CALCULATION OF INTERFACE ROUGHNESS SCATTERING-LIMITED ELECTRON MOBILITIES AT LOW TEMPERATURES IN GaAs AND InAs QUANTUM WELLS

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***Abstract**: In this paper, we present a study of the effects of interface roughness scattering-limited electron mobilities in GaAlAs/GaAs/GaAlAs and InGaSb/InAs/InGaSb quantum wells. We propose that interface roughness-related scatterings are generally key scattering mechanisms at low temperatures in heterostructures, especially thin quantum wells. Roughness is also shown to produce misfit deformation potential and misfit piezoelectric field as scattering sources in strained heterostructures. The analysis of our results clearly indicates that the significance of interface roughness scattering and, in particular, the influence of interface roughness correlation length and height is considerable. A comparison of our calculated results with published experimental data is shown to be in good agreement.*

***Keywords:** Interface roughness, scattering, correlation length, quantum wells, heterostructures.*

1. Introduction

It is well known [1] that transport properties of a two-dimensional electron gas (2DEG) in a semiconductor quantum well (QW) can be strongly affected by the quality of interfaces between the well and barrier layers. For any QW, interface roughness was shown [2, 3] to produce random fluctuations in the well width, which modulate the confinement energy and resulted in a scattering potential for the 2D motion of confined charge carriers. In recent years, a lot of investigations have been made to control and enhance the mobility of two-dimensional electrons (2DEGs). Some scattering mechanisms that limit the mobility of 2DEG have been studied, such as the ionized impurities scattering, the interface roughness scattering, the surface roughness scattering and the dislocation scattering [4]. In these scattering mechanisms, interface-roughness scattering (IRS) is known to limit carrier mobilities at low temperatures and the interface roughness and surface roughness scattering are sensitive to the sheet charge density of 2DEG.

In this paper, we calculated low temperatures mobilities in *GaAs/ GaAsAl* and *InGaSb/InAs* QWs as limited by the IRS by solving the associated Poisson equation for the Hartree potential. The interface profile is described by some roughness distribution in the in-plane. This is specified by two size parameters: a roughness amplitude Δ and a

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correlation length Λ. The former is the average height of roughness in the quantization direction. The latter is the size of a region in the in-plane, where the roughness at different points is correlated, so this defines whether the nature of roughness scatterings is of short-range or long-range.

2. Theoretical determinations

We consider a rectangular quantum well of width *L*. The wave function for the electrons is taken to be:

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

here, *B* and *c* are variational 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 [5] 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. The transport lifetime limited by some disorder is represented (via scattering rate 1/τ) in terms of its autocorrelation function (ACF) as follows:

$$\frac{1}{\tau} = \frac{1}{(2\pi)^2 \hbar E_F} \int_0^{2k_F} dq \int_0^{2\pi} d\varphi \frac{q^2}{(4k_F^2 - q^2)^{1/2}} \frac{\left\langle |U(q)|^2 \right\rangle}{\varepsilon^2(q)} \tag{2}$$

Here $q = (q, \varphi)$ is the 2D momentum transfer due to a scattering event in the *x-y* plane (in polar coordinates): $q = |q| = 2k_F \sin(\vartheta / 2)$ with ϑ as a scattering angle. The Fermi energy is given by $E_F = \hbar^2 k_F^2 / 2m^*$ with $k_F = \sqrt{2\pi p_s}$ as the Fermi wave number. In the ACF, $\left\langle |U(q)|^2 \right\rangle$, the angular brackets stand for an ensemble average. *U(q)* is the 2D Fourier transform of the unscreened scattering potential weighted with an envelop wave function,

$$U(q) = \int_{-\infty}^{\infty} dz |\zeta(z)|^2 U(q,z). \tag{3}$$

Next, we derive the ACF for surface roughness scattering. The weighted potential in wave vector space for SR scattering, e.g., from the top interface is given in terms of the local value of the wave function therein $\zeta_- = \zeta\left(z = -L/2\right)$ by

$$U_{SR}(q) = V_0 |\zeta_-|^2 \Delta_q, \tag{4}$$

where Δ_q is a 2D Fourier transform of the roughness profile:

$$\left\langle |\Delta_q|^2 \right\rangle = \pi \Delta^2 \Lambda^2 F_{SR}(q\Lambda), \tag{5}$$

Here, the roughness form factor $F_{SR}(q\Lambda)$ depends merely on Λ and is of some shape, E.g., Gaussian [1], power-law [6]… Δ is simply a scaling factor, so fixing the scattering strength, while Λ appears not only in the scaling combination $\Delta\Lambda$ but also in $F_{SR}(q\Lambda)$, so fixing both the strength and angular distribution of scattering. For theoretical analysis of the roughness effects [1-7], one must adopt some interface profile with Λ and Δ as input parameters. It is very important to have Λ and Δ individually in order to test the validity of the roughness model and the key scattering mechanisms adopted in the theory.

