Influence of surface roughness on the conductivity of metallic and semiconducting quasi-two-dimensional structures

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(Received 7 August 1990; revised manuscript received 3 December 1990)

At low temperature, the conductivity σ of metallic films or of semiconducting quantum wells is limited by surface-roughness scattering. The expression for σ includes an autocorrelation function (ACF) associated with the roughness. We report a theoretical study of the dependence of σ on the shape, and the correlation length ξ of the ACF. It is concluded that σ depends strongly on the choice of the ACF for $\xi \gg k_F^{-1}$, where k_F is the Fermi wave vector. For metallic films, the mean variation of σ with thickness d cannot be approximated by the usual power law, $\sigma \propto d^s$; similar effects are obtained for semiconducting quantum wells.

Because of substantial technological progress in the controlled fabrication of quasi-two-dimensional samples, recent experiments on the conductivity of metallic films[1-5] and of semiconducting quantum wells[6] have produced conclusive evidence of scattering by the roughness of the surfaces or interfaces. Concurrently, quantum-mechanical derivations of the conductivity, based either on Green's function[7,8] or on coupled Boltzmann-like equations,[9,10] have been proposed. The boundaries of a perfect quasi-two-dimensional structure are planes whose equations are $z=\pm d/2$, where d is the thickness of the metallic film or the width of the semiconducting quantum well and both are perpendicular to a chosen direction, the z axis. In real structures, the surfaces are no longer planes and, for instance, the equation of the upper surface is modified to $z=d/2+f(\boldsymbol{\rho})$, where $\boldsymbol{\rho}$ is a two-dimensional vector that is the projection onto the plane perpendicular to the z axis of the vector $\mathbf{r}$ defining a point on the surface. In such a model, the surface roughness is entirely described by a continuous function $f(\boldsymbol{\rho})$ and[10,11] all the electronic properties are expressed through the autocorrelation function (ACF) of $f(\boldsymbol{\rho})$, which is defined by

$$\frac{1}{S}\int_S f(\boldsymbol{\rho})f(\boldsymbol{\rho}+\boldsymbol{\rho}')d^2\rho' = \Delta^2 G(\rho/\xi) , \tag{1}$$

where ξ is the roughness correlation length. In the above definition, the function $G(\rho/\xi)$ depends only on the magnitude ρ (and not on the direction of $\boldsymbol{\rho}$) because, for simplicity, we have assumed that the roughness is isotropic. Moreover, $G(\rho/\xi)$ has significant values only for $\rho<\xi$. The parameter Δ is the root mean square of the height of the variation of the real surface from a plane. For the $CoSi_2$/Si interface ξ is usually of the order of one interatomic distance;[1-5] for samples with excellent surfaces, ξ may be quite large.[12-13] This condition is also supported by mobility experiments at the GaAs/AlAs interface[6] or by high-resolution transmission electron microscopy at the Si/SiO_2 interace.[14] On the contrary, Δ varies in a small range between one and two interatomic distances. In the following we show the influence upon the electrical conductivity of (i) the magnitude of the roughness correlation length as compared with the electron wavelength at the Fermi energy and (ii) the shape of the ACF. We begin with the conductivity expression for scattering by surface roughness derived earlier [Eq. (10) of Ref. 10]:

$$\sigma = \frac{e^2 d^5}{4\pi^6 \hbar \Delta^2} \sum_{\nu=1}^{N} \sum_{\nu'=1}^{N} k_\nu^2 k_{\nu'}^2 (D^{-1})_{\nu\nu'} . \tag{2}$$

In Eq. (2), N is the number of subbands filled by the electron gas, k_ν is the Fermi wave vector of subband ν,

$$k_\nu = [(2m/\hbar^2)(E_F - E_\nu)]^{1/2}$$

(E_F is the Fermi energy and E_ν the minimum energy of subband ν), and D^{-1} is the inverse of the matrix D, which is defined by its elements as

$$D_{\nu\nu'} = \frac{d^6 \xi^2 m^2}{4\pi^6 \hbar^4} A_\nu \int_0^{2\pi} d\theta \left[\delta_{\nu\nu'} k_\nu^2 \sum_{\mu=1}^{N} A_\mu F(\xi k_{\nu\mu}) - A_{\nu'} k_\nu k_{\nu'} \cos\theta F(\xi k_{\nu\nu'}) \right] , \tag{3}$$

where

$$k_{\nu\nu'} = (k_\nu^2 + k_{\nu'}^2 - 2k_\nu k_{\nu'} \cos\theta)^{1/2}$$

and $F(q)$ is the Fourier transform of $G(\rho)$:

$$F(q) = \int d^2\rho\, e^{i\mathbf{q}\cdot\boldsymbol{\rho}} G(\rho) .$$

Because the ACF is $\Delta^2 G(\rho/\xi)$, it is more useful to define the Fourier transform of $G(\rho/\xi)$ by

$$\int d^2\rho\, e^{i\mathbf{q}\cdot\boldsymbol{\rho}} G(\rho/\xi) = \xi^2 \int d^2\rho\, e^{i\xi\mathbf{q}\cdot\boldsymbol{\rho}} G(\rho) = \xi^2 F(\xi q) .$$

