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Apparent barrier height in scanning tunneling microscopy

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The apparent barrier height in the scanning tunneling microscope, defined in terms of the rate of change (at constant bias) of the logarithm of current with tip-sample separation, is calculated as a function of separation. It is found to be substantially lower than the sample work function in the range of tip-sample separations commonly used experimentally, and becomes very small in the region just before contact between tip and sample.

It is often stated that the rate of change of the logarithm of current with tip-sample separation (at a small constant bias) in the scanning tunneling microscope provides a measure of the height of the tunneling barrier. If we note[1] that for a one-dimensional square barrier of height ϕ above the Fermi level the tunneling current I at a small bias V is proportional to $V\exp(-1.025s\sqrt{\phi})$, where s is the barrier thickness in Å and where ϕ is given in eV, then it is clear that for constant bias, $\phi = 0.952(d\ln I/ds)^2$. In view of this, an apparent barrier height is often defined in scanning tunneling microscopy as

$$\phi_A(\mathrm{eV}) = 0.952\left[\frac{d\ln I}{ds(\text{Å})}\right]^2 . \tag{1}$$

[In atomic units, where $|e| \equiv \hbar \equiv m \equiv 1$, the corresponding formulas are $I \propto V\exp(-2s\sqrt{2\phi})$ and $\phi_A = \frac{1}{8}(d\ln I/ds)^2$.] A number of authors present "local barrier-height" images of surfaces (that is, images of ϕ_A) as an alternative to the more commonly shown "topographic" images.[2-5]

In this paper we will study the apparent barrier height ϕ_A as a function of separation for a single-atom tip and a perfectly flat uniform sample surface. We will consider, in particular, the case of two planar parallel metallic electrodes, one of which has an adsorbed atom (representing the tip), with a small fixed bias voltage between them; and we will use the jellium model[6] to represent the metallic electrodes themselves, taking the two to be identical [with $r_s = 2$ bohrs (Ref. 7)].

Now it is clear that for tip-sample separation $s \rightarrow \infty$, $\phi_A(s) \rightarrow \Phi$, the sample surface work function.[8] The question we address here is whether or not $\phi_A(s)$ will be close to Φ for the range of tip-sample separations commonly used in scanning tunneling microscopy. We will begin by discussing ϕ_A for the case of the two electrodes in the absence of the atom, in order to illustrate several simple but general aspects of the problem. Before presenting the actual computational results for this case, however, we give a short analytic discussion.

The tunneling current, omitting pre-exponential factors, with energies in eV and distances in Å, can be written approximately for small bias as[1]

$$I \propto V\exp\left[-1.025\int_0^s dz\,[v(z)-\varepsilon_F]^{1/2}\right] , \tag{2}$$

where $v(z)$ is the barrier potential and $v(0) = v(s) = \varepsilon_F$. This last equality sets the origin of z and defines s as the barrier thickness at the Fermi energy ε_F. In most cases, s will differ by some nearly constant distance from an electrode separation defined geometrically (such as the distance between the positive background edges of the two electrodes).

Now since the barrier potential $v(z)$ is symmetric about the midpoint of the gap $z = s/2$, if we assume that $v(z)$ has its maximum there, we can combine Eqs. (1) and (2) to obtain

$$\phi_A^{1/2} = \phi_{\max}^{1/2} + \int_0^{s/2} dz\,[v(z)-\varepsilon_F]^{-1/2}\frac{\delta v(z)}{\delta s} , \tag{3}$$

where $\phi_{\max} = v(s/2) - \varepsilon_F$ is the maximum barrier height. The quantity $\delta v(z)$ is the variation in the potential that occurs when the electrode separation is increased by δs (keeping the left-hand turning point always at $z = 0$). If it were to be true that the potential quickly reached a constant value moving away from each electrode toward the center of the barrier, and that the variation in $v(z)$ consisted only of an expansion of the width of this constant-potential region, then $\delta v(z)/\delta s$ would vanish over the range of integration in the second term of Eq. (3). This would leave $\phi_A = \phi_{\max}$, the barrier height in the constant-potential region, as we would expect intuitively for this simple case (where we note again that we have made the further simplification of omitting preexponential factors in the expression for the tunneling current).

