arrows indicate relevant transitions. The index (n, m) represents the number of nodes n of the wave functions in the y direction and m in the z direction.

and the second quantization state in z direction. It is seen in Fig 2 that the eigen energies are lowered when the gate voltage is swept in the forward direction, and that many subbands move below the Fermi level (0 eV of the vertical scale), resulting in an enhancement of carrier population and the reduction of subband spacing. A typical result of the electron wave functions in the QW is shown in Fig 3, where the subband energies and potential profile are also plotted by dotted lines and dashed curve, respectively. As shown in Fig 3, the potential profile along z direction is quasi-triangular and the first peek (lefthand side) of the wave functions appears at almost the same position. Since the matrix elements (the form factors) are expressed by the overlap integral [4], we may expect a large value for the overlap integral between eigen states of same confinement in the y direction and different confinement in the z direction and the strong transition between the (n,0) and (n,1) states. In the following we present a calculated result of the conductivity in the QW structure.

3. CALCULATION OF CONDUCTIVITY IN A QUANTUM WIRE

The form factor $G_{ii'}$ and the scattering probability $W_{ii'}$ between subband *i* and *i'* are given by the following equations [4].

$$G_{ii'}(q_x) = \int d\rho_1 \int d\rho_2 K_0(q_x |\rho_1 - \rho_2|) \Psi_{i'}^*(\rho_1) \Psi_i(\rho_1) \Psi_i^*(\rho_2) \Psi_{i'}(\rho_2)$$
(1)

$$W_{ii'}(k,k') = \alpha \omega_0 \sqrt{\frac{2\hbar\omega_0}{m^*}} \left(N_0 + \frac{1}{2} \pm \frac{1}{2} \right) G_{ii'}(q) \delta(\varepsilon(k') - \varepsilon(k) + E_{i'} - E_i \pm \hbar\omega_0)$$
(2)
(q = k - k'),

where $\Psi_i(\rho)(\rho = (y, z))$ is the wave function of the eigen state i = (n, m) and K_0 is the modified



Figure 3: Calculated electron wave functions (solid lines) and potential profile (dashed line) along z direction of the QW shown in Fig 1 at $V_g = 0.0$ V. Ψ_{00} and Ψ_{01} are the wave functions of the (0, 0) state (ground state) and the (0, 1) state, respectively.



Figure 4: Calculated conductance as a function of gate voltage in the QW shown in Fig 1 at T = 150 K.

Bessel function of the second kind, α is the Fröhlich's coupling constant, $m^* = 0.067m_0$ is the electron effective mass and $\hbar\omega_0 = 36.2 \text{ meV}$ is the LO-phonon energy in GaAs bulk, N_0 is phonon number, and E_i denotes subband energy of eigen state *i*. The \pm sign in equation (2) corresponds to the emission and the absorption of LO-phonon, respectively.

The electron conductivity in a QW is calculated as a function of gate voltage using the Boltzmann transport equation and the detailed balance principle. Figure 4 shows the calculated result of conductance-gate voltage characteristic of a QW at T = 150 K. It is very interesting to point out that the calculated magnitude of the conductivity is very close to the experimental result of Ismail [2], where he used similar structure of a quantum wire. He observed a dip in the conductance-gate voltage characteristic, whereas the present calculation shows several weak dips in the region from 0.1 to 0.3 V. The increase in the conductivity with the gate voltage is interpreted in terms that the electron density increases with increasing the gate voltage. In order to see the weak structure in the conductance curve more clearly, we deduced the oscillatory components by deducting a smooth curve of the least square fit from the conductance. The oscillatory component thus obtained is plotted in Fig 5, where we see more detailed structure. Although the oscillatory structure is very complicated, some of them are well explained with the help of the results shown in Fig. 2, where the arrows show the resonant transition of the electrons (the length of the arrow is the ${
m LO}$ phonon energy). From a comparison between Fig. 2 and Fig. 5, the oscillatory structures at about 0.2 and 0.24 V are ascribed to the resonant transition from the subband with the index m = 0 to the subbands with the index m = 1. Other transitions indicated by the arrows in Fig 2 are expected to be weaker because of the small value of the form factor as discussed in previous section. From the present work we find that the strength of transitions between the subbands in a QW structure strongly depends on form factors. We present the calculated form factors in Fig 6 for a gate voltage $V_{\rm g} = 0.2 \, \rm V$. It is clearly seen in Fig 6 that the form factor for the transition between the (0,0)state and the (0,1) state is large enough to dominate the reduction in the conductance because the energy separation between the subbands is very close to the LO phonon energy at this gate voltage. Similar situation occurs at the gate voltage $V_g = 0.24$. These oscillatory structures are found to be



very weak compared with the experimental result reported by Ismail [2]. Taking into account the difficulty in obtaining a uniform QW structure, the energy subband structure of a real QW is not so sharp compared with the ideal one used in the present calculation and the broadened nature of the density of states will allow the LO phonon scattering in wider range of energy, resulting in a broadened conductance minima.

4. CONCLUSION

Self-consistent calculation was carried out to obtain electronic eigen states in a QW and the conductance was evaluated by calculating the electron mobility based on Boltzmann transport equation. The calculated conductance was found to exhibit minima as the resonant intersubband transition occurs. The dominant contribution to the minima arises from the intersubband transition between the (0,0) and (0,1) subbands in the QW structure used in the present calculations.

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