When surfaces localize electrons strictly inside the region $-d/2<z<d/2$ (infinite quantum well),

$A_\nu=\hbar^2\pi^2\nu^2/(md^3)$.

For a small correlation length such that $\xi k_1 \ll 1$ (as $k_1 > k_\nu$ for $\nu > 1$, this condition implies $\xi k_{\nu\nu'} \ll 1$ for $\nu,\nu' \le N$), we have already shown[10] that the conductivity depends on the value $F(0)=\int G(\rho)d^2\rho$ and reduces to

$$\sigma=\frac{e^2}{\hbar}\frac{d^5}{2\pi^6\Delta^2\xi^2}\frac{\pi}{F(0)}\frac{6}{N(N+1)(2N+1)}\sum_{\nu=1}^{N}\frac{k_\nu^2}{\nu^2}\ . \tag{4}$$

In this limit, details of the function $G(\rho)$ are not important; only its mean value occurs through the factor $\pi/F(0)$, which is of the order of unity for different ACF. Finally, σ varies with Δ and ξ only through the product $(\xi\Delta)^{-2}$.

If the condition $\xi k_1 \ll 1$ is not satisfied, we need to know the complete Fourier transform of $G(\rho)$. For our purpose we have chosen to study two types of ACF: (i) a Gaussian[6,10,14] and (ii) an exponential.[14]

In the Gaussian model, we assume that

$$G(\rho/\xi)=G_g(\rho/\xi)\equiv\exp(-\rho^2/\xi^2)\ .$$

Its Fourier transform is

$$\xi^2F_g(\xi q)=\pi\xi^2\exp(-\xi^2q^2/4)\ .$$

When we introduce this expression into Eq. (3), we obtain for the matrix elements $D_{\nu\nu'}$,

$$D^g_{\nu\nu'}=\tfrac{1}{2}\xi^2\nu^2k_\nu\left[\delta_{\nu\nu'}k_\nu\sum_{\mu=1}^{N}\mu^2\exp[-\tfrac{1}{4}\xi^2(k_\nu^2+k_\mu^2)]I_0(\tfrac{1}{2}\xi^2k_\nu k_\mu)-\nu'^2k_{\nu'}\exp[-\tfrac{1}{4}\xi^2(k_\nu^2+k_{\nu'}^2)]I_1(\tfrac{1}{2}\xi^2k_\nu k_{\nu'})\right]\ , \tag{5}$$

where $I_0(x)$ and $I_1(x)$are modified Bessel functions.

In the exponential model,

$$G(\rho/\xi)=G_e(\rho/\xi)\equiv\exp(-\rho/\xi)$$

whose Fourier transform is

$$\xi^2F_e(\xi q)=2\pi\xi^2(1+\xi^2q^2)^{-3/2}\ .$$

We deduce for $D_{\nu\nu'}$ the expression

$$D^e_{\nu\nu'}=\frac{2\xi^2\nu^2k_\nu}{\pi}\left[\delta_{\nu\nu'}k_\nu\sum_{\mu=1}^{N}\mu^2\frac{\mathrm{E}(\beta_{\nu\mu})}{\alpha^3_{\nu\mu}(1-\beta^2_{\nu\mu})}-\frac{2\nu'^2k_{\nu'}}{\alpha^3_{\nu\nu'}\beta^2_{\nu\nu'}}\left[\frac{1-\frac{1}{2}\beta^2_{\nu\nu'}}{1-\beta^2_{\nu\nu'}}\mathrm{E}(\beta_{\nu\nu})-\mathrm{K}(\beta_{\nu\nu'})\right]\right]\ , \tag{6}$$

where $\mathrm{K}(x)$ and $\mathrm{E}(x)$ are, respectively, the complete elliptic integral of the first and of the second kind, while

