Temperature-dependent transport properties of two-dimensional hole gas in Ge channel modulation-doped square quantum wells

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Abstract. We present a theoretical study of the transport properties of two-dimensional hole gas (2DHG) in Ge channel modulation-doped square quantum wells, with very high room-temperature drift mobilities. Within the variational approach, we obtain analytic expressions for the carrier distribution, and autocorrelation functions for various scattering mechanisms. The results were used to determine the hole mobility where only the relevant scattering processes, namely acoustic phonons (Deformation potential and Piezoelectric coupling), ionized impurity, surface roughness were considered. The partials and total mobility dependences on temperature were found. It is shown that acoustic phonon and surface roughness scattering are the dominant mechanism. The interpretation of these results is carried out and the scattering mechanisms limiting the 2DHG mobility in Ge quantum wells of SiGe heterostructure are discussed.

1. Introduction
Heterostructures containing strained Ge or SiGe quantum wells have received enormous attention within recent years due to their importance in device applications [1, 2, 3, 4, 5]. The systems show high hole mobilities and are potential candidates for replacing conventional p-Si metal oxide-semiconductor field effect transistors. The strained Ge channel modulation doped (MOD) heterostructures with very high hole mobilities have been reported by several groups. It has been known for many years that surface roughness scattering plays a dominant role in limiting the mobility at low temperatures in MBE grown samples [4, 6]. At temperatures higher than 150K, the acoustic phonon scattering begins to dominate and it is one of the most important mechanisms, along with the optical phonon scattering, limiting the room temperature hole mobility [2, 7]. The good agreement of fitting results with the 2DHG mobility at higher temperatures suggests that the mobility near room temperature in the strained Ge channel is indeed limited by the acoustic phonon scattering, optical phonon scattering and surface roughness scattering.

In the past few years some people [4, 8, 9] have presented a first successful attempt at giving a theory of the mobilities of carriers confined in a modulation-doped square quantum wells. We are able to explain the mobility of the one-side doped square quantum well dependence on carrier density and channel width. However, this investigation do not take into account mobility dependence on temperature.

Thus, the goal of this paper is to provide a theory of the main scattering mechanisms on the high-temperature transport properties of charge carriers in a single-side modulation
doped infinite square QW. We develop a variational approach to the description of quantum confinement in bent-band infinite square QWs. For Ge channel modulation-doped square quantum wells, we incorporate all possible scattering mechanisms, especially acoustic phonons (dominant at high temperatures). The paper is organised as follows. In the second section, we supply the theory for calculating the scattering mechanisms for Ge channel modulation-doped square quantum wells. In section 3, Results and discussion, comparison with the recent experimental data. Lastly, a conclusion is given in section 4.

2. Theory

We are now dealing with a heterostructures containing the Ge strained channel of single-side modulation-doped SiGe/Ge/SiGe square quantum wells, 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 confinement may be plausibly described by an asymmetric wave function as follows: [8]

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

with \(L\) as the channel width. Here, \(B\) and \(c\) are variational parameters to be determined.

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 \(\langle |U(q)|^2 \rangle\). Here is a two-dimensional Fourier transform of the unscreened scattering potential weighted with an envelope wave function,

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

Within the linear transport theory, the mobility \(\mu\) at very low temperatures is determined by the transport lifetime: \(\mu = e\tau/m^*\), with \(m^*\) as the in-plane effective mass of the carrier. The transport lifetime \(\tau\) limited by some disorder is represented (via scattering rate \(1/\tau\)) in terms of its autocorrelation function (ACF) as follows: [10]

\[
\frac{1}{\tau} = \frac{1}{(2\pi)^2 \hbar E_F} \int_0^{2k_F} dq \int_0^{2\pi} d\phi \frac{q^2}{(4k_F^2 - q^2)^{1/2}} \frac{\langle |U(q)|^2 \rangle}{\varepsilon^2(q)}. 
\]  

Here \(q = (q, \varphi)\) is the 2D momentum transfer due to a scattering event in the \(x-y\) plane (in polar coordinates): \(q = |q| = 2k_F \sin(\theta/2)\) with \(\theta\) as a scattering angle. The Fermi energy is given by \(E_F = \hbar^2 k_F^2/2m^*\), with \(k_F = k_F^{TF}\) as the Fermi wave number. The first subband carrier density \(p_s\) determined by the Fermi-Dirac distribution at finite temperatures is given by [11]

\[
p_s = \frac{k_B T m^*}{\pi \hbar^2} \ln[1 + \exp\left(\frac{E_F - E_0}{k_B T}\right)],
\]  

where \(E_0\) is the first subband energy, \(k_B\) is the Boltzmann constant and \(T\) the absolute temperature. The dielectric function \(\varepsilon(q)\) takes account of the screening of scattering potentials by the 2D carriers. As usual, this is evaluated within the random phase approximation, [12]

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

with \(q_s = 2m^* e^2/\varepsilon_L \hbar^2\) as the inverse 2D Thomas-Fermi screening length. The local field corrections are due to a many-body exchange effect, quantified by [13] \(G(q) = q/2\sqrt{q^2 + k_F^2}\).
The screening form factor \( F_S(q) \) takes account of the extension of the carrier state along the growth direction, defined by the wave function: [12]

\[
F_S(q) = \int_{-\infty}^{+\infty} dz \int_{-\infty}^{+\infty} dz' \zeta^2(z) \zeta^2(z') e^{-q|z-z'|}.
\] (6)

With the use of the wave function from eq. 1 we obtain the screening form factor for the 2DHG in Ge channel modulation-doped square quantum wells.

