

The main scattering mechanisms in Single-side modulation doped square quantum wells

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Abstract. We present a theory of the transport of carrier confined in the conduction band of a single-side modulation doped square quantum wells. Beside the well-known the scattering mechanisms such as surface roughness (*SR*), remote impurities (*RI*), and misfit deformation potential (*DP*), the theory induces acoustic phonon due to the deformation potential and acoustic phonon due to the piezoelectric coupling. In the result, we prove that acoustic phonon scattering has revealed very large mobility values. We have also consider acoustic-phonon partial mobility dependence on temperature for single-side modulation doped square quantum wells.

1. Introduction

The calculation of the carrier mobility in semiconductor heterostructures has received great attention in recent year due to their importance in device applications. In order to upgrade the electron mobility of the above-quoted QWs, one needs to identify the key scattering mechanisms limiting the transport properties of their two-dimensional electron and holes gas (2DEG and 2DHG), and reduce their detrimental effects. It is well known [1, 2] that the best way for this purpose is to study the dependence of 2DEG and 2DHG mobility on experimental conditions such as sample temperature, carrier density, and channel width.

It is worth mentioning that although the above dependencies were explored by a number of authors, they still remain as challenging problems. Firstly, the key scattering mechanisms for these QWs are a subject under debate. The previous interpretations of some experimental findings are quite different even due to one and the same research group [7, 8]. From the two-dimensional holes gas mobility dependence on temperature (100K) and on channel width some authors [3, 4, 8] assumed surface roughness scattering to be the key mechanism. However, from the carrier density dependence of the mobility and the transport to quantum lifetime ratio, the others [8] assumed ionized impurity scattering to be dominant. Secondly, in their calculations the roughness-related misfit deformation potential scattering has been ignored, which was proven to be important for strained Si [16] and SiGe [19] channels.

Just recently, some theoretical [18, 20] studies have indicated the well-known the scattering mechanisms such as surface roughness, misfit deformation potential and remote impurity.. To date, the theory of the key scattering mechanisms has been developed for a single-side modulation doped square quantum wells [20], however, there is not theory for mobility dependence on temperature. Thus, the goal of this paper is to provide a theory of the main scattering mechanisms in Single-side modulation doped square quantum wells, we develop a variational approach to the description of quantum confinement in bent-band infinite square QWs. For



strained GaAs channel in GaAs/ AlGaAs single asymmetric quantum well, we incorporate all possible scattering mechanisms, especially optical phonons (dominant at high temperatures).

2. Theoretical determinations

As a prototype, we are dealing with a heterostructure made of cubic crystals, which is composed of a strained well layer grown pseudomorphically along the axis between two barrier ones. The well layer forms a conduction channel of width L in the region $|z| < L/2$. The sample is modulation doped in a region of thickness L_d in the surface-side barrier $z < -L/2$ and separated from the channel by a spacer layer of thickness L_s . The confinement may be plausibly described by an asymmetric wave function as follows:[21]

$$\zeta(z) = \begin{cases} B\sqrt{\pi/L}\cos(\pi z/L)e^{-cz/L} & \text{for } |z| \leq L/2, \\ 0 & \text{for } |z| > L/2, \end{cases} \quad (1)$$

with L as the well width. Here, B and c are parameters to be determined. The former may be given in terms of the latter via the normalization of the wave function. Thus, there is a single independent parameter, say c , which is, following Eq. (1), regarded as a measure of the band-bending effect on the carrier distribution. The band-bending parameter c is determined from the requirement that the wave function of the ground-state subband is to minimize the total energy per particle. In the bent-band model, besides the barrier potentials this energy includes the Hartree potential created by ionized impurities and charge carriers. In Ref. [21] we achieved an analytic expression for this energy, which enables a tractable variational evaluation of c .