Now for large s, the major contribution to $\delta v(z)/\delta s$ in Eq. (3) arises from the fact that $v(z)$ includes the image potential seen by the tunneling electrons. However, Binnig *et al.*[9] have pointed out that for the case with one-dimensional symmetry, even though at large separations there are contributions of $O(s^{-1})$ to each of the two terms in Eq. (3) due to the image effect, they cancel each other, leaving only a term of $O(s^{-2})$ in ϕ_A. Therefore, we will neglect image effects at large distances from the electrodes in our calculations of ϕ_A.[10] At shorter distances, the surface potential no longer has an image form in any case.[11]

We now present the results of our actual computations for the pair of electrodes in the absence of the atom. The tunneling current $I(s)$ is calculated as described in Ref. 12, and ϕ_A is obtained from $I(s)$ using Eq. (1). Figure 1 shows these results for ϕ_A, with $\phi_{\max}$ given for comparison,[13] as a function of the separation between the positive

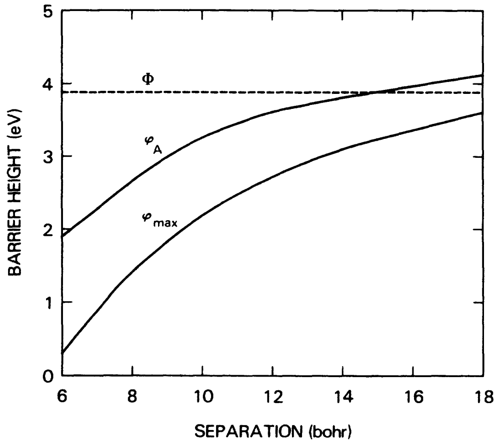

FIG. 1. Apparent barrier height ϕ_A and maximum barrier height ϕ_{max} for two electrodes ($r_s=2$ jellium model) in the absence of adsorbed atom. Separation given is between positive-background edges of the electrodes. The work function Φ for a single such electrode is shown for comparison. (1 bohr = 0.529 Å.)

background edges of the two electrodes.[14] Note that ϕ_A goes from 1.9 eV for the smallest separation shown in Fig. 1 to 4.1 eV for the largest separation shown. The work function Φ for one of the electrodes by itself is 3.9 eV,[6] so we see that ϕ_A can in fact go slightly above this value (it reaches a maximum of 4.3 eV somewhat further out); of course at sufficiently large separations, we must have $\phi_A \rightarrow \Phi$.[15] Note also that the actual maximum barrier height ϕ_{max} goes from 0.3 to 3.6 eV over the separation range shown; for sufficiently large separations, $\phi_{max} \rightarrow \Phi$ also.

The striking fact about Fig. 1 is that ϕ_{max} is well below the work function Φ for separations in the range relevant to scanning tunneling microscopy. The difference between ϕ_A and ϕ_{max} arises from the second term in Eq. (3), with an additional contribution from the preexponential factor[15] omitted from Eqs. (2) and (3). To the extent to which we can loosely think of the barrier potential as arising from the potentials of the two electrodes adding in some possibly nonlinear way, we see that the behavior exhibited in Fig. 1 is a consequence of the relatively long range of the potential at a surface, even in the absence of image effects. We discuss, therefore, in more detail, the nature of this potential outside of a metal surface.

The total effective potential $v_{eff}(r)$ acting upon an electron in an inhomogeneous many-electron system is the sum of the electrostatic potential $v_{es}(r)$ and an exchange-correlation potential $v_{xc}(r)$, as discussed by Kohn and Sham.[16] The potential v_{xc} represents the interaction between an electron and its exchange-correlation hole; we recall that as an electron moves from the bulk of a metal out through a surface, the exchange-correlation hole around it lags behind, staying on the surface and becoming the image charge.

In the present calculation, we employ the widely used local-density approximation[16] for v_{xc}, in which, crudely speaking, the effect of the exchange-correlation hole associated with an electron is taken to be the same as that due to the hole that would surround the electron if it were in a homogeneous electron gas, of density equal to that of the inhomogeneous gas at the position of the electron. Clearly this is invalid when the electron and its exchange-correlation hole become separated, as they do when the electron moves into the image region far outside the surface. The image contribution to ϕ_A can be neglected however, as noted above, so that the failure of the local-density approximation to give an image contribution to the potential far outside does not represent a problem for our discussion. On the other hand, for distances much closer to the surface, the approximation is quite adequate[11] [and conversely the asymptotic image form $v_{xc}(z) \sim -e^2/4z$ breaks down]. It is only in a distance range intermediate between these two regions that the use of the local-density approximation might be expected to have any quantitative consequence for the value of ϕ_A.

The electron density $n(z)$ at our surface decays exponentially into the vacuum: $n(z) \sim \exp(-\alpha z)$. This has the consequence that $v_{es}(z) \sim \exp(-\alpha z)$. But in the local-density approximation, the exchange-correlation potential is roughly proportional to the cube root of the local electron density, so $v_{xc}(z) \sim \exp(-\frac{1}{3}\alpha z)$ in the vacuum region. It is this slow decay of v_{xc} that causes the relatively slow decay toward the vacuum level of $v_{eff} \equiv v_{xc} + v_{es}$ at a surface, as illustrated in Fig. 2.[17] This, as discussed above, is what leads to ϕ_{max} being well below Φ in Fig. 1.[18]

