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Interface Roughness Fractality Effects on the Electron Mobility in Semiconducting Quantum Wells

G. PALASANTZAS (a), J. BARNAŚ (b), and L. J. GEERLIGS (a)

(a) *Department of Applied Physics, Delft University of Technology, Lorentzweg 1, NL-2628 CJ Delft, The Netherlands*

(b) *Magnetism Theory Division, Institute of Physics, Adam Mickiewicz University, ul. Umultowska 85, PL-61-614 Poznań, Poland*

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The influence of interface electron scattering on electron mobility in semiconducting quantum wells is analyzed theoretically in the Born approximation. The interface roughness is assumed to be random self-affine fractal characterized by roughness exponent H , correlation length ξ , and rms amplitude Δ . In particular, the ratio of electron mobilities for the Fermi level slightly above and below the second miniband edge (or for the well width above and below a critical width d_c for a constant areal electron density) is calculated. It is shown that the correlation length ξ and roughness exponent H have pronounced effects on electron mobility.

1. Introduction

Electrical conductivity σ of ultra-thin metal-like films (e.g., CoSi_2) follows the universal power-law with film thickness d ; $\sigma \propto d^c$ ($c \approx 2.3$) [1, 2]. For semiconducting films a similar law with $c \approx 6$ has been found [2, 3]. Both results hold in the limit $k_F \xi \ll 1$, with k_F the Fermi wavevector and ξ the roughness in-plane correlation length. In the opposite limit, $k_F \xi \gg 1$, the roughness correlation function plays a significant role and the mean variation of σ with film thickness can no longer be approximated by a power law [4]. However, one should note that the limit $k_F \xi \gg 1$ is not properly described by the Born approximation [5]. Apart from this, the roughness fractality, described by the roughness exponent H , has been recently shown to have significant influence on the film conductivity [6].

In metal–oxide–semiconductor inversion layers with high electron density ($> 10^{-2} \text{ nm}^{-2}$), the low temperature mobility of a two-dimensional electron gas is dominated by interfacial scattering [7]. Although, in single-heterojunction systems, like AlGaAs/GaAs , the interface roughness scattering can have rather small influence on the carrier mobility due to loose electron confinement [8], the situation is different in thin quantum wells, where small interface roughness leads to strong electron scattering and gives the dominant contribution to electrical resistivity. In fact, in GaAs quantum wells bounded on both sides by AlGaAs the roughness scattering becomes important for well thickness less than 10 nm [4, 9]. Similar influence of the interface roughness on electronic transport was also found in other systems, e.g. in HgTe/CdTe superlattices [10].

Fishman and Calecki [4] have shown that the form of roughness correlation function has significant influence on electron mobility, and consequently also on the ratio of electron mobilities for the Fermi level slightly below and above the edge of second

miniband. More precisely, in the limit $k_F \xi \ll 1$ the mobility ratio acquires a constant value (≈ 5) which is independent of the form of correlation function, while for $k_F \xi > 1$ it becomes high sensitive to the correlation form. In fact, the mobility ratio for the Gaussian correlation function $C(r) \sim \exp(-r^2/\xi^2)$ was found to be significantly different from the mobility ratio for simple exponential correlations $C(r) \sim \exp(-r/\xi)$; being typically larger in the former case for moderate correlation lengths (smaller than half the critical width above which the Fermi level crosses the second miniband) [4]. Recently, the effects of the exponential form $C(r) \sim \exp(-r/\xi)$ were examined by Kruithof et al. [11], who showed that in the low electron density regime the electron mobility was better described by such a correlation form than by the Gaussian correlation function. Apart from this, high resolution transmission electron microscopy on Si/SiO₂ interfaces as well as scanning tunneling microscopy and atomic force microscopy on quantum wells proved that the form of height–height correlation function is not Gaussian but rather simple exponential [12].

The correlation forms mentioned above can be considered as special cases of interfaces with the fractality exponents $H = 1$ and 0.5 , if they are viewed in terms of the stretched exponential correlation function $C(r) \sim \exp[-(r/\xi)^{2H}]$ used in the past to model random rough surfaces [13]. This indicates that the interface fractality can have significant impact on electron transport properties of quantum wells. However, the stretched exponential correlation function yields in the limit $H = 0$ the trivial behaviour $C(r) \sim \text{const}$, instead of logarithmic roughness. Therefore, the influence of interface fractality degree on the electron mobility in semiconducting quantum wells requires more detailed analysis for the whole range of the roughness exponents, $0 \leq H \leq 1$ (from the logarithmic to power-law roughness). This problem is addressed in the present paper, which is organized as follows. In Section 2 we present basic theoretical formulas used to calculate the film conductivity. A model self-affine interface is described in Section 3. Section 4 presents results for the mobility ratio in a quantum well, when only interface scattering is included. Summary and final conclusions are contained in Section 5.