The particles moving along the in-plane are scattered by various disorder sources, which are characterized by some random fields. Scattering by a Gaussian random field is specified by its autocorrelation function in wave vector space [15]. Here $U(\mathbf{q})$ is a two-dimensional Fourier transform of the unscreened scattering potential weighted with an envelope wave function:

$$U(\mathbf{q}) = \int_{-\infty}^{+\infty} dz |\zeta(z)|^2 U(\mathbf{q}, z). \quad (2)$$

The transport (τ_t) and quantum (τ_q) lifetimes are represented in terms of the ACF for each disorder by [12, 14]

$$\frac{1}{\tau_t} = \frac{1}{(2\pi)^2 \hbar E_F} \int_0^{2k_F} dq \int_0^{2\pi} d\varphi \frac{q^2}{(4k_F^2 - q^2)^{1/2}} \frac{\langle |U(\mathbf{q})|^2 \rangle}{\varepsilon^2(q)}, \quad (3)$$

and

$$\frac{1}{\tau_q} = \frac{1}{(2\pi)^2 \hbar E_F} \int_0^{2k_F} dq \int_0^{2\pi} d\varphi \frac{2k_F^2}{(4k_F^2 - q^2)^{1/2}} \frac{\langle |U(\mathbf{q})|^2 \rangle}{\varepsilon^2(q)}. \quad (4)$$

Here, $\mathbf{q} = (q, \varphi)$ is the 2D momentum transfer due to a scattering event in the in-plane (in polar coordinates), $q = |\mathbf{q}| = 2k_F \sin(\vartheta/2)$ with ϑ as a scattering angle. The Fermi energy is given by $E_F = \hbar^2 k_F^2 / 2m^*$, with k_F as the Fermi wave number fixed by the sheet hole density p_s : $k_F = \sqrt{2\pi p_s}$.

The dielectric function $\varepsilon(q)$ in Eqs. (3) and (4) takes account of the screening of scattering potentials by the 2D carriers. As usual, this is evaluated within the random phase approximation, [15]

$$\varepsilon(q) = 1 + \frac{q_s}{q} F_S(q) [1 - G(q)], \text{ for } q \leq 2k_F. \quad (5)$$

Here, $q_s = 2m^*e^2/\varepsilon_L\hbar^2$ is the inverse 2D Thomas-Fermi screening length, with ε_L as the dielectric constant of the well layer. The local field corrections due to a many-body exchange effect in the in-plane are quantified by $G(q) = q/2\sqrt{q^2 + k_F^2}$. The screening form factor $F_S(q)$ takes account of the extension of particle states along the growth direction. With the wave function from Eq. (1), $F_S(q)$ is analytically expressed in terms of the band-bending parameter c .

The charge carriers are in general expected to experience the following scattering mechanisms: (i) acoustic-phonon, (ii) remote impurities (*RI*), (iii) surface roughness (*SR*), and (iv) misfit deformation potential (*DP*) therefrom. The overall lifetime is determined by the ones for individual disorders according to the Matthiessen's rule [12]:

$$\frac{1}{\tau_{\text{tot}}} = \frac{1}{\tau_{AP}} + \frac{1}{\tau_{RI}} + \frac{1}{\tau_{SR}} + \frac{1}{\tau_{DP}}. \quad (6)$$

The total mobility is determined by the transport lifetime: $\mu = e\tau/m^*$, with m^* as the in-plane effective mass of the carrier. The transport lifetime limited by some disorder is represented, via the scattering rate $1/\tau$, in terms of its autocorrelation function (ACF) by [12].

3. Autocorrelation functions for scattering mechanisms

With the use of the envelop wave function from Eq. (1), we are able to derive the autocorrelation functions for all possible low-temperature scattering mechanisms in strained 1S-doped square QWs in an analytic form (remote impurity-*RI*, surface roughness-*SR*, and misfit deformation potential-*DP*) [20].

At high temperatures, we are able to derive the autocorrelation functions for Phonon scattering. It has been shown [22] that phonons scattering plays an important role in limiting the electron mobility in III-V semiconducting compounds. The most important phonon scattering processes are (i) deformation potential acoustic, (ii) piezoelectric acoustic. In this paper we calculate only the temperature dependent part of the electron mobility. The momentum relaxation time due to acoustic-phonon scattering is given by:

$$\frac{1}{\tau_{AP}} = \sum_{k'} W(k, k')(1 - \cos\vartheta), \quad (7)$$

where $W(k, k')$ is the transition probability from state k to k' and ϑ is the scattering angle. In the temperature range in which we analyze the electron mobility, acoustic-phonon scattering can be consider as elastic. We approximate the phonon-distribution function N_q by $K_b T/\hbar\omega_q$. Then $W(k, k')$ is given by [23]

$$W(k, k') = \frac{2k_B T}{\hbar^2} \int_{-\infty}^{+\infty} dz \frac{|M(q)|^2}{\omega_q S^2(|k - k'|)} |I(q_z)|^2 \delta(E_k - E_{k'}), \quad (8)$$

where q_z is the wave vector normal to the heterointerface and $|M(q)|$ is the 3D scattering matrix element. $I(q_z)$ is the overlap integral by

$$I(q_z) = \int_{-\infty}^{+\infty} dz \zeta(z) \exp(iq_z z) \zeta(z). \quad (9)$$

