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LETTER TO THE EDITOR

Tunnel current on a quantum wedge

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Abstract

Solving the Schrödinger equation directly, we study the characteristics of tunnel current on a quantum wedge. We obtain theoretical curves for the tunnel current which agree with experiment results better than those obtained using the penetration coefficient formula with an arbitrary potential.

Probing interfacial structure and its evolution during growth is essential to our understanding of and to our ability to ultimately control the morphology and physical properties of epitaxial film. Traditionally, much of the buried-interface analysis has been accomplished using destructive techniques such as cross-sectional transmission electron microscopy (TEM). However, in recent years, significant progress has been made in a number of nondestructive approaches. With the help of intense synchrotron light sources, grazing-incidence x-ray diffraction and soft-x-ray spectroscopy have been used for characterizing interfacial reconstruction and chemical composition [1]. Low-energy electron microscopy has been used to observe both atomic steps and dislocations at the Si/Ag interface [2]. Ion-implantation-induced subsurface noble-gas bubbles have been revealed by scanning tunnelling microscopy (STM) [3]. Recently, Altfeder, Chen and Matveev [4, 5] developed a new nondestructive approach for probing buried-interface structure on an atomic scale by STM [6]. Probing buried-interface structure with nondestructive approaches will have wide applications in practice. For example, we can learn some information about a biologic sample by nondestructively depositing a thin conductive (metal) film on its surface.

Using molecular beam epitaxy, Altfeder *et al* have fabricated a quantum wedge: a nano-scale flat-top lead island on a stepped Si(111) surface. Imaging the top surface of the wedge with a scanning tunnelling microscope reveals the phenomenon of electron interference fringes. The wave function of an electron confined in the quantum wedge should contain the imprints of both the vacuum and buried interfaces through the matching of the boundary conditions; the electron quantization will determine the tunnel current between the STM and the surface of the quantum wedge. In order to determine the buried interfacial structure, we have to know the relation between the tunnel current and the electron quantization. In reference [4], Altfeder *et al* obtained tunnel I–V curves calculated from the penetration coefficient formula with an arbitrary potential, quantum mechanically. Although the curves are in good qualitative agreement with the main features observed in the experiment, there is obviously some difference between the theoretical curves and the experimental curves. For the theoretical tunnel current curves, there is an abrupt variation at $V = -E_i/e$, but there is no abrupt variation for the experimental curves.

In this letter, we study the tunnel current characteristics of a quantum wedge by solving the Schrödinger equation directly, and compare our findings with experimental curves and ones derived from the penetration coefficient formula for an arbitrary potential.

The quantum wedge in reference [4] was formed by using molecular beam epitaxy as illustrated schematically in figure 1.

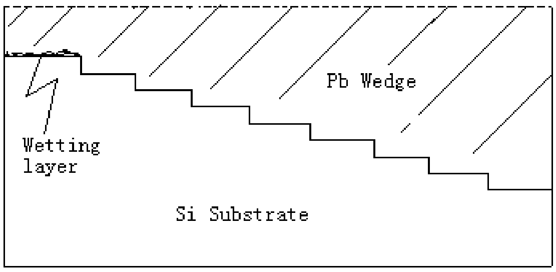

Figure 1. A quantum wedge formed using molecular beam epitaxy.

On the Si(111) surface, three-dimensional islands of Pb begin to form after an initial growth of 2–3 wetting layers, which result from the misfit between the lattice spacing of Si (3.13 Å) and Pb (2.86 Å) in the [111] direction, and the growth planes are the Pb(111) planes [7, 8].

In the following, we solve the Schrödinger equation directly to determine the penetration coefficient and the tunnel current expression for STM.

(1) For a positive tip bias V, the tunnelling potential barrier model is as shown in figure 2.