$$\alpha^2_{\nu\nu'}=1+\xi^2(k_\nu+k_{\nu'})^2$$

and

$$\beta^2_{\nu\nu'}=\frac{4\xi^2k_\nu k_{\nu'}}{\alpha^2_{\nu\nu'}}\ .$$

In the limit $\xi k_1 \ll 1$, from Eqs. (5) and (6) we recover Eq. (4) for the conductivity σ, with $F(0)=\pi$ for the Gaussian model and $F(0)=2\pi$ for the exponential one. It is precisely in this limit that experimental results on the conductivity of metallic $CoSi_2$ films were conveniently interpreted.[10] In $CoSi_2$ the carrier density is $n\approx3\times10^{22}$ cm^{-3}, which gives $k_\nu\approx1$ $Å^{-1}$, and the number of occupied subbands N varies from 3 to 30 when the thickness d changes from 10 to 100 Å. The experimental variations of σ with d, in this range, are well fitted by expression (4) with $\Delta\approx4$ Å and $\xi\approx2$Å. The case of GaAs quantum wells has been studied in Ref. 6; in the samples investigated the carrier density was approximately 3×10^{11} cm^{-2} so that the number of occupied subbands and the Fermi wave vector reduced, respectively, to $N=1$ and $k_1\approx10^{-2}$ $Å^{-1}$. Again, the variations of σ and d were fitted by expression (4) with $\Delta\approx3$ Å and $\xi\approx60$ Å.

Thus there is no appreciable difference between the Gaussian and the exponential models when the condition $\xi k_1 < 1$ is fulfilled; either can be used to interpret the experiments. Conversely, however, this means that the product $\xi\Delta$ is slightly model dependent and neither Δ nor ξ can be determined to within a factor of 2. We now show that important differences appear for samples with better surfaces, in which the correlation length can increase with the condition $\xi k_1 > 1$ being satisfied.

First we discuss the case of a metallic film. Figure 1 shows the variations of σ with d when $\xi=25$ Å and $\Delta=3$ Å for $n=3\times10^{22}$ cm^{-3} (the $CoSi_2$ case). The lower curve corresponds to an exponential ACF; it presents well-defined jumps corresponding to thicknesses for which the number of occupied subbands N is increased by 1. The upper curve corresponds to a Gaussian ACF. The previous jumps have disappeared and we notice smooth oscillations of the conductivity. Moreover, in the exponential model, the mean values of σ can be fitted by a power law $\sigma\propto d^s$ (with $s\approx\frac{3}{2}$); it is clear that such a power law cannot be used in the Gaussian case. Figures 2 and 3 show what happens to $\sigma(d)$ when the correlation length ξ increases from 5 to 35 Å. With the exponential ACF, the jumps remain visible and the shape of the different curves is unchanged. On the contrary, with a Gaussian ACF the jumps disappear for $\xi > 5$ Å; they are smeared out and extrema take place for d values which progressively are displaced towards high d values. It is

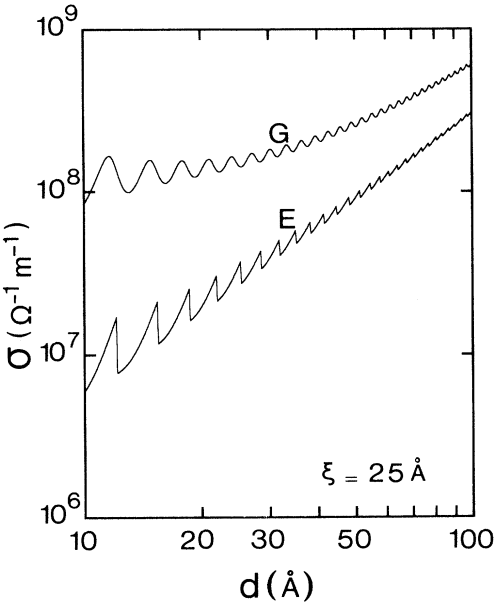

FIG. 1. Oscillations of conductivity in $CoSi_2$ plotted as a function of film thickness d for Gaussian (G) and exponential (E) autocorrelation functions (ACF) with the same correlation length $\xi=25$ Å. The exponential curve can be approximated by a straight line (i.e., defining s such that $\sigma \propto d^s$) but this is not possible for the Gaussian one (here, $\Delta=3$ Å).

possible to understand such strong differences produced by the choice of the ACF by looking at expressions (5) and (6) for the matrix elements $D^g_{\nu\nu'}$ and $D^e_{\nu\nu'}$. They occur because the Bessel functions in $D^g_{\nu\nu'}$ decrease with ξ exponentially, while the elliptic functions in $D^e_{\nu\nu'}$ decrease roughly as the inverse of $\ln\sigma$. Finally, we note that it is