The scattering matrix elements for the deformation-potential and piezoelectric coupling are, respectively, given by

$$|M(q)|^2 = \frac{D^2 \hbar \omega_q}{2c_l L^3}, \quad (10)$$

and

$$|M(q)|^2 = \frac{2\pi e^2 P^2 \hbar \omega_q}{\epsilon_0 q^2 L^3}. \quad (11)$$

Here ϵ_0 is the static dielectric constant $\epsilon_0 = 12.91$, e the elemental charge. The static screening factor at finite temperature has been calculated to be:

$$S(q) = 1 + \frac{2\pi e^2 F(q) \Pi(q)}{\epsilon_0 q}. \quad (12)$$

The screening form factor $F_S(q)$ takes account of the extension of the particle state along the growth direction, defined by

$$F_S(q) = \int_{-\infty}^{+\infty} dz \int_{-\infty}^{+\infty} dz' \zeta^2(z) \zeta^2(z') e^{-q|z-z'|}. \quad (13)$$

Here, we defined the following mathematical functions:

$$\gamma_n(x) = \left[\frac{1}{x} + \frac{(-1)^n x}{x^2 + n^2 \pi^2} \right] \sinh x; \quad \omega_n(x) = \frac{(-1)^n n \pi}{x^2 + n^2 \pi^2} \sinh x, \quad (14)$$

$F_S(t)$ defined by [21] with the wave function from Eq. (1), the calculation of Eq. (13) is lengthy, but straightforward with the aid of the functions γ_n and ω_n in Eqs. (14).

The static polarizability at finite temperature is given by [24]

$$\Pi(q, T, E_F) = \frac{1}{4k_B T} \int_0^{+\infty} \frac{\Pi(q, 0, \sigma)}{\cosh^2\left(\frac{E_F - \sigma}{2k_B T}\right)} d\sigma, \quad (15)$$

where $\Pi(q, 0, \sigma)$, is the polarizability funtion at $T = 0K$, namely,

$$\Pi(q, 0, \sigma) = \frac{m^*}{\pi \hbar^2} \left\{ 1 - \theta(q - 2k_F) \left(1 - \left(\frac{2k_F}{q} \right)^2 \right)^{1/2} \right\}. \quad (16)$$

Here $k_F = \sqrt{2m^* E_F}/\hbar$ is the Fermi wave number. In the quantum limit, the temperature can be considered low enough so that $q < 2k_F$ becomes a very good approximation to acoustic phonon and it is very useful in phonon mobility calculations since it makes the factor in brackets of Eq. (17) to be unity. Also, due to the fact that significant effects of interface-phonons were never experimentally found, the electron-phonons non interactions occurring in the 2DEG are considered identical to that of bulk GaAs.

4. Results and conclusion

4.1. Input material parameters

In this section, we apply the above-developed theory in order to understand the properties of low-temperature transport in remote doped square QWs. In Particular, we clarify the The main scattering mechanisms in Single-side modulation doped square quantum wells.

To illustrate all above-quoted scattering mechanisms, in the Figure 1, we consider a two-dimensional hole gas (2DHG) in the strained Ge channel of an $\text{Si}_{0.3}\text{Ge}_{0.7}/\text{Ge}/\text{Si}_{0.30}\text{Ge}_{0.7}$ QW. The two barriers are B-doped equally with a doping profile of $L_d = 100 \text{ \AA}$ and $L_s = 100 \text{ \AA}$. As indicated, [9] for strained Ge on cubic [001] $\text{Si}_{0.3}\text{Ge}_{0.7}$, the potential barrier height for heavy holes is rather large: $V_0 \approx 270 \text{ meV}$. Therefore, the assumption of infinite square QWs is plausibly accepted as in the previous theories. [13] For strained Ge, the out of-plane and in-plane

effective masses of the heavy hole are $m_z = 0.19 m_e$, $m^* \approx 0.1 m_e$. [17] The lattice mismatch of the QW is $\epsilon_{||} = -0.01$. The elastic stiffness constants of the Ge channel are $c_{11} = 12.85$, $c_{12} = 4.83$, $c_{44} = 6.80$ in units of 10^{10} Pa, and the shear deformation potential constants are $b_s = -2.55$, $d_s = -5.50$ in eV [9, 25].