ϕ_1, ϕ_2 are the work functions of the tungsten tip and the Pb wedge respectively, d is the width of the tunnel barrier, E_i is the energy of the ith quantum state (QS) counting from the Fermi level, which is determined by the energy quantization of the electron confined in the nanoscale wedge with thickness H, and $\Delta E = E_{i+1} - E_i \cong \pi\hbar v_F/H$, where $\hbar$ is Plank's constant and v_F is the Fermi velocity. Here we take the Fermi level as the zero point of energy and neglect the small difference between ϕ_1 and ϕ_2 for convenience, and let $\phi_1 = \phi_2 = \phi$. The stationary Schrödinger equation which is satisfied by the electron

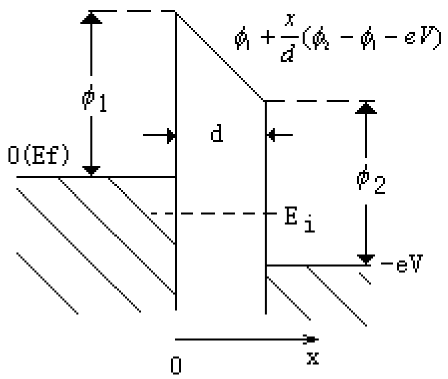

Figure 2. An electron tunnelling potential barrier ($V > 0$).

wave function ψ is given by

$$\frac{d^2\psi}{dx^2} + \frac{2\mu E_i}{\hbar^2}\psi = 0 \qquad (x < 0) \tag{1}$$

$$\frac{d^2\psi}{dx^2} + \frac{2\mu(E_i - \phi + [x/d]eV)}{\hbar^2}\psi = 0 \qquad (0 < x < d) \tag{2}$$

$$\frac{d^2\psi}{dx^2} + \frac{2\mu(E_i + eV)}{\hbar^2}\psi = 0 \qquad (x > d). \tag{3}$$

For convenience, let

$$k_{i1} = \left|\frac{2\mu E_i}{\hbar^2}\right|^{1/2} \qquad k_{i3} = \left|\frac{2\mu}{\hbar^2}(E_i + eV)\right|^{1/2}$$

where $|y|$ denotes the absolute value of y.

In the $x < 0$ region, the wave function is

$$\psi_1 = A_1 \exp(k_{i1}x) + A_2 \exp(-k_{i1}x). \tag{4}$$

In the $0 < x < d$ region, the solution of equation (2) is

$$\psi_2 = B_1 \operatorname{Ai}_1(k_2(x_{i0} - x)) + B_2 \operatorname{Ai}_2(k_2(x_{i0} - x)) \tag{5}$$

where

$$k_2 \equiv \left|\frac{2\mu eV}{\hbar^2 d}\right|^{1/3} \qquad x_{i0} = \left|\frac{(\phi - E_i)d}{eV}\right|$$

and $\operatorname{Ai}_1(x)$ and $\operatorname{Ai}_2(x)$ are two solutions of the Airy equation $d^2y/dx^2 - xy = 0$.

In the $x > d$ region, the solution of equation (3) is

$$\psi_3 = C \exp(ik_{i3}x). \tag{6}$$

Now, we get the coefficient relation of the continuity of wave function using the wave functions and their derivatives at $x = 0$ and $x = d$ as follows:

$$\frac{C}{A_2} = \frac{2k_{i1}k_2 \exp(-ik_{i3}d)I}{\Pi + i\Omega} \tag{7}$$

where

$$I = \operatorname{Ai}_1(k_2x_{i0} - k_2d)\operatorname{Ai}_2'(k_2x_{i0} - k_2d) - \operatorname{Ai}_2(k_2x_{i0} - k_2d)\operatorname{Ai}_1'(k_2x_{i0} - k_2d)$$

$$\Pi = k_{i1}k_2[\operatorname{Ai}_1(k_2x_{i0})\operatorname{Ai}_2'(k_2x_{i0} - k_2d) - \operatorname{Ai}_2(k_2x_{i0})\operatorname{Ai}_1'(k_2x_{i0} - k_2d)] - k_2^2[\operatorname{Ai}_1'(k_2x_{i0} - k_2d)\operatorname{Ai}_2'(k_2x_{i0}) - \operatorname{Ai}_1'(k_2x_{i0})\operatorname{Ai}_2'(k_2x_{i0} - k_2d)]$$