2. Conductivity of a Thin Film

Consider a thin semiconducting quantum well with two boundaries described by $z = -d/2 + h_-(\mathbf{r})$ and $z = d/2 + h_+(\mathbf{r})$, where the axis z is assumed to be normal to the film plane. We assume that the roughness is described by single-valued random functions $h_+(\mathbf{r})$ and $h_-(\mathbf{r})$ of the in-plane position vector $\mathbf{r} = (x, y)$. Apart from this, we assume that the interface roughness is isotropic, so that the height–height correlation function $C_{\pm}(r) = \langle h_{\pm}(\mathbf{r}') h_{\pm}(\mathbf{r}'') \rangle$ depends only on the relative distance $r = |\mathbf{r}' - \mathbf{r}''|$. Taking into account electron scattering due to interface roughness only, one finds in the Born approximation the following formula for the film conductivity [2]:

$$\sigma(d) = \frac{e^2 \hbar^3}{m^2 d} \sum_{\nu=1}^N \sum_{\nu'=1}^N k_{\nu}^2 k_{\nu'}^2 [C^{-1}]_{\nu\nu'}, \quad (1)$$

where the matrix elements $C_{\nu\nu'}$ are determined by inter-miniband and intra-miniband transitions, and are given by

$$C_{\nu\nu'} = \delta_{\nu\nu'} \sum_{\beta=+,-} \left[A_{\nu}^{\beta} k_{\nu}^2 \sum_{\mu=1}^N A_{\mu}^{\beta} F_{\mu\nu}^{\beta(1)} - A_{\nu}^{\beta} A_{\nu'}^{\beta} k_{\nu} k_{\nu'} F_{\nu\nu'}^{\beta(2)} \right]. \quad (2)$$

In Eq. (2) $F_{\nu\nu'}^{\beta(1)}$ and $F_{\nu\nu'}^{\beta(2)}$ are defined as

$$F_{\nu\nu'}^{\beta(1)} = \int_0^{2\pi} d\theta \langle |h_\beta(k_{\nu\nu'})|^2 \rangle \quad (3a)$$

and

$$F_{\nu\nu'}^{\beta(2)} = \int_0^{2\pi} d\theta \langle |h_\beta(k_{\nu\nu'})|^2 \rangle \cos \theta, \quad (3b)$$

where $k_{\nu\nu'} = (k_\nu^2 + k_{\nu'}^2 - 2k_\nu k_{\nu'} \cos \theta)^{1/2}$, and $\langle |h_\beta(k)|^2 \rangle$ is the Fourier transform of the height–height correlation function $C_\beta(r)$ (for $\beta = +$ and $-$). Apart from this, in Eq. (1) N is the number of occupied minibands, while $k_\nu = [(2m/\hbar^2)(E_F - E_\nu)]^{1/2}$, with E_F and E_ν standing for the Fermi energy and the ν -th discrete level (miniband edge), respectively. Finally, the constants A_ν^β in Eq. (2) are determined by the confining potential and the wavefunctions taken at the β -th interface.

Since our main objective is the analysis of roughness fractality, we restrict our consideration to the limit of infinite confining potential. The influence of the height of confining potential on electrical conductivity was studied by Gottinger et al. [17], who showed that the weaker the confining potential, the smaller is the surface contribution to electrical resistivity. Thus, one may expect that in quantum wells with finite confining potential the main features due to roughness fractality are qualitatively similar to those in wells with infinite confining potential. This conjecture is supported by the observation that the role of confining potential is similar to the role of the roughness amplitude. Assuming infinite confining potential one finds $E_\nu = (\hbar^2/2m)(\nu\pi/d)^2$ and $A_\nu^+ = A_\nu^- \equiv A_\nu = \hbar^2\pi^2\nu^2/md^3$.

For a film of thickness d and for the corresponding bulk carrier density n , the Fermi energy E_F and the number N of occupied minibands can be determined from the condition $nd = (m/\pi\hbar^2) \left(NE_F - \sum_{\nu=1}^N E_\nu \right)$.

