Solid State Communications, Vol. 70, No. 3, pp. 371–374, 1989.
Printed in Great Britain.

0038–1098/89 $3.00 + .00
Pergamon Press plc

THEORY OF INTERFACE-ROUGHNESS INDUCED SUBBAND-EDGE ENERGY RENORMALIZATION IN THIN QUANTUM WELLS

A. Gold

Physik Department E16, Technische Universität München, D-8046 Garching, Federal Republic of Germany, and Groupe de Physique des Solides de l'Ecole Normale Supérieure, Université de Paris VII, tour 23, 2 place Jussieu, F-75251 Paris Cédex 05, France

(*Received* 24 *November* 1988 *by B. Mühlschlegel*)

We calculate the density of states of a two-dimensional electron gas in a quantum well with effective barrier height and width in the presence of interface-roughness scattering. The subband-edges energies of the subbands $n = 1, 2, \ldots$ shift with disorder. Analytical and numerical results for the renormalization of the subband-edge energies are presented for an unscreened and a screened potential. The effects of finite confinement are discussed.

IT IS important to understand the interfaces of quantum wells grown by molecular beam epitaxy. Some unexpected results have been found in thin quantum wells. The photoluminescence line width increases with decreasing quantum well width L [1]. A strong decrease in the mobility with decreasing L has been reported for thin quantum wells [2–4]. We have argued [3] that this anomaly is due to interface-roughness scattering and for the mobility we predicted the relation: $\mu \propto L^6$. Recent experimental results [4, 5] confirm the strong decrease of the mobility with decreasing quantum well width.

The band gap renormalization in quantum wells due to electron–electron interaction has been calculated [6, 7] and measured [8, 9]. In this paper we present a calculation on the band-gap renormalization and the shift of subband-edge energies due to disorder, which is induced by interface-roughness scattering.

We consider a two-dimensional electron gas in the lowest subband of a quantum well with a width L and with infinite barriers. The roughness of the quantum well interface is parameterized by the height Δ and the length Λ. A Gaussian-like decay of the fluctuations is assumed [10]. The random potential $U(\mathbf{q})$ due to this interface-roughness is written as [3]

$$\langle |U(\mathbf{q})|^2 \rangle = \frac{\pi^5}{m_z^2} \frac{\Delta^2 \Lambda^2}{L^6} e^{-q^2\Lambda^2/4}. \tag{1}$$

m_z is the mass perpendicular to the well. We assume that $\langle U(\mathbf{q} = 0) \rangle = 0$.

In a quantum well with infinite barriers the subband structure is given by $E_n = \pi^2 n^2 / 2 m_z L^2$. The fluctuation of the first subband energy due to fluctuations of the quantum well width is given by $dE_1 = -(\pi^2/m_z L^3)\, dL$.

The density of states is determined by the imaginary part of the one-electron Green's function $G(\mathbf{k}, z)$. As usual we express $G(\mathbf{k}, z)$ as

$$G(\mathbf{k}, z) = \frac{-1}{z - k^2/2m^* + \Sigma(\mathbf{k}, z)}. \tag{2a}$$

$\mathbf{k}$ is the wave vector and z is the complex energy of the quasiparticle (we use $\hbar = 1$). m^* is the electron mass parallel to the interface. $\Sigma(\mathbf{k}, z)$ is calculated in the selfconsistent Born approximation [11]:

$$\Sigma(\mathbf{k}, z) = 2 \sum_{\mathbf{q}} \langle |U(\mathbf{k} - \mathbf{q})|^2 \rangle G(\mathbf{q}, z). \tag{2b}$$

The factor 2 in equation (2b) is due to the two interfaces. We assume that both interfaces are parameterized by the same interface-roughness parameters. However, experimental results indicate that the two interfaces might be different under special growth conditions [12].

In the following we will neglect the k-dependence of the self-energy: $\Sigma(z) = \Sigma(\mathbf{k} = 0, z)$. For a discussion on the validity of this approximation, see [13]. For a short-range random potential ($\Lambda = 0$) the self-energy is independent of the wave number [13–16]. Then the "ultraviolet" divergency of the q-integral in equation (2b) is a result of the short-range random potential. Any realistic potential has a finite range q_c and the q-integral has a cutoff at a certain wave number q_c. We use $q_c = 2/\Lambda$ and we replace $\exp(-q^2\Lambda^2/4)$ by $\Theta(1 - q^2\Lambda^2/4)$ and $\Theta(x)$ is the unit step function. From equation (2) we then get for $\Sigma(z) =$