As indicated in [7], we derived a formula, which allows us to safely calculate the local value in Eq. (7) for any confinement with the use of some approximate wave function,

$$V_0 |\zeta_{\mp}|^2 = \frac{\hbar^2}{2m_z} |\zeta_{\mp}|^2 \tag{6}$$

$$\begin{aligned} V_0 \zeta_{\mp}^2 &= \left[E(c) - V_H(z_0) \right] \zeta^2(z_0) \pm \frac{\pi^2 e^2 B^2 p_s}{2\varepsilon_L} \\ &\times \Bigg\{ 4g'_+ \Gamma_1(\pm c, \pm\delta) + \frac{\pi B^2}{c^2 + \pi^2} \Bigg[\left(2c + \frac{\pi^2}{c} \right) \\ &\times \Gamma_1(\pm 2c, \pm\delta) + \frac{c}{2} \left[\Gamma_2(\pm 2c, \pm\delta) - \Gamma_0(\pm 2c, \pm\delta) \right] \\ &\mp \frac{\pi}{2} \left[\Omega_2(\pm 2c, \pm\delta) + 2\Omega_1(\pm 2c, \pm\delta) \right] \Bigg] \Bigg\}. \end{aligned} \tag{7}$$

The inverse of the transport lifetime τ_t is then given by:

$$\frac{1}{\tau_t} = \frac{1}{2\pi\hbar E_F} \int_0^{2k_F} dq \frac{q^2}{(4k_F^2 - q^2)^{1/2}} \frac{\left\langle |U(q)|^2 \right\rangle}{\varepsilon^2(q)} = \int_0^{\pi} p(\theta)(1 - \cos\theta) d\theta \tag{8}$$

The inverse of the quantum lifetime τ_q is then given by:

$$\frac{1}{\tau_q} = \frac{1}{2\pi\hbar E_F} \int_0^{2k_F} dq \frac{2k_F^2}{(4k_F^2 - q^2)^{1/2}} \frac{\left\langle |U(q)|^2 \right\rangle}{\varepsilon^2(q)} = \int_0^{\pi} P(\theta) d\theta. \tag{9}$$

Within the linear transport theory the mobility at very low temperatures is determined by $\mu = e\tau / m^*$ with m* as the in-plane carrier effective mass of the well layer. Then, the mobility can be expressed as

$$\mu_{t,q} = \frac{e}{m^*}\tau_{t,q} \tag{10}$$

Use Eqs. (3) - (12), we examine the ratio between any two different lifetimes (or mobilities) limited by the same roughness parameters Λ and Δ. Since Δ drops out of the ratio, this depends on Λ only, so denoted simply by $R_{t,q}(\Lambda)$. The ratio of the transport to quantum lifetimes, is defined for a quantum with a given value of the well width and carrier density [8],

$$R_q(\Lambda) = \frac{\tau_t(\mathrm{L}, \mathrm{p}_S; \Delta, \Lambda)}{\tau_q(\mathrm{L}, \mathrm{p}_S; \Delta, \Lambda)} = \frac{\mu_t(\mathrm{L}, \mathrm{p}_S; \Delta, \Lambda)}{\mu_q(\mathrm{L}, \mathrm{p}_S; \Delta, \Lambda)} \tag{11}$$

with L and p_S as parameters.

$$R_t(\Lambda) = \frac{\tau_t(\mathrm{L'}, \mathrm{p'}_S; \Delta, \Lambda)}{\tau_t(\mathrm{L}, \mathrm{p}_S; \Delta, \Lambda)} = \frac{\mu_t(\mathrm{L'}, \mathrm{p'}_S; \Delta, \Lambda)}{\mu_t(\mathrm{L}, \mathrm{p}_S; \Delta, \Lambda)} \tag{12}$$

with L, p_S and L', p'_S as parameters.

As observed from Eqs. (1) - (12), the mobilities and their ratio are specified by the envelope wave function. Thus, the mobilities ratio is fixed by the confinement model. If the barrier height and band-bending sources are known, this ratio is a well-defined function of the correlation length. On the other hand, its value is inferred from the data about the mobilities dependence on the well width and carrier density. So, one can get a separate estimation of Λ from the $R_{t,q}$ versus curve. With a fixed Λ, one can completely estimate Δ by a subsequent fit to some lifetime. As a result, one is able to individually evaluate the two size parameters of the roughness.

