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Self-affine roughness effects on electron transmission and electric current in tunnel junctions

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Interface roughness effects on electron transmission in tunnel junctions are investigated theoretically in the limit of thick barriers. The barrier roughness is described in terms of self-affine fractal scaling by the roughness exponent H , rms roughness amplitude w , and correlation length ξ . For realistic parameters diffuse transmission usually exceeds specular transmission. It is shown that for small roughness exponents ($H < 0.5$) the transmission coefficient increases with decreasing ratio w/ξ . For large roughness exponents (or smoother interfaces at short wavelengths) the transmission coefficient has a maximum at a certain value of the ratio w/ξ . With increasing w/ξ the tunneling current behaves similarly as the transmission coefficient. © 2000 American Institute of Physics. [S0021-8979(00)05814-X]

I. INTRODUCTION

Quantum-mechanical tunneling of electrons between two metal electrodes separated by a thin insulating layer was extensively studied in the past two decades. Now, the electron tunneling is also used as a spectroscopic tool for investigations of condensed matter systems.¹ Although tunneling experiments were usually carried out in systems with significant electrode/barrier interface roughness, most of theoretical works were performed on the assumption of flat interfaces. In junctions with thick barriers and flat interfaces the tunneling current is dominated by electrons incident almost normally on the barrier, which is known as the tunneling cone effect.^{1,2} This effect was used very often to describe experimental data. For example, it was used to describe recently observed tunneling phenomena in high temperature superconductors with highly anisotropic quasiparticle spectrum.³

The tunneling cone effect is no longer applicable to junctions with rough interfaces, which significantly complicates interpretation of tunneling phenomena. When the electrode/barrier interface roughness fluctuations exceed the electron wavelength, the diffuse transmission dominates the specular one.⁴ It was also shown that for sufficiently small local interface slopes the tunneling cone effect can still exist, although the tunneling current is entirely diffuse.⁴

However, no quantitative calculations of the transmission coefficient were performed, that could be correlated with the roughness parameters measured experimentally, e.g., by x-ray and electron scattering techniques.⁵ Such quantitative calculations of the transmission coefficient and tunneling current in thick junctions with rough barriers are the

main objective of the present article. The roughness fluctuations are quantified in terms of self-affine fractal roughness which has been observed in a wide range of thin film surfaces (interfaces).^{5,6} This kind of roughness is described by the roughness exponent H ($0 \leq H < 1$), rms roughness amplitude w , and in-plane correlation length ξ . We show that the local interface slope, electron transmission coefficient, and tunneling current significantly depend on the value of the roughness exponent H .

The article is organized as follows. In Sec. II we describe briefly the electron transmission through rough barriers. Self-affine model of electrode/barrier interfaces is described in Sec. III. Electron transmission and tunneling current in junctions with self-affine fractal interfaces is calculated in Sec. IV, where also numerical results are presented and discussed. Conclusions and final remarks are in Sec. V.

II. TRANSMISSION COEFFICIENT FOR THICK ROUGH BARRIERS

In this section we summarize briefly the results obtained by Walker⁴ for Gaussian interfaces. Assume that the metal/insulator interfaces are located, respectively, at $z_1 = -d + h_1(\mathbf{r})$ and $z_2 = h_2(\mathbf{r})$, where d denotes the average barrier thickness, $\mathbf{r} = (x, y)$ is the in-plane position vector, whereas $h_1(\mathbf{r})$ and $h_2(\mathbf{r})$ are random functions of $\mathbf{r}$ with $\langle h_{1(2)}(\mathbf{r}) \rangle = 0$.

For an electron of mass m and energy E the transmission coefficient D through a rectangular insulating barrier of height V_0 is given by⁴

$$D(E, \mathbf{k}) = V(\mathbf{k}) + \int_{k' < k_M} \Sigma(\mathbf{k}', \mathbf{k}) d^2 \mathbf{k}', \quad (1)$$

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where $\mathbf{k}$ (and also $\mathbf{k}'$) is the in-plane wave vector and $k_M = \sqrt{2mE/\hbar^2}$. The term $V(\mathbf{k})$ describes specular transmission of electrons through the potential barrier, when the in-plane wave vector is conserved (specular term), while the second term on the right side of Eq. (1) describes diffuse transmission (diffusive term) with $\Sigma(\mathbf{k}', \mathbf{k})d^2\mathbf{k}'$ denoting the fraction of electrons transmitted into states contained in $d^2\mathbf{k}'$.