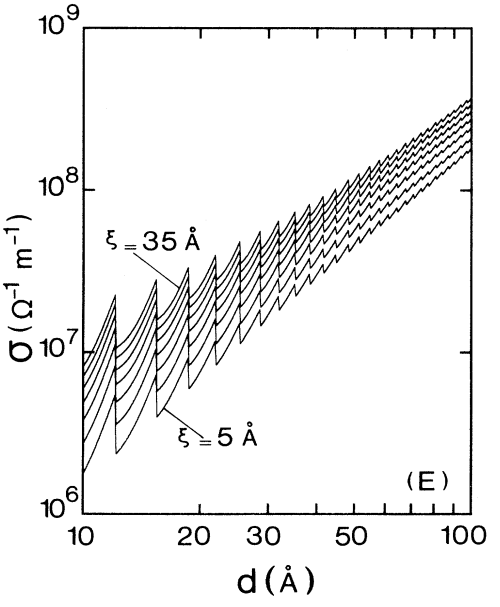

FIG. 2. Oscillations of conductivity in $CoSi_2$ plotted as a function of thickness d for an exponential (E) ACF with different correlation lengths: $\xi=5$, 10, 15, 20, 25, 30, and 35 Å. $\Delta=3$ Å.

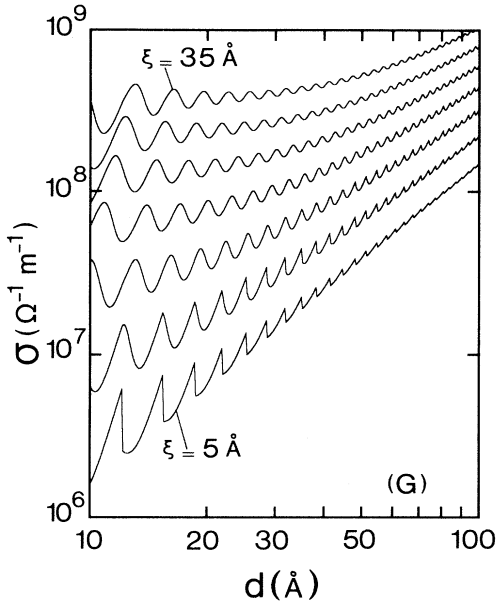

FIG. 3. Same as in Fig. 2 but for Gaussian (G) ACF.

not possible to fit the mean variations of σ with d by a power law, $\sigma \propto d^s$, for all values of ξ. For the Gaussian model, ξ must be smaller than 10 Å. For the exponential case, the restriction is less drastic; $\xi<30$ Å. When the mean slope $s=d\ln\sigma/d\ln d$ can be defined, Fig. 4 shows the variation of s with the correlation length ξ. We observe that s can decrease from 2.3 for small values of ξ to 1.5 for $\xi\approx10$ Å. It follows that explaining recent results[12,13] on $CoSi_2$ with a Gaussian or an exponential ACF requires only high values of ξ, and it is not possible to decide between the two functional forms on the basis

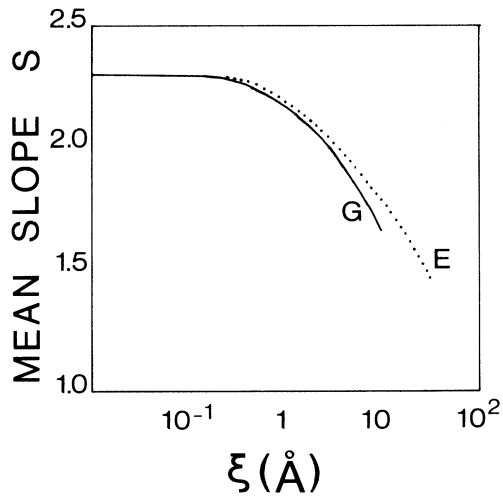

FIG. 4. Exponent s of the power law $\sigma \propto d^s$ as a function of the correlation length for Gaussian and exponential ACF in $CoSi_2$. It is not possible to define s for ξ larger than 10 Å for a Gaussian type and for ξ larger than 30 Å for an exponential one; see Fig. 1 as an example. Heavy line (G), Gaussian type; dotted line (E), exponential type.