At low temperatures, we used the autocorrelation functions for *interface roughness scattering*. It has been shown [5] that *interface roughness* scattering plays an important role in limitting the electron mobility in III-V semiconducting compounds. In order to understand the calculated mobilities, it is useful to consider some of the intermediate results of the calculation such as the relaxation rates, the ratio between any two different lifetimes (or mobilities). The lifetimes and their ratio are specified by the envelop wave function. Thus, the lifetime ratio is fixed by the confinement model. If the barrier height and band-bending sources are known, this ratio is a completely-defined function of the correlation length, $R_{t,q}(\Lambda)$.

3. Results and Discussion

In order to display the behavior of the carrier mobility as a function of quantum wells parameters, we now apply our method to search for the roughness parameters in some experiments of interest. The *4.2 K* transport of electrons in a square QW of *AlGaAs/GaAs/AlGaAs* is dominated by Gaussian-profile SR scattering in the flat-band model [9,10]. The *10 K* transport of electrons in a square QW of *InGaSb/InAs/InGaSb* is dominated by Gaussian-profile SR scattering in the flat-band model [2], [11].

Now we apply the above method to search for the roughness parameters in some recent experiments [2], [10-12] .

It was indicated [2], [11] that the electrons in the InAs strained channel are charge carriers, whose transport at *4.2 K* is ruled by SR scattering and roughness-induced misfit deformation one. In equations (8) and (9) we derived the overall transport (τ_q) and quantum (τ_q) lifetimes limited by both scatterings from both interfaces of the QW.

We begin with showing the ratio between the transport (τ_q) and quantum (τ_q) lifetimes for electrons vs the correlation length Λ.

This ratio is plotted in Fig.1 versus the correlation length Λ for different well widths and electron densities from the measured data in SL2 [2]:

$$L = 53.6\,Å,\ p_S = 1.2\times10^{12}cm^{-2}, \varepsilon_L = 15.2 \text{ (dash-line);}$$

$$L = 53.6\,Å,\ p_S = 1.4\times10^{12}cm^{-2}, \varepsilon_L = 15.2 \text{ (solid line).}$$

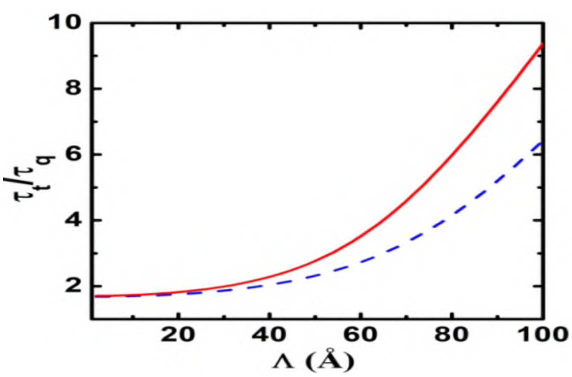

***Fig.1**. Transport lifetime ratios $R_q(\Lambda)$ for electrons in the InAs strained bent-band square QW vs the correlation length Λ for a given well width and different electrons densities*

As observed from Fig.1, the ratio between the transport lifetimes and quantum lifetimes is generally increased with the correlation length Λ at their values in use. The ratio with well widths $L' = 53.6\,Å$ and electron densities $p'_S = 1.5\times10^{12}cm^{-2}$ (solid line) has much higher value than the the ratio with well widths $L = 53.6\,Å$ and electron densities $p_S = 1.2\times10^{12}cm^{-2}$ (dash line).

From the measured data in [2], we consider the mobility for a two-dimensional electrons gas (2DEG) in the *InGaSb/InAs/InGaSb* square QWs in Fig. 2 for different well widths and electron densities: $L =$ 53.6 $Å$, $p_S = 1.2.10^{12}\,cm^{-2}$ and $L' =$ 72.7 $Å$; $p'_S = 1.5\times10^{12}\,cm^{-2}$.

As observed from Fig.2, the mobility for different well widths and electron densities is generally increased with the correlation length Λ at their values in use. The mobility with well widths $L' =$ 72.7 $Å$ and electron densities $p'_S = 1.5\times10^{12}\,cm^{-2}$ (solid line) has much higher value than the the mobility with well widths $L =$ 53.6 $Å$ and electron densities $p_S = 1.2\times10^{12}\,cm^{-2}$ (dash line).