$\hat{\Sigma}(\hat{z})E_0$ [15]

$$\hat{\Sigma}(\hat{z}) = U_1^2 \ln\left(1 - \frac{1}{\hat{z} + \hat{\Sigma}(z)}\right) \tag{3a}$$

$$U_1 = \frac{\pi^2}{2}\frac{m^*}{m_z}\frac{\Delta\Lambda^2}{L^3}. \tag{3b}$$

$E_0 = 4a^{*2}R/\Lambda^2$ is the energy unit. $a^* = \varepsilon_L/m^*e^2$ and $R = m^*e^4/2\varepsilon_L^2$ are the Bohr radius and the effective rydberg, respectively. ε_L is the dielectric constant of the host lattice.

For a long-range random potential ($1/\Lambda = 0$) we get for the self-energy [17]

$$\Sigma(\mathbf{q}, z) = 2\pi^4 \frac{1}{m_z^2}\frac{\Delta^2}{L^6} G(\mathbf{q}, z). \tag{4}$$

Explicitly we derive the following expression (in reduced units with $\hat{q} = \Lambda q/2$):

$$\hat{\Sigma}(\hat{q}, \hat{z}) = (\hat{q}^2 - \hat{z})/2 + ((\hat{z} - \hat{q}^2)^2/4 - 2U_1^2)^{1/2}. \tag{5}$$

We have solved equation (3) to calculate the density of states. The energy $\delta\varepsilon_1$ defines the disorder induced shift of the conduction band edge to lower energies and is given by

$$\delta\hat{\varepsilon}_1 = \tfrac{1}{2} - (\tfrac{1}{4} + U_1^2)^{1/2} - U_1^2 \ln\left[\frac{U_1^2}{\frac{1}{2} + U_1^2 - (\frac{1}{4} + U_1^2)^{1/2}}\right]. \tag{6}$$

In the limits of small and large U_1 one gets $\delta\hat{\varepsilon}_1 = 2U_1^2 \ln U_1 + O(U_1^2)$ and $\delta\hat{\varepsilon}_1 = -2U_1 + 1/2 + O(1/U_1)$, respectively. The reason why $\delta\varepsilon_1$ is linear in U_1 for $U_1 \gg 1$ is because we used the dressed electron propagator ($\Sigma(z) \neq 0$) on the right hand side of equation (2b).

We restrict our results to $k_F\Lambda \ll 1$, k_F is the Fermi wave number. For the Fermi energy ε_F we find the relation $\varepsilon_F \ll E_0/4$. The relation $k_F\Lambda \ll 1$ is well satisfied in undoped or weakly doped quantum wells. We point out that in all reduced energy variables, which linearly depend on U_1, the Λ disappears in the real energy variables.

For long-range interface roughness potentials we get from equation (5) for the disorder induced shift of the conduction band edge $\delta\hat{\varepsilon}_1 = -2(1 + 2^{1/2})U_1$, which is the strong coupling result in mass-shell approximation.

Energy $\varepsilon_{1C} = \delta\varepsilon_1$ describes the shift of the conduction band edge with disorder. Of course, similar results (but with the hole masses) hold for the renormalization of the valence band edge, denoted by ε_{1V}. The disorder renormalized band-gap E_{GR} is expressed in terms of the gap of the clean material E_{G0} via

$$E_{GR} = E_{G0} - |\varepsilon_{1V}| - |\varepsilon_{1C}|. \tag{7}$$

In a recent work [5] the interface-roughness parameters have been determined by comparing mobility measurements on thin GaAs quantum wells (40 Å < L < 60 Å) with the theory of [3]: $\Delta \approx 2.4$ Å, $\Lambda \approx 65$ Å. In similar experiments [4] $\Delta = 3$Å and $\Lambda = 70$ Å have been found. With equation (6) we get $\varepsilon_{1C} = -35$ meV and -8 meV for $L = 50$ Å and 70 Å, respectively. This example shows that strong band gap renormalization effects are expected from interface-roughness scattering. Screening effects reduce these numbers. We mention that in the experiments of [4, 5] $k_F\Lambda \approx 1$.

Our calculation was done for a non-interacting electron gas. In this model the electrons are localized for arbitrary weak disorder because of weak localization effects [18]. Then, screening effects should be negligible. A complete picture of the localization phenomena in an interacting electron gas is missing [18]. We argued that a metal-insulator transition occurs in thin quantum wells because of the interface-roughness scattering [3].