$$\Omega = k_{i1}k_{i3}[\operatorname{Ai}_1(k_2x_{i0})\operatorname{Ai}_2(k_2x_{i0} - k_2d) - \operatorname{Ai}_1(k_2x_{i0} - k_2d)\operatorname{Ai}_2(k_2x_{i0})] + k_2k_{i3}[\operatorname{Ai}_2(k_2x_{i0} - k_2d)\operatorname{Ai}_1'(k_2x_{i0}) - \operatorname{Ai}_1(k_2x_{i0} - k_2d)\operatorname{Ai}_2'(k_2x_{i0})]$$

where $\operatorname{Ai}'(x)$ denotes the derivative of the Airy function. Then we can obtain the penetration coefficient D—that is, the ratio of the probability flow densities of the incident and penetrating waves:

$$D = \sum_i \frac{k_{i3}|C|^2}{k_{i1}|A_1|^2} = \sum_i \frac{4k_{i1}k_{i3}k_2^2I^2}{\Pi^2 + \Omega^2}. \tag{8}$$

The tunnel current I is proportional to the penetration coefficient D.

(2) If the tip bias is negative, the potential barrier model is as shown in figure 3.

The stationary Schrödinger equations which are satisfied by the electron wave function ψ are the same as equations (1)–(3), but now $V < 0$, $E_i > 0$, the tunnel current is along the $-x$-direction, the wave function ψ_1 is a complex function, and ψ_3 is an exponentially decreasing function.

Using the continuity of wave functions and their derivatives at $x = 0$ and $x = d$, we can obtain the penetration coefficient as above:

$$D = \sum_i \frac{k_{i1}|A|^2}{k_{i3}|C|^2} = \sum_i \frac{4k_{i1}k_{i3}k_2^2 I^2}{\Pi^2 + \Omega^2} \tag{9}$$

where

$$I = \mathrm{Ai}_1(k_2x_{i0})\,\mathrm{Ai}_2'(k_2x_{i0}) - \mathrm{Ai}_2(k_2x_{i0})\,\mathrm{Ai}_1'(k_2x_{i0})$$

$$\Pi = -k_{i1}k_2[\mathrm{Ai}_1(k_2x_{i0}+k_2d)\,\mathrm{Ai}_2'(k_2x_{i0}) - \mathrm{Ai}_2(k_2x_{i0}+k_2d)\,\mathrm{Ai}_1'(k_2x_{i0})] + k_2^2[\mathrm{Ai}_1'(k_2x_{i0})\,\mathrm{Ai}_2'(k_2x_{i0}+k_2d) - \mathrm{Ai}_1'(k_2x_{i0}+k_2d)\,\mathrm{Ai}_2'(k_2x_{i0})]$$

$$\Omega = k_{i1}k_{i3}[\mathrm{Ai}_1(k_2x_{i0})\,\mathrm{Ai}_2(k_2x_{i0}+k_2d) - \mathrm{Ai}_1(k_2x_{i0}+k_2d)\,\mathrm{Ai}_2(k_2x_{i0})] - k_2k_{i3}[\mathrm{Ai}_2(k_2x_{i0})\,\mathrm{Ai}_1'(k_2x_{i0}+k_2d) - \mathrm{Ai}_1(k_2x_{i0})\,\mathrm{Ai}_2'(k_2x_{i0}+k_2d)].$$

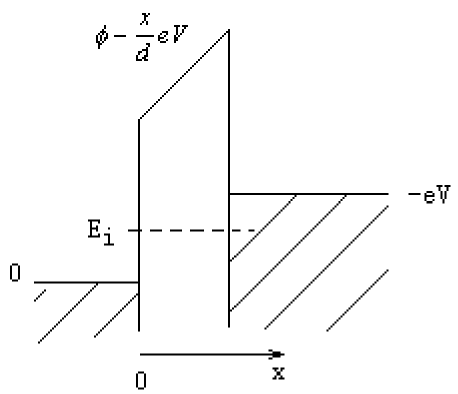

Figure 3. An electron tunnelling potential barrier ($V < 0$).

