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LETTER TO THE EDITOR

STM imaging of a nanometre conducting structure in the exponential approximation

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Abstract. The correspondence between the STM image and the contours of a nanometre conductor lying under a planar insulating surface is investigated theoretically. A simple model is considered in which the cross sections of the potential barriers in the vacuum and the insulator are rectangular. Both the direct and inverse problems are solved in analytical parametric form using the exponential approximation for the tunnelling current.

Considerable success has already been achieved in the creation of nanometre structures of preselected form [1, 2]. Recently, in [3], different configurations with the characteristic dimension of 60 Å were reproduced on a metallic surface from STM-fabricated craters with depth and width ≃20 Å. Similar operations can naturally be carried out also on a thin conducting film lying on an insulating substrate, thereby realising nanometre lithography. When an insulating film fixing the conductor is superimposed, an important problem in the investigation of such a formation arises.

Consider a nanometre conductor placed near an insulator surface as shown in figure 1(*a*). The insulating film is assumed to be transparent to tunnelling electrons. Thus it is possible to record a current between the nanometre conductor and the STM tip by bringing the tip near to the surface of the film.

Let us assume, for simplicity, that the vacuum–insulator interface is planar (in general its shape can be determined by STM or AFM [4]). We will consider large-scale (nanometre) contours of the insulator–conductor interface, $f_2(x)$, with dimensions much larger than the interatomic distance and electron wavelength. Therefore, the length of the current-carrying tunnel space in the vacuum and insulator must be large compared with these distances.

The method used below, which connects the STM image to nanometre conductor contours, is essentially one of the simplest versions of tunnelling microscope theory [5–7]. In the present paper (unlike in [5–7]) the exponential approximation for the tunnel current is used under the natural assumption that the corresponding pre-exponent, which depends on the surface geometry and electron local density of states, is a function of the tip coordinates that varies considerably more slowly than the action taken along the most probable tunnelling path (MPTP).

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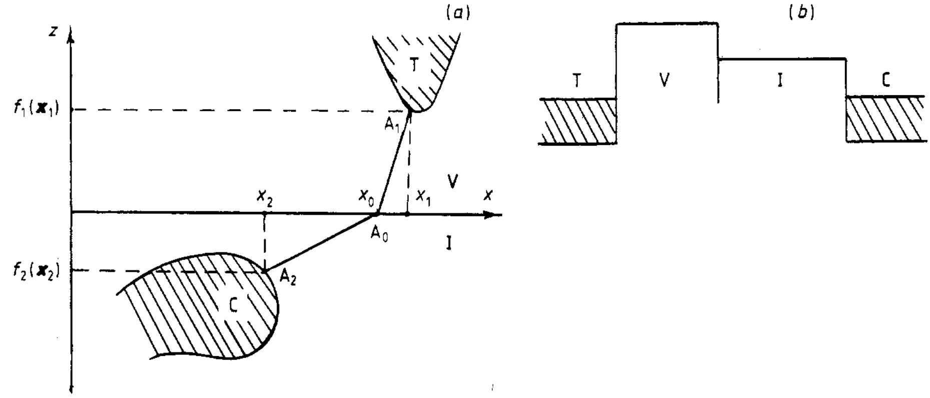

Figure 1. (*a*) Planar picture of the disposition of the nanometre conductor C in the insulator I and of the STM tip T in the vacuum V. The broken line $A_1A_0A_2$ is the MPTP. Axis *y* is perpendicular to the page. (*b*) Potential energy diagram section along the MPTP.

Consider the model where the cross sections of the barriers in the vacuum and insulator are rectangular (figure 1(*b*))†. In the exponential approximation, the tunnel current $j \simeq \exp(-2s)$, where

$$s(\boldsymbol{x}_0, \boldsymbol{x}_1, \boldsymbol{x}_2) = \gamma_1(f_1^2(\boldsymbol{x}_1) + |\boldsymbol{x}_0 - \boldsymbol{x}_1|^2)^{1/2} + \gamma_2(f_2^2(\boldsymbol{x}_2) + |\boldsymbol{x}_0 - \boldsymbol{x}_2|^2)^{1/2} \tag{1}$$

is the absolute value of the action taken along the MPTP. Here $(\boldsymbol{x}_1, f_1(\boldsymbol{x}_1))$, $(\boldsymbol{x}_2, f_2(\boldsymbol{x}_2))$ and $(\boldsymbol{x}_0, 0)$ are the rectangular coordinates of the points of intersection of the MPTP with the surface of the STM tip, the surface of the nanometre conductor, and the surface of the insulator, respectively (figure 1). γ_1 and γ_2 are absolute values of the corresponding wave numbers. We use the vector notation $\boldsymbol{x} = (x, y)$.