In the most simple approximation in order to treat the electron–electron interaction effects we have to screen the random potential and we have to include the exchange and correlation contribution Σ_{xc} to the self-energy. Σ_{xc} for quantum wells was calculated before [6, 7] and will be neglected: $\Sigma_{xc} = 0$. Σ_{xc} gives rise to a rigid shift of the band and this shift must be added to the disorder induced shift. For the screening function we use $\varepsilon(q) = 1 + q_s/q$ [19]. q_s is the Thomas–Fermi wave number. In units of $2/\Lambda$ we find $\hat{q}_s = g_v\Lambda/a^*$. g_v is the valley degeneracy. The self-consistent Born approximation is expressed as

$$\hat{\Sigma}(\hat{z}) = -2U_1^2 \int_0^1 d\hat{q}\, \frac{\hat{q}^3}{(\hat{q}_s + \hat{q})^2}\, \frac{1}{\hat{z} - \hat{q}^2 + \hat{\Sigma}(\hat{z})}. \tag{8}$$

We have solved equation (8) and the result for $\delta\varepsilon_1$ is shown in Fig. 1. As expected we find that screening reduces the effects of the interface-roughness scattering.

Equation (1) describes the interface-roughness scattering in the lowest subband $n = 1$ of a quantum well with infinite barriers. For a quantum well with finite barriers the wave function penetrates into the barriers and the interface-roughness scattering potential becomes weaker as in case of infinite barriers. The interface-roughness scattering potential for the n-th subband and finite barriers is given by

$$\langle U_n(\mathbf{q})U_m(-\mathbf{q})\rangle = \langle|U(\mathbf{q})|^2\rangle F_n(V, L)F_m(V, L). \tag{9}$$

Equation (9) describes the scattering potential for intersubband scattering ($n \neq m$) and for intrasubband scattering ($n = m$). Interface-roughness scattering is strongly increased in higher subbands.

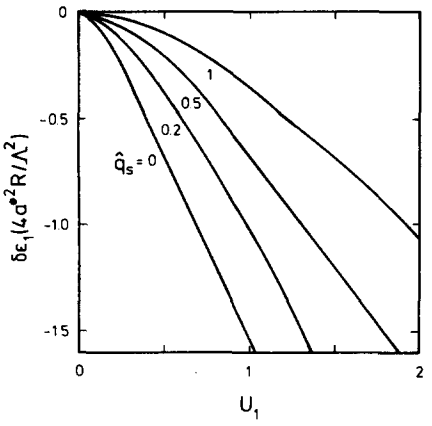

Fig. 1. $\delta\varepsilon_1$ vs disorder U_1 for the screened interface roughness potential according to equation (8) and various values of the screening parameter $\hat{q}_s$.

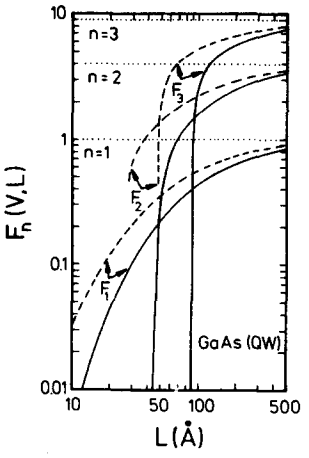

Fig. 2. $F_n(V, L)$ vs quantum well width L for V = 300 meV (solid lines), V = 1000 meV (dashed lines), and n = 1, 2, 3. The dotted lines are for $V \to \infty$.

The functions $F_n(V, L)$ are determined by the wave function at the interface [20]. We calculate $F_n(V, L)$ for a quantum well with barrier height V and width L. Band-bending effects are neglected. For n = 1, 3, 5 . . one gets

$$F_n(V, L) = \frac{4}{\pi^2} \frac{(1 - m_b/m_z)y^2 \sin^2(y) + C* \cos^2(y)}{1 + \dfrac{\sin(2y)}{2y} + \dfrac{m_z}{m_b} \dfrac{\cos^2(y)}{y \operatorname{tg}(y)}} \tag{10a}$$

and y ($\pi(n - 1)/2 < y < \pi n/2$) is defined by the solution of

$$y * \operatorname{tg}(y) = (C - y^2)^{1/2} * (m_z/m_b)^{1/2} \tag{10b}$$

and

$$C = \frac{1}{4} \frac{m_z}{m^*} \frac{L^2}{a^{*2}} \frac{V}{R}. \tag{10c}$$

For n = 2, 4, 6. . we get

$$F_n(V, L) = \frac{4}{\pi^2} \frac{(1 - m_b/m_z)y^2 \cos^2(y) + C* \sin^2(y)}{1 - \dfrac{\sin(2y)}{2y} - \dfrac{m_z}{m_b} \dfrac{\sin^2(y)}{y \operatorname{ctg}(y)}} \tag{11a}$$