The holes in the Ge strained channel of modulation-doped SiGe/Ge/SiGe square QWs are expected to experience the following scattering sources: (i) acoustic phonons (AP), (ii) ionized impurity (II), (iii) surface roughness (SR) therefrom. The overall lifetime is determined by the ones for individual disorders according to the Matthiessen’s rule,

\[
\frac{1}{\tau_{tot}} = \frac{1}{\tau_{AP}} + \frac{1}{\tau_{SR}} + \frac{1}{\tau_{II}}.
\] (7)

2.1. Acoustic phonons (AP)
First, we will be dealing with scattering of the 2DHG at high temperature. It has been shown [14] 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. The momentum relaxation time due to acoustic-phonon scattering is given by [15]

\[
\frac{1}{\tau_{AP}} = \sum_{k'} W(k, k')(1 - \cos \vartheta),
\] (8)

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

Then, \( W(k, k') \) is given by [15]

\[
W(k, k') = \frac{2k_B T}{\hbar^2} \int_{-\infty}^{+\infty} dz \zeta(z) [M(q)]^2 \frac{1}{\omega_q S^2(q_{\perp})} |I(q_z)|^2 \delta(E_k - E_{k'}),
\] (9)

where \( q_z \) and \( q_{\perp} \equiv k - k' \) are the vertical and the horizontal components of the phonon wave vector, respectively, \( |M(q)| \) is the 3D scattering matrix element, \( S(q_{\perp}) \) is the static screening factor, \( I(q_z) \) is the overlap integral and \( \delta(E) \) is the Dirac delta function. The overlap integral is given by [15]

\[
I(q_z) = \int_{-\infty}^{+\infty} dz \zeta(z) e^{iq_z z} \zeta(z).
\] (10)

The scattering matrix elements for the deformation-potential (DP) and piezoelectric coupling (PZ) are, respectively, given by [15]

\[
|M(q)|^2 = \frac{D^2 \hbar \omega_q}{2c_l L^3},
\] (11)

and

\[
|M(q)|^2 = \frac{2\pi e^2 P^2 \hbar \omega_q}{\epsilon_0 q^2 L^3},
\] (12)

where \( D \) is the deformation potential constant, \( c_l \) is the longitudinal elastic constant, \( P \) the piezoelectric constant, \( L \) the sample volume, \( \omega_q \) is the frequency of the phonons in the state, \( \epsilon_0 \)
is the static dielectric constant $\varepsilon_0 = 12.91$, and $e$ the elemental charge. 

The static screening factor at finite temperature has been calculated to be:

$$S(q) = 1 + \frac{2\pi e^2 F_S(q)\Pi(q)}{\varepsilon_0 q},$$

(13)

$F_S(q)$ is defined by [8] with the wave function from Eq. (1), the calculation $F_S(q)$ of Eq. (6) is lengthy, but straightforward with the aid of the functions $\gamma_n$ and $\omega_n$ in Eqs. (14).

here, we defined the following mathematical functions [4]

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

(14)

The static polarizability at finite temperature is given by [15]

$$\Pi(q, T, E_F) = \frac{1}{4k_B T} \int_0^{+\infty} \Pi(q, 0, \xi') d\xi',$$

(15)

where $\Pi(q, 0, \xi')$, is the polarizability function at $T = 0K$, namely,

$$\Pi(q, 0, \xi') = \frac{m^*}{\pi\hbar^2} \left\{1 - \theta(q - 2k_F) \left[1 - \left(\frac{2k_F}{q}\right)^2\right]^{1/2}\right\},$$

(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. (16) to be unity.

2.2. Surface roughness (SR)

Next, we will be dealing with scattering of the 2DHG from a rough potential barrier. The scattering potential is due to roughness-induced fluctuations in the position of the barrier [12]. The autocorrelation function for surface roughness scattering in a square QW of an arbitrary depth was derived in Ref. [16]. The result reads as follows:

$$U_{SR}(q) = V_0|\xi|^2\Delta_q,$$

(17)

where $\Delta_q$ is a 2D Fourier transform of the roughness profile. The autocorrelation function for Surface roughness scattering in Ge channel modulation-doped square quantum wells is in Ref. [4].