If the STM tip radius is small compared with the typical value of the curvature radius of the conductor investigated then the function $f_1(\boldsymbol{x})$ defines the trajectory of the tip coinciding with the STM image. The tip coordinates $(\boldsymbol{x}_1, f_1(\boldsymbol{x}_1))$ and conductor contours $f_2(\boldsymbol{x})$ being given, the MPTP is the broken line determined by minimising the action (1) over $\boldsymbol{x}_2$ and $\boldsymbol{x}_0$. This leads to the simultaneous equations

$$\begin{gathered}\gamma_1(\boldsymbol{x}_0 - \boldsymbol{x}_1)/(f_1^2(\boldsymbol{x}_1) + |\boldsymbol{x}_0 - \boldsymbol{x}_1|^2)^{1/2} \\ + \gamma_2(\boldsymbol{x}_0 - \boldsymbol{x}_2)/(f_2^2(\boldsymbol{x}_2) + |\boldsymbol{x}_0 - \boldsymbol{x}_2|^2)^{1/2} = 0 \\ \boldsymbol{x}_0 = \boldsymbol{x}_2 + f_2(\boldsymbol{x}_2)f_{2\boldsymbol{x}}(\boldsymbol{x}_2).\end{gathered} \tag{2}$$

The first of these equations is a well known (from geometrical optics) condition describing the inverse proportionality of cosines of incident ray angles to the corresponding wave numbers. The second equation represents the perpendicularity of the MPTP and $f_2(\boldsymbol{x})$ at their point of intersection $(\boldsymbol{x}_2, f_2(\boldsymbol{x}_2))$. The action s in these equations for the exponential approximation considered is constant because the value of the current in the STM measurements is constant. The STM image $f_1(\boldsymbol{x}_1)$ can be expressed in terms of conductor contours $f_2(\boldsymbol{x}_2)$ by solving (2) in the parametric form:

$$\begin{gathered}f_1 = \gamma_1^{-2}[\gamma_1^2 + (\gamma_1^2 - \gamma_2^2)|f_{2\boldsymbol{x}}(\boldsymbol{x}_2)|^2]^{1/2}[\gamma_2 f_2(\boldsymbol{x}_2) + s(1 + |f_{2\boldsymbol{x}}(\boldsymbol{x}_2)|^2)^{-1/2}] \\ \boldsymbol{x}_1 = \boldsymbol{x}_2 + f_{2\boldsymbol{x}}(\boldsymbol{x}_2)[(1 - \gamma_2^2/\gamma_1^2)f_2(\boldsymbol{x}_2) - (s\gamma_2/\gamma_1^2)(1 + |f_{2\boldsymbol{x}}(\boldsymbol{x}_2)|^2)^{-1/2}].\end{gathered} \tag{3}$$

Here $f_1 > 0$ and $f_2 < 0$ always. Equations (2) and (3) allow us to perform the scale

† Such an approximation appears to be satisfactory for materials with small carrier concentrations. In a more general case, barrier bending and non-plane vacuum–insulator interfaces can be considered using more complicated models and computer investigation. In this communication we restrict ourselves to the indicated simplest model.

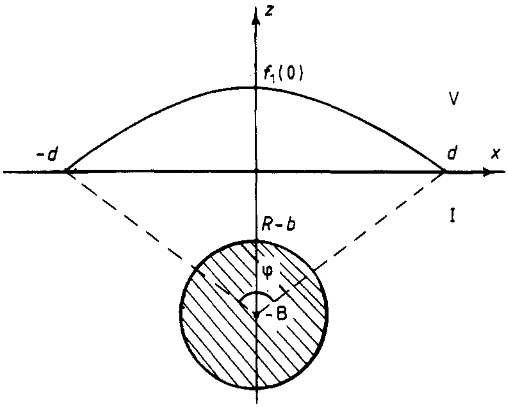

Figure 2. STM tip trajectory for the cylindrical conductor.

transformations $f_j \to f_j\gamma_1/s$ and $x_j \to x_j\gamma_1/s$, which permits us to exclude the dependence on s thus leaving only the dependence on γ_2/γ_1. For $\gamma_1 = \gamma_2$, equations (3) describe the image of a conductor surface without an insulating film. Equations (3) can be easily simplified for the case $\gamma_2/\gamma_1 \ll 1$ which holds, e.g., when the conductor and insulator are made from semiconductor materials of $Al_xGa_{1-x}As$ type.

If the surface of the conductor has slight bending, then omitting the terms containing the derivative f_{2x} we have

$$f_1(x) = s/\gamma_1 + (\gamma_2/\gamma_1)f_2(x). \tag{4}$$

Thus the slope of the conductor surface with slight bending, when imaged, diminishes by γ_2/γ_1 times.

