Quantum Well Geometrical Effects on Two-Dimensional Electron Mobility in AlGaAs/GaAs Hetero-Structures

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A Monte Carlo analysis to study the quantization effects on the low-field electron mobility in various rectangular and triangular AlGaAs/GaAs heterojunction quantum wells has been performed at T=77K and T=300K. The influence of the electron envelop wave-function and the subband structure on the two-dimensional electron scattering rates is evaluated. Our result shows that a maximum two-dimensional electron mobility at T=300K occurs in a quantum well structure where the energy difference between the first subband and the second subband is about two polar optical phonon energy.

Recently, much research effort has been devoted to the use of heterostructures to achieve an enhancement of the electron mobility speed devices. in ultra-high Among the successful demonstrations of the heterojunction field effect transistors are AlGaAs/GaAs Modulation Doped FET's $\begin{bmatrix} 1 \end{bmatrix}$, AlGaAs/InGaAs/GaAs Pseudomorphic MODFET's [2], Multiple Quantum Well FET's [3] and GaAs Gate Heterojunction FET's [4]. Although all of the above structures employ the concept of the "two-dimensional electron gas" (2DEG), the and the subband wave-functions electron structures in these 2DEG devices are quite different. Since the electron scattering rate closely related to the wave-function is distribution and the subband structure, the two-dimensional electron mobility may change significantly with the quantum well geometry. In this paper, we are to investigate the quantum well confinement effects on the 2DEG mobility. It is our intention to find an optimized AlGaAs/GaAs quantum well structure for the mobility enhancement by tailoring the subband structure and the electron wave-function.

A 2DEG Monte Carlo method is employed to study electron transport in the subbands of quantum wells. Polar optical phonon (POP) scattering and accoustic phonon (ACP) scattering are considered as far as the low-field mobility is concerned. Polar optical phonon energy, $\hbar w$, is 35mev. The 2DEG scattering rate is modulated with respect to the bulk electron scattering rate in two aspects, overlap integral and density of states. As the width of a the intra-subband increases, quantum well scattering rate is lowered due to the spread of an electron wave-function and thus a reduced wave-function overlap integral. The electron

scattering rate therefore declines with a well width until at a certain width the electron transition to the next subband (inter-subband scattering) takes place. As a result, the 2DEG scattering rate exhibits a sawtooth-like feature as a quantum well width is increased (Fig. 1).



Fig. 1 POP and ACP scattering rates versus a quantum well width at an electron energy of 80meV. The solid line is the 2DEG ACP scattering rate, the dashed line is the 2DEG POP scattering rate and the dotted lines represent the bulk electron scattering rates. T=300K

Our study reveals that there exists a window of a well width in which the 2DEG scattering rate can be lower than that of bulk electrons. This suggests that an enhancement of the 2DEG mobility can be optimized in certain geometry quantum wells.

Two sorts of quantum well structures are studied at T=77K and T=300K. The first kind has a 500Å n⁺ Al_{0.3}Ga_{0.7}As /30Å i-Al_{0.3}Ga_{0.7}As /GaAs /i-Al_{0.3}Ga_{0.7}As rectangular quantum well. The doping concentration in the n⁺ AlGaAs layer is 1x10¹⁸ 1/cm³. A 30Å undoped spacer is included.

The GaAs well width is varied in the simulation. The second kind structures have a n⁺ GaAs gate/i-Al_{0.4}Ga_{0.6}As/i-GaAs configuration [4]. The quantum well is triangle-like at the AlGaAs/GaAs interface. In these structures, the interface field is varied to adjust the subband structure and the spread of the electron wave-function. In the simulation, the Schrödinger and the Poisson equations are solved self-consistently. Fig. 2 shows the 2DEG mobility as a function

Fig. 2 shows the 2DEG mobility as a function of a well width. The self-consistent conduction band-edge diagram and the subband structure are illustrated in the inset of this figure. The peak mobility occurs at a width of 120Å.



Fig. 2 Calculated 2D electron mobility as a function of a well width. The inset of the figure shows the conduction band-edge and the quantum states.

In Fig. 3, we redraw the 2DEG mobility against the energy difference between E_0 and E_1 . A maximum mobility around $E_1-E_0=2\hbar w$ is noticed. This result can be explained as follows; The electron energy distribution at a low field has a significant drop about $1\hbar w$ above the ground state due to polar optical phonon emission. In other words, the majority of electrons are restricted in the energy range from E_0 to $E_0+\hbar w$. If the subband structure has $E_1-E_0 > 2\hbar w$, the majority of the electrons are virtually immune from inter-subband transition caused by POP absorption. Only electrons with an energy above $E_0 + \hbar w$ suffer from inter-subband scattering. As the difference between E_1 and E_0 approaches $2\hbar w$, the majority of electrons in the first subband begin to encounter POP absorption. Consequently, the mobility drops at $E_1-E_0=2\hbar w$.

In order to verify our explanation, we simulate the 2DEG mobility in the same structure at T=77K in Fig. 4. As expected, the $2\hbar w$ peak disappears due to the reduction of the POP absorption rate at lower temperature.



Fig. 3 2D electron mobility versus the energy difference between the first subband and the second subband at 300K



Fig. 4 2D electron mobility as a function of a well width at 77K



Fig. 5 2D electron mobility versus the energy separation between E_1 and E_0 in the triangular quantum wells. The inset illustrates the conduction band-edge profile and the subband structure.

In the second kind of quantum well structures, the 2DEG mobility versus the energy separation between E_1 and E_0 is shown in Fig. 5. A triangle-like quantum well geometry with the subband structure is illustrated in the inset of Fig. 4. A similar result of a peak mobility at E_1 - E_0 =2 $\hbar w$ is observed again. However, the peak mobility

(8250 cm²/V-sec) in the triangle-like quantum well is somewhat lower than that (8600 cm²/V-sec) in the rectangle-like quantum well.

As a conclusion, our study shows that the 2DEG mobility varies significantly with the quantum well structures from 7250 cm²/V-sec in a 50Å rectangular well to 8600 cm²/V-sec in a 120Å rectangular well. The maximum mobility can be achieved in a quantum well structure where the energy difference between the first and the second subbands is $2\hbar w$, or 70meV in GaAs wells.

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