Using the parameters $\Delta E_i = \Delta = 1.2$ eV, $d = 10$ Å, $\phi = 4.0$ eV, we produced a tunnel I–V curve, which is shown in figure 4.

In order to make a comparison with tunnel current curves derived from the penetration coefficient formula for an arbitrary potential, quantum mechanically, for this model, we give our tunnel current curve in figure 5 derived according to the following formula which is taken from reference [4] (their equation (3)):

$$I_{(V)} = \pm A \sum_i \exp\left[-\frac{2}{\hbar}\int_0^d \sqrt{2m\left(\phi - E_i - \frac{x}{d}eV\right)}\,\mathrm{d}x\right] \tag{10}$$

where $\pm$ indicate the polarity of the bias, A is a constant, m a free-electron mass, e the charge of an electron. The sum is taken over E_i between 0 and $-eV$.

Comparing figure 4 and figure 5 to the experimental results shown in figure 5(B) in reference [4], we see that the tunnel current curve in figure 4 fits experiment better than that in figure 5, especially for positive bias; the tunnel current shows gradual change near the energy

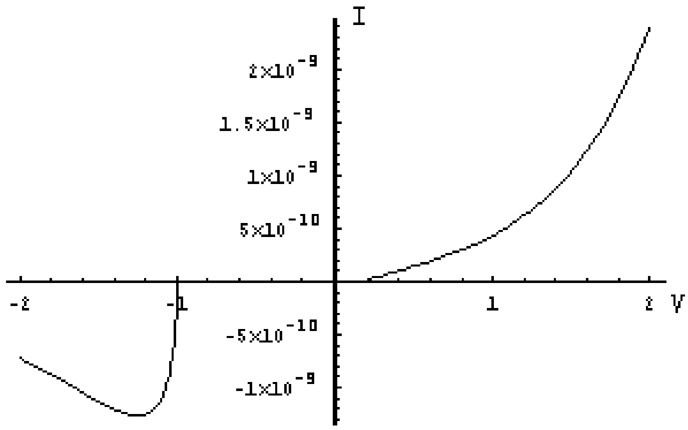

Figure 4. A tunnelling spectrum derived using equations (8) and (9).

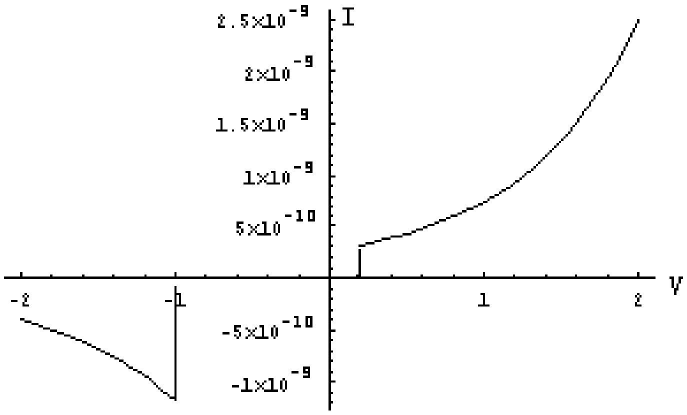

Figure 5. The tunnel I–V curve calculated from equation (10) with the parameters $\Delta = 1.2$ eV, $d = 10$ Å, $\phi = 4.0$ eV.

level. However, there is an abrupt change of the tunnel current curve at $V = -E_i/e$ in figure 5, which means that the above model can describe the effect of quantum tunnelling between the STM and quantum wedge well, but formula (10) should be replaced by equations (8) and (9) for this system. In fact, A in formula (10) is not a constant, but is dependent on the bias V; moreover, it is an approximation appropriate only under the condition that the potential changes slowly.

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