In the Figure 2, we consider a two-dimensional electron gas (2DHG) in the strained GaAs channel of an $GaAs/AlGa_{1-x}As_x$ square QWs whose following physical parameters were taken elsewhere [26].

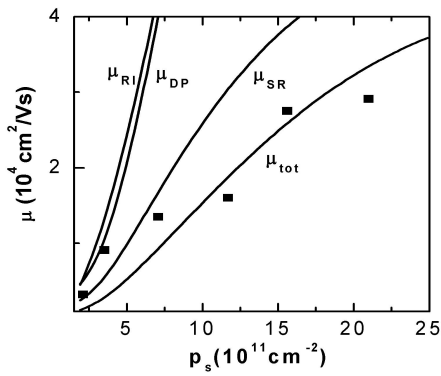


Figure 1. Partial and total mobilities of holes in a $Si_{0.33}Ge_{0.67}/Ge/Si_{0.33}Ge_{0.67}$ square QW with a channel width $L = 75$ Å vs hole density p_s . The single-side modulation doping is with $L_d = 100$ Å and $L_s = 100$ Å. The 8K experimental data [6] are marked by squares.

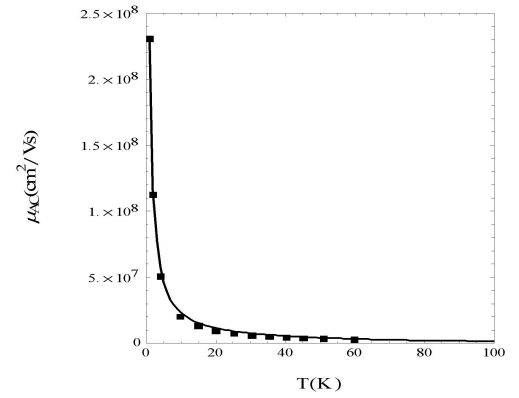


Figure 2. Acoustic-phonon partial mobility in a $GaAs/AlGa_{1-x}As_x$ square QW with a channel width $L = 152$ Å vs temperature T . There common parameters are $L_d = 100$ Å, $L_s = 100$ Å. The experimental data [10] are marked by squares.

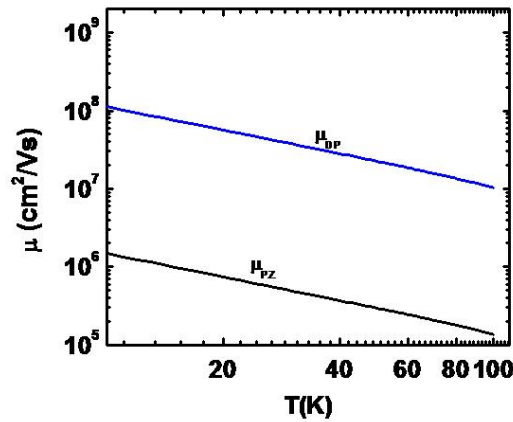


Figure 3. Acoustic-phonon (DP plus PZ coupling) partial mobility dependence on temperature for single-side doped square quantum well.

At high temperatures the carriers in the single-side doped square QWs are expected to experience the following scattering sources: acoustic phonons (Deformation potential- DP) and Piezoelectric coupling- PZ). From Figure 3, the key scattering mechanisms is acoustic phonons due to the piezoelectric coupling (PZ), acoustic phonons due to Deformation potential (DP) is in general less relevant.

4.2. Conclusions

From the lines thus obtained, we may draw the following conclusions:

- (i) As clearly observed from Figure 1, the calculated overall mobility may reproduce very well the observed hole density p_s dependence of the 2DHG mobility. The key scattering mechanisms are surface roughness and misfit deformation potential, remote impurities are in general less relevant.
- (ii) We calculated the dependences on temperature of acoustic-phonon scattering and the total mobility from Figure 2 and Figure 3. We show that phonon scattering plays an important role in limiting the electron mobility in square QWs. We analyzed the behavior of the mobility for temperature values up to 100K.
- (iii) Our theory is able to well reproduce the recent experimental data about transport of electrons and holes in one-side doped square QWs.

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