3. Interface Roughness Model

For clarity of notation we suppress in this section the interface index β . A wide variety of thin film surfaces and interfaces grown under non-equilibrium conditions are well described in terms of self-affine fractal scaling defined in terms of fractional Brownian motion [14]. For self-affine fractal surfaces, the roughness spectrum $\langle |h(k)|^2 \rangle$ has the asymptotic scaling behaviour [14, 15]

$$\langle |h(k)|^2 \rangle \propto \begin{cases} k^{-2-2H} & \text{if } k\xi \gg 1, \\ \text{const} & \text{if } k\xi \ll 1. \end{cases} \quad (4)$$

The roughness exponent H is a measure of interface irregularity [13 to 16]; small values of H ($H \approx 0$) characterize jagged or irregular surfaces at small length scales ($r < \xi$), while large values of H ($H \approx 1$) correspond to interfaces which are smoother at $r < \xi$. Moreover, the roughness exponent H is related to the local fractal dimension D ($D = 3 - H$) [14].

The self-affine asymptotic limits of $\langle |h(k)|^2 \rangle$ in Eq. (4) are satisfied by the simple Lorentzian model [16]

$$\langle |h(k)|^2 \rangle = (2\pi) \frac{\Delta^2 \xi^2}{(1 + ak^2 \xi^2)^{1+H}}. \quad (5)$$

Indeed, for $k\xi \gg 1$ we have $\langle |h(k)|^2 \rangle \propto k^{-2-2H}$, while for $k\xi \ll 1$ one finds $\langle |h(k)|^2 \rangle \propto \Delta^2 \xi^2$. As for growing self-affine surfaces $\Delta \propto \xi^H$ [14, 15], the latter formula as a function of ξ reads $\langle |h(k)|^2 \rangle \propto \xi^{2+2H}$. The parameter a in Eq. (5) is determined by the equation $a = (1/2H)[1 - (1 + aQ_c^2\xi^2)^{-H}]$ if $0 < H \leq 1$, and $a = (1/2)\ln(1 + aQ_c^2\xi^2)$ for $H = 0$ (logarithmic roughness) [16]. Here $Q_c = \pi/a_0$, with a_0 of the order of the interatomic spacing. For $H = 0.5$ and $\xi \gg a_0$, the Fourier transform of $\langle |h(k)|^2 \rangle$ yields the simple exponential correlation form $C(r) \sim \exp(-r/\xi)$ [16].

4. Semiconducting Quantum Wells with $N = 1$ and 2

For semiconducting quantum wells the areal electron density n_s ($n_s = nd$) can be rather small, so that the number of occupied minibands N is also small; say $N = 1$ or 2 . The electronic conductivity is determined by intra- and inter-miniband transitions, and therefore significantly depends on the number N of occupied minibands. Let us denote by d_c the critical width of the well (for a constant areal electron density n_s) above which the Fermi level E_F crosses the second miniband, i.e. $N = 2$ for $d > d_c$ and $N = 1$ for $d < d_c$. The role of inter-miniband transitions is characterized by the ratio of electron mobilities for the well thickness below and above the critical width d_c , $\mu(d_c - \varepsilon)/\mu(d_c + \varepsilon) \equiv \mu(d_c^-)/\mu(d_c^+) = \sigma(d_c - \varepsilon)/\sigma(d_c + \varepsilon)$. Here ε is a small thickness difference, $\varepsilon \ll d_c$.

To calculate the mobility ratio defined above, we shall calculate first the electron conductivity for $N = 1$ and 2 . Assume for simplicity a symmetrical well, i.e., the same roughness amplitudes Δ , correlation lengths ξ and roughness exponents H for both interfaces. For infinite confining potential on both sides of the well one finds the following formula for the conductivity $\sigma(d_c - \varepsilon)$:

$$\sigma(d_c - \varepsilon) = G_0 \frac{2n_s(d_c - \varepsilon)^5}{\pi^2[F^{(1)} - F^{(2)}]}, \quad (6)$$

where $G_0 = e^2/2\pi\hbar$. $F^{(1)}$ and $F^{(2)}$ are defined here as $F^{(1)} = F_{11}^{+(1)} = F_{11}^{-(1)}$ and $F^{(2)} = F_{11}^{+(2)} = F_{11}^{-(2)}$, respectively, while $F_{11}^{\pm(1)}$ and $F_{11}^{\pm(2)}$ can be calculated from Eqs. (3a) and (3b) for $k_{11} = [4\pi n_s(1 - \cos\theta)]^{1/2}$.