For a large slope f_{2x}, equations (3) give

$$|f_{1x}(x)| = \gamma_2(\gamma_1^2 - \gamma_2^2)^{-1/2} \tag{5}$$

regardless of the actual form of $f_2(x)$. The slope of the STM tip trajectory cannot exceed the value $\gamma_2(\gamma_1^2 - \gamma_2^2)^{-1/2}$. This follows from the remarkable relation

$$f_{1x}(x_1) = \gamma_2 f_{2x}(x_2)/[\gamma_1^2 + (\gamma_1^2 - \gamma_2^2)|f_{2x}(x_2)|^2]^{1/2} \tag{6}$$

which can be obtained by taking derivatives of both parts of (3) with respect to x_2. Using (6) we can easily invert equations (3) and obtain the parametric expression for $f_2(x_2)$ symmetrical to (3):

$$f_2 = \gamma_2^{-2}[\gamma_2^2 + (\gamma_2^2 - \gamma_1^2)|f_{1x}(x_1)|^2]^{1/2}\,[\gamma_1 f_1(x_1) - s(1 + |f_{1x}(x_1)|^2)^{-1/2}] \tag{7}$$

$$x_2 = x_1 + f_{1x}(x_1)[(1 - \gamma_1^2/\gamma_2^2)f_1(x_1) + (s\gamma_1/\gamma_2^2)(1 + |f_{1x}(x_1)|^2)^{-1/2}].$$

These equations can also be obtained from (3) by making the substitutions $f_1 \leftrightarrow -f_2$, $x_1 \leftrightarrow x_2$. It follows from (7) that the MPTP is perpendicular to the STM tip trajectory at their intersection point $(x_1, f_1(x_1))$.

Let the conductor surface be planar, $f_2(x) = a \cdot x$. Then it can be obtained from (3) that

$$f_1(x) = [s(1 + a^2)^{-1/2} + \gamma_2 a \cdot x]/[\gamma_1^2 + (\gamma_1^2 - \gamma_2^2)a^2]^{1/2}. \tag{8}$$

So the planar surface is transformed into a planar image.

Let us consider the image of the cylindrical conductor when $f_2(x) = (R^2 - x^2)^{1/2} - b$ (figure 2). In order to avoid cumbersome formulae we shall not reproduce the expression for $f_1(\boldsymbol{x})$ which can be found by solving the algebraic equation to the fourth order. The STM image of the conductor can be obtained in a restricted sector defined by the angle φ (figure 2). The image enlarges the conductor surface along $\boldsymbol{x}$ by a factor of $\zeta = (d^2 + b^2)^{1/2}/R$, and has the maximum distance from the sample surface equal to $f_1(0)$. It is easy to obtain the following expressions for the parameters introduced:

$$\begin{aligned} &\varphi = 2\cos^{-1}[\gamma_2 b/(s+\gamma_2 R)] \qquad && d = [(s/\gamma_2 + R)^2 - b^2]^{1/2} \\ &\zeta = s/\gamma_2 R + 1 && f_1(0) = (1/\gamma_1)[s + \gamma_2(R - b)]. \end{aligned} \tag{9}$$

For example, a sector with $\varphi = \pi/2$ can be observed only when $s \geqslant (\sqrt{2}b - R)\gamma_2$; then $f_1(0) \geqslant (\sqrt{2} - 1)\gamma_2 b/\gamma_1$. Thus, if the conductor parameters R and b are known, we can select the value of s (and hence the current j) so that the surface of the conductor can be measured in a preselected sector φ. In the above-mentioned case $\gamma_2/\gamma_1 \ll 1$, the image of the cylindrical surface is hyperbolic:

$$f_1(\boldsymbol{x}) = (\gamma_2/\gamma_1)[R - (b^2 + x^2)^{1/2}] + s/\gamma_1. \tag{10}$$

The case of a straight thin conducting wire parallel to the surface $(\boldsymbol{x}, 0)$ is essentially the limiting case of the cylindrical conductor as $R \to 0$. In order to search out the $f_1(\boldsymbol{x})$ we must put $f_2(\boldsymbol{x}_2) = -b$ in equations (3) and exclude f_{2x}. Unfortunately the result is very cumbersome because the problem is again reduced to an algebraic equation to the fourth order. Equations (9) and (10) are valid for a wire when R tends to zero.

Note that for a given current j, part of the conductor surface remains inaccessible to observation. In some cases it is possible to observe more distant parts of the surface by reducing the current j. In other cases, when the conductor surface has both convexities and concavities, the enlargement of the tunnelling space can lead to a diminishing of its visible part. Nevertheless, the fact that equations (3) can be inverted seems remarkable.

In summary, by means of a simple model example we have demonstrated the possibility of performing a theoretical determination of the correspondence between contours of nanometre conductors under tunnel-penetrative film and the STM image.

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