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METAL INSULATOR TRANSITION DUE TO SURFACE ROUGHNESS SCATTERING IN A QUANTUM WELL

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We calculate the critical width a_c for a quantum well structure as function of the two-dimensional electron density. For $a > a_c$ the electron gas has a finite dc conductivity at temperature zero, and for $a < a_c$ the dc conductivity is zero. Homogeneous background doping, remote doping, and surface roughness scattering are considered. Due to surface roughness we find a strong increase of a_c at high electron concentration, in novel contrast to heterostructures. Explicit results are presented for GaAs and InAs quantum wells and compared with experimental results. Experiments are suggested to test the predictions of the localization theory.

THE PROBLEM OF electron localization in a random potential is a controversial one. There exists some agreement that a non-interacting electron gas at temperature zero is localized for arbitrarily weak disorder due to the so-called $2k_F$ scattering [1]. For an interaction electron gas the localization problem is unsolved [2].

In the scaling approach of Finkelstein [3], the conductivity scales to a finite conductivity and no mobility edge was found there.

Another approach, based on the diffusive motion of the electrons, was formulated by Gold and Götze [4]. They generalized the localization theory for a non-interacting electron gas [5] within the random phase approximation to an interacting electron gas. A metal insulator transition (MIT) in two dimensions was found at a finite amount of disorder. The disorder was assumed to be due to charged impurities. When the calculated phase diagram for the MIT was compared with experimental data on silicon metal oxide semiconductor systems [6], a very good agreement was established [4].

In this paper we generalize this localization theory to quantum wells and we discuss the scattering due to homogeneous distributed bulk impurities, due to a sheet of impurities parallel to the electron gas, and due to surface roughness scattering. In heterostructures and metal oxide semiconductor systems the disorder due to surface roughness increases with increasing electron density, because the electrons are pushed more strongly to the interface [7]. For the same reason the screening properties of the electron gas increase and a very rough surface is necessary to get localization at high electron density [8]. In quantum wells the disorder due to surface roughness scattering is independent of the electron density. Furthermore, the quantum well thickness can be controlled during fabrication, and in thin quantum wells the surface roughness scattering may become very strong. It is the aim of this paper to point out that localization effects due to surface roughness scattering can be studied in thin but realistic quantum well structures. Quantitative predictions on the MIT in such systems are given for the first time.

We consider a quantum well structure in the z-direction, infinite barriers are at $z = 0$ and $z = a$. The electrons in the quantum well are free to move in the xy-plane. In the z-direction the envelope wavefunction is given by the quantum well width a via

$$\psi(z) = \begin{cases} 0 & z < 0 \\ \sqrt{\frac{2}{a}} \sin\left(\frac{\pi z}{a}\right) & 0 \leqslant z \leqslant a \\ 0 & z > a \end{cases} \tag{1}$$

Here one subband is considered.

Three kinds of disorder are expected to be relevant in such systems. First we assume disorder due to homogeneously distributed bulk impurities of a (three-dimensional) density N_B. The random potential $U(q)$ for wavenumber q is given by

$$\langle |U_1(q)|^2 \rangle = N_B a \left(\frac{2\pi e^2}{\epsilon_L} \frac{1}{q}\right)^2 F_B(q). \tag{2a}$$

ϵ_L is the background dielectric constant and $F_B(q)$ is a form factor due to the finite width of the quantum well [7]. Explicit results will be published elsewhere [9]. Second we take into account disorder due to a two-dimensional sheet of impurities in the xy-plane at $z = z_i$ with density n_i

$$\langle |U_2(q)|^2 \rangle = n_i \left(\frac{2\pi e^2}{\epsilon_L} \frac{1}{q}\right)^2 F_{RD}(q, z_i)^2. \tag{2b}$$

F_{RD} (for remote doping) is again a form factor due to a

and the finite distance between the electrons and the impurities. Third we account for the surface roughness scattering at $z = 0$ and $z = a$. Following Prange and Nee [10] (see also [7] and [11]) one gets

$$\langle |U_3(q)|^2 \rangle = \frac{2\pi^5}{a^6} \frac{1}{m_z^2} (\Delta\Lambda)^2 e^{-q^2\Lambda^2/4}. \tag{2c}$$

The roughness is characterized by the height Δ and the length Λ of the Gaussian fluctuations of the interface. m^* is the transport mass and m_z is the mass perpendicular to the interface.

The electron–electron interaction is treated in random phase approximation generalized by local field corrections $G(q)$. The dielectric constant $\epsilon(q)$ of the electron gas is given by

$$\epsilon(q) = 1 + V(q)[1 - G(q)]X^0(q). \tag{3a}$$

Due to the finite thickness of the quantum well the Coulomb potential is generalized to

$$V(q) = \frac{2\pi e^2}{\epsilon_L} \frac{1}{q} F_c(q). \tag{3b}$$

$G(q)$ is the Hubbard correction [12] and $X^0(q)$ is the polarizability of the electron gas [13].