For $d = d_c + \varepsilon$, when the second miniband is also occupied ($N = 2$), the conductivity $\sigma(d_c + \varepsilon)$ is given by

$$\sigma(d_c + \varepsilon) = G_0 \frac{(d_c + \varepsilon)^5}{2(D_{11}D_{22} - D_{12}^2)} (k_1^4 D_{11} + k_2^4 D_{22} - 2k_1^2 k_2^2 D_{12}), \quad (7)$$

where D_{11} , D_{12} and D_{22} are defined as

$$D_{11} = k_1^2 \{ [F_{11}^{(1)} - F_{11}^{(2)}] - 4F_{12}^{(1)} \}, \quad (8a)$$

$$D_{12} = -k_1 k_2 F_{12}^{(1)}, \quad (8b)$$

$$D_{22} = k_2^2 \{ 16[F_{22}^{(1)} - F_{22}^{(2)}] - 4F_{12}^{(1)} \}. \quad (8c)$$

Here $F_{\nu\mu}^{(1)} = F_{\nu\mu}^{+(1)} = F_{\nu\mu}^{-(1)}$ ($\nu\mu = 1, 2$) and the parameters $k_{\nu\mu}$ which enter the formula for $F_{\nu\mu}^{(1)}$ and $F_{\nu\mu}^{(2)}$ according to Eqs. (3a) and (3b), are given by the following expressions: $k_{11} = \sqrt{2}k_1(1 - \cos\theta)^{1/2}$, $k_{12} = [2\pi n_s - \{2(\pi n_s)^2 - [9(\pi/d_c + \varepsilon)^4/2]\} \cos\theta]^{1/2}$, and $k_{22} = \sqrt{2}k_2(1 - \cos\theta)^{1/2}$, with k_1 and k_2 defined as $k_1 = [\pi n_s + (3/2)(\pi/(d_c + \varepsilon))^2]^{1/2}$

Fig. 1. Conductivities $\sigma(d_c + \varepsilon)$ and $\sigma(d_c - \varepsilon)$ vs. correlation length ξ , calculated for $H = 0.7$, $d_c = 10$ nm, $a_0 = 0.3$ nm, $\Delta = 0.3$ nm, and $\varepsilon = 0.1$ nm

and $k_2 = [\pi n_s - (3/2)(\pi/(d_c + \varepsilon))^2]^{1/2}$. Analytic calculations of the integrals which occur in $F_{v\mu}^{(1)}$ and $F_{v\mu}^{(2)}$ (and consequently also of the matrix elements $D_{v\mu}$) can be performed for limiting values of the roughness exponent, i.e. for $H = 0$ (logarithmic roughness) and $H = 1$ [6].

Results of numerical calculations are presented in Fig. 1, where $\sigma(d_c \pm \varepsilon)$ as a function of the correlation length ξ is shown for the carrier density $n_s = 4.8 \times 10^{12} \text{ cm}^{-2}$, for which the critical well width d_c is equal to 10 nm. The conductivity has generally a broad minimum at a correlation length close to $\lambda_F/4$ ($\lambda_F \approx d_c$) [3, 6]. This behaviour is reflected in the matrix elements $C_{v\mu}$, which for small ξ and fixed $k_{v\mu}$ increase proportionally to ξ^2 (since $\langle |h(k_{v\mu})|^2 \rangle \sim \xi^2$), and then, after reaching maximum at a certain point, decrease with further increase of the correlation length ξ (since $\langle |h(k_{v\mu})|^2 \rangle \propto \xi^{-2H}$ for $k_{v\mu}\xi \gg 1$).

Equations (6) and (7) lead to the following formula for the mobility ratio:

$$\frac{\mu(d_c^-)}{\mu(d_c^+)} = \frac{4n_s}{\pi^2} \left(\frac{d_c - \varepsilon}{d_c + \varepsilon} \right)^5 \frac{(D_{11}D_{22} - D_{12}^2)}{[F^{(1)} - F^{(2)}]} (k_1^4 D_{11} + k_2^4 D_{22} - 2k_1^2 k_2^2 D_{12})^{-1}. \quad (9)$$

In the limit $k_F \xi \ll 1$ one finds $\lim_{\varepsilon \rightarrow 0} [\mu(d_c^-)/\mu(d_c^+)] = 5$, independently of the form of the height-height correlation function [5, 12]. Since $\langle |h(k)|^2 \rangle \sim \Delta^2$, the roughness amplitude dependence of the conductivity is a rather trivial one, namely $\sigma \sim \Delta^{-2}$. This leads effectively to the mobility ratio $\mu(d_c^-)/\mu(d_c^+)$ independent of Δ . Therefore, the only nontrivial dependence is the one on the roughness exponent H and the roughness correlation length ξ .