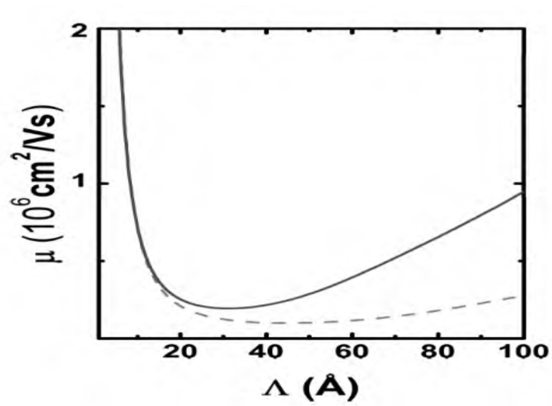

Fig.2. *Mobility* μ_t *for electrons in the InAs strained bent-band square QW vs the correlation length* Λ *for a given well width and different electrons densities*
$L =$ 53.6 $Å$; $p_s = 1.2\times10^{12}\,cm^{-2}$ *and* $L' =$ 72.7 $Å$; $p'_S = 1.5\times10^{12}\,cm^{-2}$

Fig.3 showing the the ratio of mobilities for a two-dimensional electrons gas (2DEG) in the *InGaSb/InAs/InGaSb* square QWs [2]. One gets $R_t(\Lambda) = 1.42$ and then $\Lambda = 54$ Å. This is nearly equal to $\Lambda = 54$ Å given previously [13].

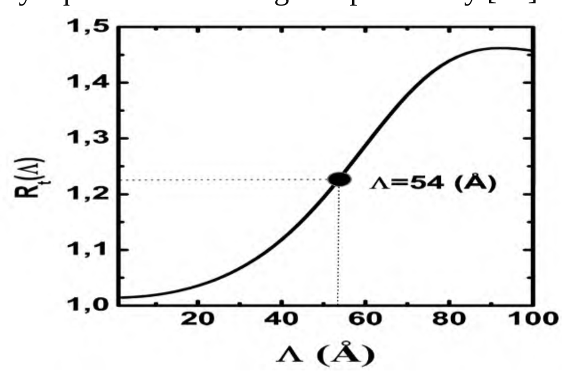

Fig.3. *The ratio of mobilities* $R_t(\Lambda)$ *for electrons in the InAs strained bent-band square QW vs the correlation length* Λ *for a given well width and different electrons densities. The ratio inferred from the measured data [13] are marked by circle.*

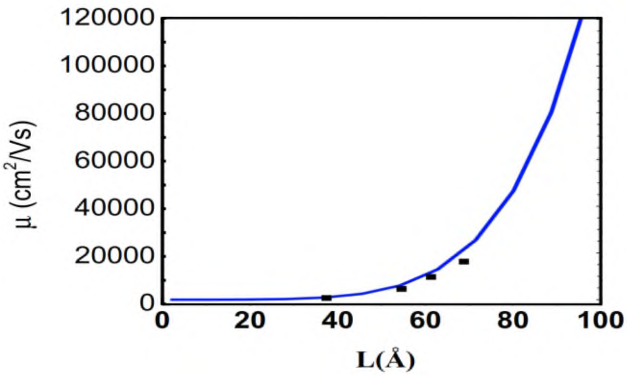

***Fig.4**. Mobilities of carriers in a AlGaAs/GaAs/AlGaAs square QW. The experimental data [10] are marked by square.*

It was shown in [10], [12] that the *4.2 K* transport of the electrons in the *GaAs* relaxed channel in *AlGaAs/GaAs/AlGaAs* square QW is ruled by SR scattering. We emphasize that the results provide a comprehensive road map of the μ-dependence on QW width for a variety of structures. The mobility in the GaAs square QW exhibits a dependence on the well width L which is different from that in the flat-band model. This is increased with a rise of L more slowly than the classic L^6 -law and is a nonmonotonic function of L.

4. Conclusions

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

(i) As clearly observed from (11), (12) we have proposed an efficient ratio for individual estimation of the two size parameters of interface profiles, based on the processing of transport data by a two-step fitting of: (i) Λ to some lifetime ratio and then Δ to some lifetime and mobilites. Our method is applicable to the ratio of any two lifetimes and mobilities which are different in parameters or quantum confinement, but limited by the same interface profile.

(ii) From the study of roughness-induced linewidths in intersubband absorption, we may speculate that the linewidth ratio is also a single-valued function of Λ. Since the roughness amplitude drops out of the ratio, this depends on the well width, sheet carrier density, and correlation length as shown explicitly. Our theory is able to well reproduce the recent experimental data about transport of electrons in a *AlGaAs/GaAs/AlGaAs* square QW.

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