According to [5] the MIT is characterized by

$$A = 1, \tag{4a}$$

and [4]

$$A = \frac{1}{4\pi n^2} \int_0^\infty dq q \frac{\langle |U(q)|^2 \rangle}{\epsilon(q)^2} X^0(q)^2. \tag{4b}$$

n is the electron density. If we take into account the various scattering mechanisms, we neglect correlations between them and write

$$\langle |U(q)|^2 \rangle = \sum_{i=1}^{3} \langle |U_i(q)|^2 \rangle. \tag{4c}$$

In the following we discuss equation (4) for the various scattering mechanisms. Numerical results are presented for GaAs and InAs quantum wells. With g_v as the valley degeneracy we use for GaAs $g_v = 1$, $\epsilon_L = 12.8$, and $m^* = m_z = 0.067\, m_e$. m_e is the free electron mass. For InAs we use $g_v = 1$, $\epsilon_L = 15$, and $m^* = m_z = 0.037$.

We estimate the parameter A for homogeneous background scattering as follows. We use $X^0(q) = \rho_F \theta(2k_F - q)$, ρ_F is the (two-dimensional) density-of-states, $\epsilon(q) = q_s/q$, q_s is the screening wavenumber, and $F_b(q \to 0) = 1/qa$. Then we get

$$A_1 = \frac{1}{(2\pi g_v)^{1/2}} \frac{N_B}{n^{3/2}} \qquad 2k_F \ll q_s. \tag{5}$$

For $A_1 = 1$ we find for $N_D = 10^{17}$ cm^{-3} and $g_v = 1$ a crictical electron density $n_c = 1.2 \times 10^{11}$ cm^{-2}. For

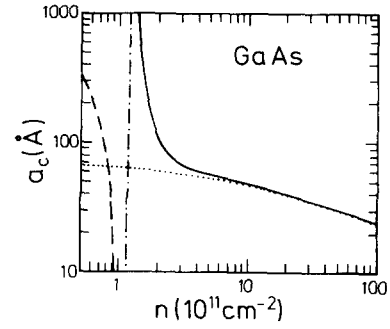

Fig. 1. Critical quantum well width a_c vs density according to equation (4) as the full line. The dotted line is for surface roughness scattering ($\Delta = 6$ Å, $\Lambda = 30$ Å), the dashed line is for remote doping ($n_i = n$, $z_i = a_c/2$) and the dashed dotted line is for background doping ($N_B = 10^{17}$ cm^{-3}).

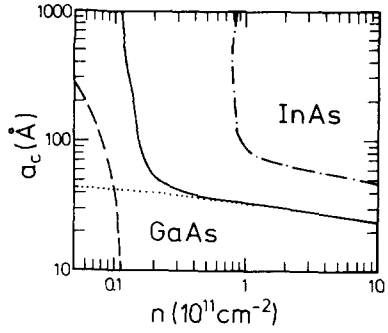

Fig. 2. Critical quantum well width a_c vs density according to equation (4) as full line for GaAs. The dotted line is for surface roughness scattering ($\Delta = 2$ Å, $\Lambda = 10$ Å) and the dashed line is for remote doping ($n_i = n$, $z_i = -100$ Å). The line for background doping ($N_B = 10^{15}$ cm^{-3}) is not shown. The dashed dotted line is for InAs and surface roughness scattering ($\Delta = 6$ Å, $\Lambda = 30$ Å) and homogenous background doping ($N_B = 10^{17}$ cm^{-3}).

$n > n_c$ the system is a conductor, but for $n < n_c$ the d.c. conductivity is zero, the system is an insulator. For $N_D = 10^{15}$ cm^{-3} and $g_v = 1$ one gets $n_c = 5.4 \times 10^9$ cm^{-2}. Numerical results for the critical quantum well width a_c vs density for GaAs and $N_D = 10^{17}$ cm^{-3} are shown in Fig. 1 as the dashed dotted line. For $a > a_c$ the system is metallic, for $a < a_c$ the system is an insulator.

One can also show that for remote impurity scattering with $a \to 0$ and $z_i = a/2$ one gets

$$A_2 = \frac{g_v^3}{\pi^{1/3} 3^{1/2} g} \frac{n_i}{n} \left(\frac{1}{na^{*2}}\right)^{4/3}. \tag{6a}$$

a^* is the Bohr radius. For $n_i = n$ and $A_2 = 1$ we reformulate equation (6a) into a Mott criterium [14]

$$n_c^{1/2} a^* = 0.309. \tag{6b}$$

One expects that a finite quantum well would increase the metallic phase and a crossover to a three-dimensional

behavior is simulated. This is shown in Fig. 1 as the dashed line. If $z_i < 0$ the metallic phase should increase drastically in comparison to equation (6b). Numerical results are shown in Fig. 2 as the dashed line (compare with Fig. 1). $z_i = -100$ Å is used there.