Fig. 2 presents the mobility ratio $\mu(d_c^-)/\mu(d_c^+)$ versus correlation length ξ , calculated for $\varepsilon = 0.1$ nm and for indicated values of the roughness exponent. The curve for $H = 0.7$ corresponds to the conductivities shown in Fig. 1. An interesting feature shown in Fig. 2 is the maximum in the mobility ratio, which occurs at a correlation length $\xi < d_c/2$. With increasing H the maximum becomes steeper and shifts to larger ξ .

Fig. 2. Mobility ratio $\mu(d_c^-)/\mu(d_c^+)$ vs. correlation length ξ for indicated values of the roughness exponent H . The other parameters are as in Fig. 1

Dependence of the mobility ratio $\mu(d_c^-)/\mu(d_c^+)$ on the roughness exponent H is shown explicitly in Fig. 3. For short correlation lengths the mobility ratio increases monotonously with increasing roughness exponent H , while for correlation lengths close to the critical width d_c , a broad maximum appears. The position of this maximum shifts to smaller values of H , when the correlation length increases.

Consider now the influence of the parameter ε on the mobility ratio. This is shown explicitly in Fig. 4. It is worth noting that for correlation lengths smaller than the critical

Fig. 3. Mobility ratio $\mu(d_c^-)/\mu(d_c^+)$ vs. roughness exponent H for indicated values of the correlation length ξ . The other parameters are as in Fig. 1

Fig. 4. Mobility ratio $\mu(d_c^-)/\mu(d_c^+)$ vs. ξ for indicated values of the correlation length ξ and for $H = 0.6$. The other parameters are as in Fig. 1

width ($\xi < d_c$), the mobility ratio decreases exponentially with increasing ξ , $\mu(d_c^-)/\mu(d_c^+) = A(H, \xi) + B(H, \xi) \exp[-\xi/\varepsilon_0(H, \xi)]$, with $\varepsilon_0(H, \xi) > d_c$. Indeed, the exponential fits of the curves for $\xi = 1$ and 5 nm in Fig. 4 yield $\varepsilon_0(H, \xi) = 11.18$ nm and 19.94 nm, respectively, which are larger than d_c ($d_c = 10$ nm).

Screening effects can be included by introducing the dielectric function $\varepsilon(q) = 1 + q_s/q$, where q_s is the screening number. The role of screening is shown in

Fig. 5. Mobility ratio $\mu(d_c^-)/\mu(d_c^+)$ vs. correlation length ξ for indicated values of the roughness exponent H and for screening wave-number $q_s = 0.1$ nm⁻¹ (solid lines). The corresponding curves in the limit of no screening are also shown (dashed lines). The other parameters are as in Fig. 2

Fig. 5, where the mobility ratio $\mu(d_c^-)/\mu(d_c^+)$ is plotted versus correlation length ξ for indicated roughness exponents H . For comparison the corresponding results in the limit of no screening are also indicated by the dotted curves.

5. Summary

We investigated interface scattering effects on electronic transport properties of semi-conducting quantum wells. The interface roughness was assumed to be random self-affine fractal with an analytic roughness spectrum. The analysis was limited to the cases where only one or two lowest minibands were occupied. To characterize the role of inter-miniband transitions, we calculated the mobility ratio $\mu(d_c^-)/\mu(d_c^+)$ for the Fermi levels slightly above and below the second miniband edge. Such a ratio can be measured experimentally by varying the well width. From the calculations follows that the mobility ratio is very sensitive to the roughness parameters H and ξ . The roughness exponent H has a significant influence on the mobility ratio for correlation lengths either moderately lower than or significantly larger than d_c , while the roughness correlation length ξ has a more pronounced effect on the mobility ratio for large roughness exponents H (≈ 1). The discontinuity of the electron mobility when the Fermi level crosses the second miniband edge is due to additional scattering channels opened by inter-miniband transitions. Apart from this, we showed that the mobility ratio decreases exponentially with increasing well width difference ϵ .

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