The specular term $V(\mathbf{k})$ is given by⁴

$$V(\mathbf{k}) = FB_1B_2P_I(\mathbf{k}), \quad (2)$$

where

$$B_{1(2)} = \exp[-k_v^2 w_{1(2)}^2], \quad (3a)$$

$$P_I(\mathbf{k}) = [(2\pi)(\Delta k_I)^2]^{-1} \exp[-k^2/2(\Delta k_I)^2], \quad (3b)$$

$$F = (2\pi)(\Delta k_I)^2 \exp[-2k_I d + 2k_I^2(w_I^2 + w_2^2)], \quad (3c)$$

and the following definitions have been introduced: $k_v = \sqrt{2mV_0/\hbar^2}$, $k_I = \sqrt{2m(V_0 - E)/\hbar^2}$, $(\Delta k_I)^2 = k_I/(2d)$ and $w_{1(2)} = \langle h_{1(2)}(r)^2 \rangle^{1/2}$.

In the tangent plane approximation the diffusive term $\Sigma(\mathbf{k}', \mathbf{k})$ is given by^{4,7}

$$\begin{aligned} \Sigma(\mathbf{k}', \mathbf{k}) = F \left[B_1 P_2(\mathbf{k}' - \mathbf{k}) P_I(\mathbf{k}) + B_2 P_I(\mathbf{k}') P_1(\mathbf{k}' - \mathbf{k}) \right. \\ \left. + \int P_2(\mathbf{k}' - \mathbf{k}'') P_I(\mathbf{k}'') P_1(\mathbf{k}'' - \mathbf{k}) d^2\mathbf{k}'' \right], \quad (4) \end{aligned}$$

where

$$P_{1(2)}(\mathbf{k}) = [(2\pi)(\Delta k_{1(2)})^2]^{-1} \exp[-k^2/2(\Delta k_{1(2)})^2], \quad (5a)$$

$$(\Delta k_{1(2)})^2 = k_v^2 \rho_{1(2)}, \quad (5b)$$

and $\rho_{1(2)} = \langle (\partial h_{1(2)}/\partial x)^2 \rangle = \langle (\partial h_{1(2)}/\partial y)^2 \rangle$ are the mean-square slopes (equal in the x and y directions for isotropic rough interfaces in the x - y plane). It is also worth to mention that the tangent plane approximation is valid when spatial scale of the roughness is larger than the electron wavelength λ , effectively $\xi \gg \lambda$,⁴ and when the roughness fluctuations are relatively small, $w_{1(2)} \leq \lambda$.

III. ROUGHNESS MODEL

A wide variety of surfaces (interfaces) which occur in nature are well described by a kind of roughness associated with self-affine fractal scaling.^{4,5} Examples include the nanometer scale topology of vapor deposited films, eroded and fractured surfaces, etc.⁹ In this section we suppress the index describing different interfaces. For self-affine fractals the roughness spectrum $\langle |h(\mathbf{k})|^2 \rangle$ scales as^{5,8}

$$\langle |h(\mathbf{k})|^2 \rangle \propto \begin{cases} k^{-2-2H} & \text{if } k\xi \gg 1 \\ \text{const} & \text{if } k\xi \leq 1 \end{cases}, \quad (6)$$

with the roughness exponent H being a measure of the degree of surface irregularity^{4,5,8} (small values of H characterize more jagged or irregular surfaces at roughness wavelengths smaller than ξ). The scaling behavior given by Eq. (6) can be described by the simple Lorentzian model⁹

$$\langle |h(\mathbf{k})|^2 \rangle = \frac{A}{(2\pi)} \frac{w^2 \xi^2}{(1 + ak^2 \xi^2)^{1+H}}, \quad (7)$$

with $a = (1/2H)[1 - (1 + ak_c^2 \xi^2)^{-H}]$ if $0 < H < 1$, and $a = (1/2)\ln[1 + ak_c^2 \xi^2]$ if $H = 0$. Apart from this, $k_c = \pi/a_o$, with a_o being of the order of the interatomic distance, and A is the macroscopic area of the flat interface. The Fourier transform of $\langle |h(\mathbf{k})|^2 \rangle$ yields the analytically solvable height-height correlation function $C(\mathbf{r}) = \langle h(\mathbf{r})h(\mathbf{0}) \rangle = [w^2/a\Gamma(1+H)](r/2a^{1/2}\xi)^H K_H(r/2a^{1/2}\xi)$ with $K_H(x)$ being the second kind Bessel function of order H and Γ denoting the gamma function. Other roughness models which satisfy the scaling relation in Eq. (6) can be found in Refs. 9–11.