2.3. Ionized impurities (II)

As well known, [11, 17] the relaxation time function for scattering from a random distribution of charged impurities is supplied by

$$\frac{1}{\tau_{II}} = \frac{4\pi\hbar N_I}{m^*k_B^2}\int_0^{2k} \frac{A_1(q)(e^{-2qL_s} - e^{-2qL_D})}{S^2(q)\sqrt{4k^2 - q^2}} dq,$$

(18)

with

$$A_1(q) = \left[\int_{-\infty}^{+\infty} |\xi|^2 e^{-qz^2} dz^2\right]^2.$$

(19)
The calculation of $A_1(q)$ with plausible wave function is given in Eq. (1) is lengthy, but straightforward with the aid of the functions $\gamma_n(x)$ in Eqs.(14), $A_1(q)$ is given by

$$\frac{1}{\tau_I} = \frac{N_1 L m_p}{p_s e I^2} \int_0^{t_{max}} dt A_1(t) \frac{e^{-2tL_s/L} - e^{-2tL_D/L}}{S^2(t,T)t \sqrt{t^2 + t_{max}^2 - t^2}}. \quad (20)$$

The total mobility is now written as [11, 15]

$$\frac{1}{\mu_{tot}} = \frac{1}{\mu_{AP}} + \frac{1}{\mu_{SR}} + \frac{1}{\mu_{II}} = \frac{1}{\mu_{DP}} + \frac{1}{\mu_{PZ}} + \frac{1}{\mu_{SR}} + \frac{1}{\mu_{II}}, \quad (21)$$

where $\mu_{tot} = e/m^* \tau_{tot}$.

3. Results and Discussion

In what follows, we apply the above-developed theory to understand the properties of room temperature transport in symmetrically modulated square QWs. In particular, we clarify the merit of symmetric doping over asymmetric doping. In order to illustrate this point, we study 2DHG in the Ge strained channel of an Si$_{1-x}$Ge$_x$/Ge/Si$_{1-x}$Ge$_x$ QW. As indicated, [18] for strained Ge on cubic [001] Si$_{1-x}$Ge$_x$ with Ge content $x = 0.7$, the potential barrier height for holes is rather large: $V_0 = 270$ meV. Thus, the assumption of infinite square QWs may be believably accepted as in earlier theories [19, 20].

For the numeric calculations we need some material parameters as input. We omit the small difference between the dielectric constants of the channel and barrier layers, using their average. For strained Ge, the out of-plane and in-plane hole effective masses are $m_z = 0.19 m_e$, $m^* \approx 0.1 m_e$ [21]. The elastic stiffness constants 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 [22].

In Figure 1, we consider a two-dimensional hole gas (2DHG) in the Si$_{1-x}$Ge$_x$/Ge/Si$_{1-x}$Ge$_x$ square QWs whose following physical parameters were taken elsewhere [11, 23]. Over the wide temperature range of $10 - 300$ K carriers in Ge strained channel modulation-doped square QWs are expected to experience the following scattering sources: acoustic phonons (Deformation potential-DP and Piezoelectric coupling-PZ), Surface roughness-SR. These mobility dependences on temperature for Ge channel modulation-doped structure are shown in Figure 1. As clearly observed from Figure 1, the total mobility decreased in the temperature values 10-300 K. The total phonon mobility (DP plus PZ) begins to contribute to the total mobility for $T > 20$. The acoustic phonon partial mobilities present a decay that will control the behavior of the total mobility for temperatures above 30K. At temperatures higher than 100K, the acoustic-phonon scattering begins to dominate and it is one of the most important mechanisms limiting the room-temperature hole mobility. The main scattering mechanisms are acoustic phonons and surface roughness, ionized impurity is in general less relevant.

Figure 2 shows the experimental data of the 2DHG mobility as a function of temperature obtained with holes in a Si$_{0.3}$Ge$_{0.7}$/Ge/Si$_{0.3}$Ge$_{0.7}$ square QW with a channel width $L = 75$ Å vs hole density $p_s = 1.5 \times 10^{12}$ cm$^{-2}$. The solid line refer to the total mobilities $\mu_{tot}$ limited by scattering from acoustic phonons, surface roughness, and ionized impurity. The experimental data are marked by circle [23]. The good agreement of fitting results with the 2DHG mobility at higher temperatures suggests that the mobility near room temperature in our strained Ge channel is indeed limited by the acoustic-phonon scattering and surface-roughness scattering.

4. Conclusions

To summarize, in the present paper we have developed a theory of room-temperature transport in Ge channel modulation-doped structure QWs.
Figure 1. Partials and total mobility dependencies on temperature for Ge strained channel modulation-doped square quantum wells.

Figure 2. Temperature-dependent Hall mobility of 2D hole gas in Ge channel modulation-doped square quantum wells.

(i) We calculated the dependencies on temperature of acoustic-phonon scattering and the total mobility from Figure 1 and Figure 2. We show that surface-roughness and acoustic-phonon scattering play dominant role in limiting the mobility at room temperatures. We analyzed the behavior of the mobility for temperature values up to 300 K.

(ii) Our results were compared with experimental data [23]. 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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5. References
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