For surface roughness scattering we get with $X^0(q) = \rho_F \theta(2k_F - q)$, $2k_F \Lambda \ll 1$, and $\epsilon(q) = 1 + q_s/q$

$$A_3 = 2\pi^3 \frac{\Delta^2 \Lambda^2}{a^6} \left(\frac{m^*}{m_z}\right)^2 \begin{cases} g_v/n & 2k_F \gg q_s \\ a^{*2}/g_v^2 & 2k_F \ll q_s \end{cases} . \quad (7)$$

Numerical results for $A_3 = 1$ are shown in Figs. 1 and 2. For GaAs and $\Delta = 6$ Å and $\Lambda = 30$ Å we get from equation (7) in the case $2k_F \ll q_s$ a critical quantum well thickness $a_c = 63$ Å. If we use the case $2k_F \gg q_s$ we get for $n = 10^{12}$ cm^{-1} $a_c = 52$ Å. Numerically we find 48 Å, see Fig. 1.

For all three scattering mechanisms the MIT line is shown in Fig. 1 and Fig. 2 as full lines. In Fig. 1 the MIT is at low density dominated by homogeneous background doping ($N_B = 10^{17}$ cm^{-3}) and at high density by surface roughness scattering. In Fig. 2 the MIT at low density is determinated by remote doping ($N_B = 10^{15}$ cm^{-3}). We mention that a_c for surface roughness scattering depends only weakly on the parameters Δ and Λ: $a_c \propto (\Delta\Lambda)^{1/3}$.

The dashed dotted line in Fig. 2 is for InAs for homogeneous background doping and surface roughness scattering. For $n = 0.85 \times 10^{11}$ cm^{-1} one gets as function of a a very interesting feature. Two phase transitions occur by lowering a. At $a = a_{c_1} = 1000$ Å a transition from an insulator to a metal occurs due to the homogeneous background doping, while at $a = a_{c_2} = 120$ Å a transition from a metal to an insulator occurs due to an increasing insulating phase because of surface roughness scattering. The range $a_{c_2} > a$ may be interpreted as the reentrance of an insulator phase. In experiment (at finite temperature) the reentrance effect should be seen as a non-monotonic behaviour of the mobility versus quantum well thickness.

According to equation (2c) the mobility μ for surface roughness scattering depends strongly on the quantum well thickness: $\mu \propto a^6$. In Fig. 3 we show the mobility versus a for InAs within our selfconsistent theory [4] as the full line for $\Delta = 6$ Å, $\Lambda = 30$ Å and as the dashed dotted line for $\Delta = 2$ Å, $\Lambda = 10$ Å for surface roughness scattering and homogenous background doping with $N_B = 10^{17}$ cm^{-3}. The dashed and dotted lines are calculated by neglecting multiple scattering effects. For the full line the MIT occurs at $a_c = 49$ Å. For great quantum well thickness the mobility is nearly independent of a and is dominated by the background doping.

Such a behaviour of μ vs a has been found recently

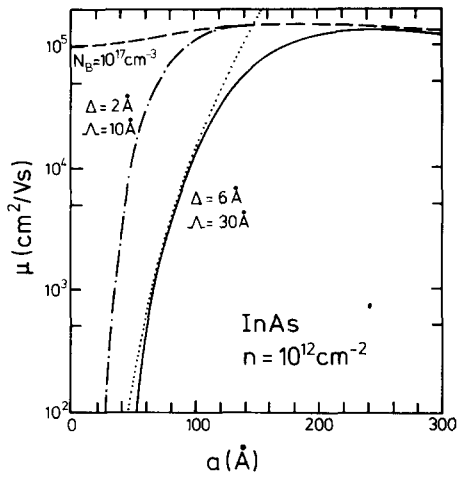

Fig. 3. Mobility vs quantum well thickness according to our selfconsistent theory [9] for surface roughness scattering and homogenous background doping ($N_B = 10^{17}$ cm^{-3}) as full and dashed dotted lines. For the dashed line (background doping) and for the dotted line (surface roughness scattering) multiple scattering effects are neglected.

in experiments [15] on quantum wells realized in GaSb/InAs/GaSb structures. But in this system also the electron density is reduced for decreasing quantum well width. This comes from the fact, that with decreasing a the energy of the ground state of the quantum well shifts to higher energy and this leads to a monotonic reduction of the electron density. In experiment the mobility reduction because of the decrease of a is much stronger than the reduction of the density and occurs at 70 Å [15]. An additional decrease of the electron density with decreasing quantum well thickness would sharpen the mobility increase in our theory, too. So we conclude, that the experimental results are at least a strong evidence for the importance of surface roughness scattering according to our theory and more experiments on this quantum wells should be done. We mention that we believe the mobility for the experiment of [15] for $a > 100$ Å is dominated by homogenous background doping, because μ does not depends on a. Impurities at the interface of the quantum well, as suggested in [15], give a stronger a dependence of the mobility than found in experiment [9].

In conclusion we have calculated the critical quantum well thickness for the metal insulator transition as function of electron density for homogenous background scattering, remote impurity scattering and surface roughness scattering for the first time. The importance of the surface roughness scattering has been demonstrated and a reentrance behaviour of the insulating phase has been found. It has been shown, that recent experiments on the mobility variation with the quantum

well width in InAs support our model. The predictions of our theory can and should be tested in experiments.

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