IV. RESULTS AND DISCUSSION

For thick tunnel junctions, $k_I d \gg 1$, the integral term in Eq. (4) can be further simplified by setting $P_I(\mathbf{k}'') \cong \delta(\mathbf{k}'')$,⁴ which leads to the following expression:

$$\begin{aligned} \Sigma(\mathbf{k}', \mathbf{k}) \cong F [B_1 P_2(\mathbf{k}' - \mathbf{k}) P_I(\mathbf{k}) + B_2 P_I(\mathbf{k}') P_1(\mathbf{k}' - \mathbf{k}) \\ + P_2(\mathbf{k}') P_1(\mathbf{k})]. \end{aligned}$$

Applying the same argument to the integral $\int_{k' < k_M} \Sigma(\mathbf{k}', \mathbf{k}) d^2\mathbf{k}'$ of Eq. (1) we obtain

$$\begin{aligned} \int_{k' < k_M} \Sigma(\mathbf{k}', \mathbf{k}) d^2\mathbf{k}' \\ \cong F \left[B_1 P_I(\mathbf{k}) \int_{k' < k_M} P_2(\mathbf{k}' - \mathbf{k}) d^2\mathbf{k}' + B_2 P_1(\mathbf{k}) \right. \\ \left. + P_1(\mathbf{k}) \int_{k' < k_M} P_2(\mathbf{k}') d^2\mathbf{k}' \right]. \quad (8) \end{aligned}$$

Furthermore, upon considering the Fourier transform $h_{1(2)}(\mathbf{r}) = [(2\pi)^{-2}] \int h_{1(2)}(\mathbf{k}) e^{-i\mathbf{k}\mathbf{r}} d^2\mathbf{k}$ of the interface fluctuation and assuming $\langle h(\mathbf{k})h(\mathbf{k}') \rangle = [A/(2\pi)^4] \times \langle |h(\mathbf{k})|^2 \rangle \delta(\mathbf{k} + \mathbf{k}')$, the interface local slopes $\rho_{1(2)}$ are given by

$$\begin{aligned} \rho_{1(2)} = \frac{(2\pi)^4}{A} \int_{0 < k < k_c} k_x^2 \langle |h_{1(2)}(\mathbf{k})|^2 \rangle d^2\mathbf{k} \\ = \frac{(2\pi)^4}{A} \int_{0 < k < k_c} k_y^2 \langle |h_{1(2)}(\mathbf{k})|^2 \rangle d^2\mathbf{k}. \quad (9) \end{aligned}$$

On substituting Eq. (7) into Eq. (9) we obtain the following analytical expression for the slopes:

$$\begin{aligned} \rho_{1(2)} = \frac{w_{1(2)}^2}{4a_{1(2)}^2 \xi_{1(2)}^2} \left\{ \frac{(1 + a_{1(2)} k_c^2 \xi_{1(2)}^2)^{1-H_{1(2)}} - 1}{1 - H_{1(2)}} \right. \\ \left. + \frac{(1 + a_{1(2)} k_c^2 \xi_{1(2)}^2)^{-H_{1(2)}} - 1}{H_{1(2)}} \right\}. \quad (10) \end{aligned}$$

Figure 1 shows the slope $\rho = \rho_1 = \rho_2$ calculated for conformal interfaces; $w_1 = w_2 = w$, $\xi_1 = \xi_2 = \xi$, and $H_1 = H_2 = H$ (consequently, $a_1 = a_2 = a$). As one can see, the surface local slope significantly depends on the roughness exponent H , especially for small values of H (even when the ratio w/ξ is small).

FIG. 1. rms of the local interface slope as a function of the correlation length ξ calculated for $w=0.3$ nm, $a_0=0.3$ nm, and the other parameters as indicated.

Calculations of the diffuse component show that the dominant term (for interface roughness amplitudes comparable or larger than the atomic spacing a_0) comes from the third term of Eq. (8). Thus, one can write a simplified analytical expression for the transmission coefficient

$$D(E, \mathbf{k}) \cong \exp[-2k_I d + 2k_I^2(w_1^2 + w_2^2) - k_v^2(w_1^2 + w_2^2) - k^2/2(\Delta k_I^2)] + (\Delta k_I)^2(\Delta k_1)^{-2} \times \exp[-2k_I d + 2k_I^2(w_1^2 + w_2^2) - k^2/2(\Delta k_1)^2] \times \{1 - \exp[-k_M^2/2(\Delta k_2)^2]\}, \quad (11)$$

which in combination with Eq. (10) yields an analytic expression for the transmission coefficient as a function of all the three roughness parameters; w , H , and ξ .