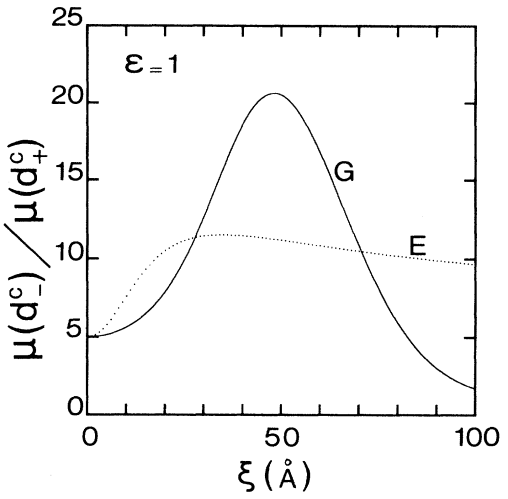

FIG. 5. Mobility ratio R of mobilities in a semiconductor for the Fermi level just below and above the bottom of the second conduction subband vs correlation length for two ACF. Heavy line (G), Gaussian type; dotted line (E), exponential type. In this figure the screening is not taken into account; $\epsilon=1$, $d^c=100$ Å. $n_s=4\times10^{12}$ cm^{-2}. (See text.)

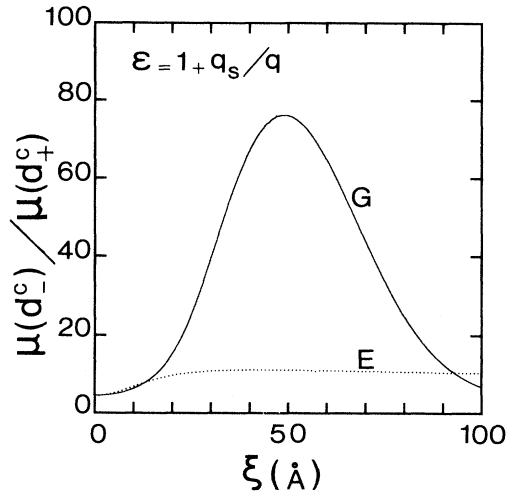

FIG. 6. Same as in Fig. 5, but screening is taken into account through the dielectric function $\epsilon=1+q_s/q$. $q_s=(50\ \text{Å})^{-1}$ in GaAs.

of these experimental results.

We now discuss the influence of the choice of ACF on a property which could be measured in a semiconducting quantum well. At fixed electron surface density n_s, it is in principle possible to vary the well width in such a way that the Fermi level crosses the bottom of the second subband. This condition occurs for a critical width labeled d^c. For instance, with a density $n_s=4\times10^{12}$ cm^{-2}, the critical width is $d^c=100$ Å (in the model of Ref. 6). At the crossing of the Fermi energy we expect a jump of the conductivity, as explained before. We can calculate the ratio

$$R=\lim_{\epsilon\to0}\frac{\sigma(d^c-\epsilon)}{\sigma(d^c+\epsilon)}$$

of the conductivities (or mobilities in a semiconductor) just below and just above the crossing between E_F and E_2 and study how R depends on the shape of the ACF and on ξ. In order to use our preceding results [Eqs. (2) and (3)], we assume that the roughness at the quantum-well interfaces is isotropic; thus we exclude an interface terracing form which is obtained with epitaxial growth in a direction which is slightly tilted relative to the nominal crystalline axis. Then in the limit $\xi k_1\ll1$, we deduce from Eq. (4) that

$$\lim_{\epsilon\to0}\sigma(d^c-\epsilon)=\frac{e^2}{\hbar}\frac{\pi}{F(0)}\frac{(d^c)^5}{2\pi^6\Delta^2\xi^2}k_1^2$$

and

$$\lim_{\epsilon\to0}\sigma(d^c+\epsilon)=\frac{e^2}{\hbar}\frac{\pi}{F(0)}\frac{(d^c)^5}{2\pi^6\Delta^2\xi^2}\frac{1}{5}k_1^2\ ;$$

Thus, $R=5$, in the limit $\xi k_1\ll1$, for all ACF types. We have shown in Figs. 5 and 6 the variations of R with ξ for the Gaussian and exponential models. Figures 5 and 6 differ by the screening effect which is absent in the first one and taken into account through a dielectric function,[15] $\epsilon=1+q_s/q$, in the second. We notice a curious effect in the screening which accentuates the variations of the ratio $R(\xi)$ for the Gaussian case and, in contrast, decreases the variations with the choice of an exponential ACF.

In conclusion, the above discussion shows that the choice of the shape for the ACF describing surface roughness may be important in the study of transport properties of quasi-two-dimensional structures. Care must be taken before deducing values of roughness correlation lengths from conductivity measurements.

We are very indebted to H. von Känel for communication of results prior to publication. We thank J. E. Nicholls and W. G. Clark for a critical reading of the manuscript. The Laboratoire de Spectrométrie Physique and Groupe de Physique des Solides are Laboratoires associés au C.N.R.S.

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