and y ($\pi(n - 1)/2 < y < \pi n/2$) is defined by the solution of

$$-y/tg(y) = (C - y^2)^{1/2} * (m_z/m_b)^{1/2}. \tag{11b}$$

For the electron mass in the barrier m_b we use m_b = 0.067 + 0.071x. The effective height of the barrier V is given by the height of the barrier V_0 and the Fermi energy: $V = V_0 - \varepsilon_F$. We used V_0 = 1.04 eV $* x$. $F_n(V, L)$ for n = 1, 2, and 3 is shown in Fig. 2 for a confining energy V = 300 meV, which is a realistic value for $Al_xGa_{1-x}As/GaAs/Al_xGa_{1-x}As$ quantum wells (a^* = 103 Å, R = 5.56 meV) with $x \approx 0.3$. The dashed lines are for V = 1000 meV, a realistic value for the system AlAs/GaAs studied in [4]. For $V \to \infty$ we get $F_n(V, L) = n^2$, see the dotted lines in Fig. 2. The strong decrease of $F_n(V, L)$ for $n \geqslant 2$ at a certain quantum well width is due to the fact that there the binding energy goes to zero.

Equations (6, 8) and Fig. 1 can be used to estimate the band-gap renormalization and the subband-edge energies in the presence of disorder, however, U_1 must be replaced by

$$U_n(V, L) = U_1 * F_n(V, L). \tag{12}$$

The decrease of $F_1(V, L)$ with decreasing quantum well width ($F_1(V, L) \propto L^\alpha$ in some small range of L ($L_1 < L < L_2$)) changes the power law for the mobility to $\mu \propto L^{6-2\alpha}$.

In Fig. 3 we show the shift of the subband-edge energies of the first ($\delta\varepsilon_1$) and second subband ($\delta\varepsilon_2$) versus quantum well width for GaAs quantum wells and confining potential V = 1000 meV. The dashed lines represent subband-edge energies in the presence of an unscreened interface-roughness scattering (Δ = 3 Å, Λ = 60 Å). The solid lines are for a screened interface-roughness scattering potential. The effects of disorder are stronger for the higher subbands and for an unscreened potential. The subband-edge energies, measured from the bottom of the quantum well, increase with decreasing width. With no disorder present the energy of the first subband-edge is 70 meV for L = 70 Å and 610 meV for L = 10 Å. The energy of the second subband-edge is 280 meV for L = 70 Å and 870 meV for L = 30 Å.

In conclusion, we have shown that in thin quantum wells the interface-roughness scattering renormalizes

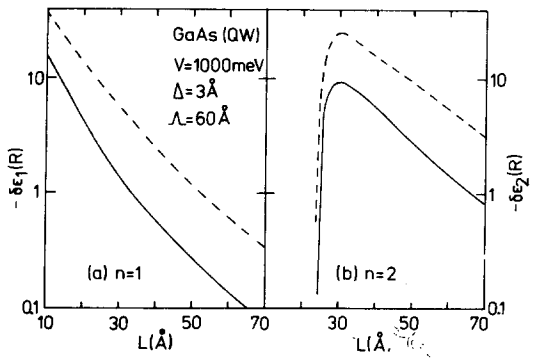

Fig. 3. Energy shifts of the first ($\delta\varepsilon_1$, $n = 1$) and second ($\delta\varepsilon_2$, $n = 2$) subband-edge versus well width for confining potential $V = 1000$ meV. The dashed lines represent the shift of the subband-edge energies of the first and the second subband in the presence of unscreened interface-roughness scattering. The solid lines are for a screened interface-roughness scattering potential. Energies are measured from the bottom of the subbands with no disorder. Intersubband scattering is neglected.

the conduction band edge and that the band-gap energy and the subband-edge energies are reduced. Undoped quantum wells are favourable to measure these effects. Then an unscreened interface-roughness potential has to be considered. Screening and finite confinement reduces the expected effects. Because of the strong dependence of the interface-roughness scattering potential on the quantum well width, $U_n \approx -1/L^3 * F_n(V, L)$, the discussed effects might be measurable in thin quantum wells with large barriers.

Acknowledgement —I thank R. Gerhardts for a helpful discussion concerning long-range random potentials. This work has been supported in part by the "Ernst von Siemens Stipendium (Munich)" and the "Deutsche Forschungsgemeinschaft (Bonn)".

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