Figure 2 shows the ratio of diffuse to specular terms in Eq. (12) as a function of the in-plane roughness correlation length ξ , calculated for $k=k_M/2$ and for various roughness exponents H . For the parameters assumed in Fig. 2 the diffuse transmission is dominant. For small roughness exponents the diffuse transmission of electrons is dominant even

FIG. 2. Ratio of diffuse to specular contributions to the transmission coefficient vs roughness correlation length ξ , calculated for $w=0.2$, $d=2$ nm, $V_0=5$, $E=4$ eV, $k=k_M/2$ and for H as indicated.

FIG. 3. Transmission coefficient vs roughness correlation length ξ calculated for $w=0.4$ nm and roughness exponents as indicated. The other parameters are the same as in Fig. 2.

for very large correlation lengths, or equivalently for very small ratio w/ξ ($\ll 1$). With increasing roughness exponent ($H>0.5$) the maximum of diffuse transmission is shifted to smaller correlation lengths ξ (larger ratio w/ξ).

The ratio of diffuse to specular transmission is large and increases with increasing in-plane component of electron wave vector. This indicates that diffuse scattering destroys the tunneling cone effect and tunneling processes are possible also for large in-plane wave vector component of an incident electron.

Variation of the total transmission coefficient with increasing correlation length ξ is shown in Fig. 3 for several values of the roughness exponent H . For small values of H ($H<0.3$) the transmission coefficient increases monotonously with increasing ξ . However, for larger values of H (smoothing at short roughness wavelengths, $<\xi$) the transmission coefficient increases up to a certain point, and then decreases with a further increase in ξ .

Dependence of the transmission coefficient on the roughness exponent is shown explicitly in Fig. 4. For small values of ξ , the transmission coefficient increases monoto-

FIG. 4. Transmission coefficient vs roughness exponent H for $w=0.4$ nm and correlation lengths as indicated. The other parameters are as in Fig. 2.

FIG. 5. Tunneling current vs roughness correlation length ξ calculated for $V=10$ mV, $E_F=3$ eV, $w=0.25$, $d=2$ nm and for indicated values of the roughness exponent H .

nously with increasing roughness exponent H . However, for larger values of ξ the transmission coefficient has a maximum at a certain point. In both Figs. 3 and 4 the maximum occurs when the local interface slopes are rather small (<0.1 ; see Fig. 1), which corresponds to slow decay of the local slope with increasing ξ .

Having found the transmission coefficient, one can calculate the current density from the formula^{1,4}

$$J = \frac{2e}{h} \int dE [f(E) - f(E - eV)] \frac{1}{(2\pi)^2} \int d^2\mathbf{k} D(E, \mathbf{k}), \quad (12)$$

where V is a bias voltage, e is the electron charge ($e > 0$) and $f(E)$ denotes the Fermi distribution function. Generally, the barrier shape is modified by an externally applied bias voltage V . For small values of V one can use an average barrier approximation, according to which the barrier is still rectangular but its height is lower and equal to $V_0 - eV/2$.

Figure 5 shows the tunneling current as a function of the correlation length ξ , calculated at zero temperature ($T=0$ K). The current increases rather monotonously with increasing ξ , even for small roughness exponents H , which is in agreement with the behavior of the transmission coefficient (Fig. 3). With increasing roughness exponent H (especially close to 1, which is characteristic of a smooth hill-valley structure), the tunnel current saturates and slightly decreases at larger roughness correlation lengths ξ . Behavior of the tunneling current with increasing roughness exponent H is shown explicitly in Fig. 6 for different values of the correlation length ξ . In both cases (Figs. 5 and 6) the weak variation of the tunnel current in the saturation regime occurs for small local interface slopes, where also their variation with decreasing interface roughness is slow.

V. SUMMARY AND CONCLUSIONS

We have investigated roughness effects on the electron transmission in thick tunnel junctions with rough boundaries. The interface roughness was described in terms of self-affine fractal scaling through the roughness exponent H , rms rough-

FIG. 6. Tunneling current vs roughness exponent H for various roughness correlation length ξ calculated for the same parameters as in Fig. 5.

ness amplitude w and correlation length ξ . Analytical calculations of the transmission coefficient were performed in the diffusive limit as a function of all the roughness parameters (w , H , and ξ). For realistic parameters the diffuse transmission is much larger than the specular transmission.¹² For small roughness exponents ($H < 0.5$), the total electron transmission coefficient through the junction increases with increasing ξ , while for larger roughness exponents (or smoother surfaces at short wavelength $< \xi$) it has a maximum at a certain value of the correlation length ξ . The tunneling current increases with increasing ξ and and/or increasing roughness exponent H .

The results indicate that junction morphology can have a significant influence on electron tunneling. Therefore, precise determination of interface roughness parameters (as for example in terms of x-ray reflectivity)⁵ is necessary in order to further understand and control tunneling phenomena, which are of potential technological importance in microelectronics devices.

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