We now return to the case of two flat semi-infinite metallic electrodes in which one of them has an adsorbed atom representing the tip. We take a Na atom for the tip, and directly calculate the difference between the total tunneling current in the presence of the tip atom and in its absence, for a small fixed bias, as described in Ref. 12. (The two total currents are individually infinite because of the infinite surface area of the electrodes.) We will denote this current difference by δI. It is computed as a function of tip-sample separation s, defined as the distance from the nucleus of the tip atom to the positive background

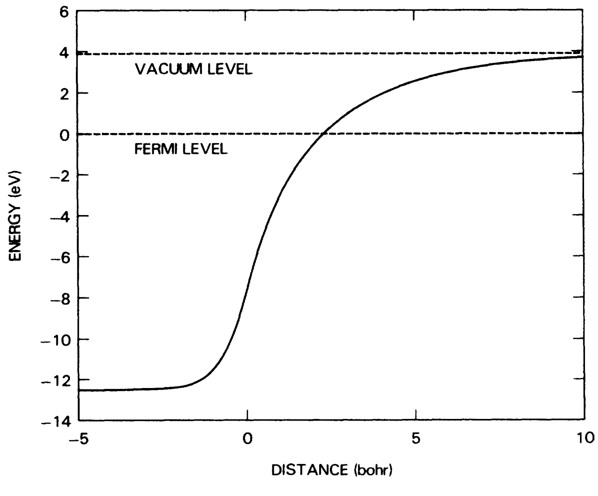

FIG. 2. Surface potential barrier v_{eff} calculated for jellium model ($r_s=2$ bohr) using local-density approximation for exchange and correlation. Distance is relative to position of positive-background edge. (1 bohr = 0.529 Å.)

edge of the sample electrode. Since the distance d from the Na nucleus to the positive background of the tip electrode is kept fixed at 3 bohrs,[19] the separation $s=d=3$ bohrs, for which the atom is midway between the two electrodes, corresponds to the nominal point of contact between tip and sample.[12]

If for purposes of comparison with experiment we wish to consider the tip atom to be adsorbed on an electrode of area A, then we can *approximate* the total current flowing between this tip electrode and the sample by $I(s)=\delta I(s)+Aj_0(s)$, where j_0 is the current density for the pair of semi-infinite metallic electrodes in the absence of the atom. If the tip were, e.g., a pyramid in the experimental configuration, with the apex atom adsorbed on a triangle of three substrate atoms, we would approximate this by simply taking A to be three times the area corresponding to the covalent radius of the substrate atoms.

The apparent barrier height $\phi_A(s)$ that we obtain from $I(s)$ via Eq. (1) is shown in Fig. 3, both for the case in which we neglect the direct effect of the substrate by taking $A=0$ (solid curve) and for the case in which we take A to be the area of three substrate atoms as described above (dot-dash curve).[20] We see that ϕ_A is well below the sample work function Φ except at the largest distances shown in the graph, where in fact, as in Fig. 1, it goes slightly above (it reaches a maximum of 4.3 eV at $s\sim 19$ bohrs). That it is below Φ for intermediate distances results from the long range of both the exchange-correlation part of the surface potential, as discussed in connection with Fig. 1, and the electrostatic potential due to the charge-transfer dipole that forms at the Na tip atom. That it is even further below at the shortest distances[21] results from the complete absence at these separations of a potential barrier to electron tunneling, as we see below (the analogous region was not shown in Fig. 1). Near the point of nominal contact ($s=3$ bohrs), the tunneling current reaches approximately a plateau,[12] and thus ϕ_A is near zero. In an experiment of Gimzewski and Möller with an Ir tip and a Ag sample, for one set of data the ϕ_A was found to be as low as ~ 1.5 eV (Ref. 21) and for another set (reproduced in Ref. 12) a current plateau was seen in the region before tip-sample contact, which corresponds to $\phi_A \sim 0$.[22]

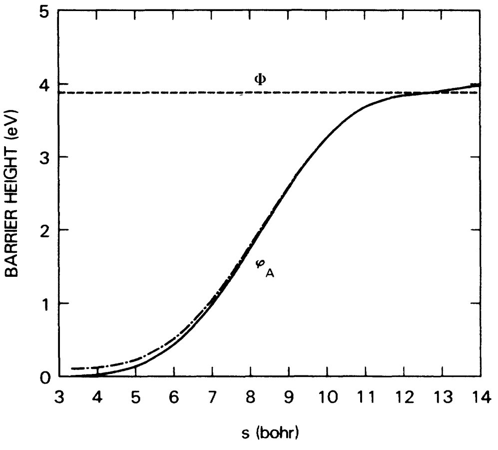

FIG. 3. Apparent barrier height ϕ_A for two electrodes ($r_s=2$ jellium model), one representing the sample, the other, with an adsorbed Na atom, representing the tip. See text for distinction between solid and dot-dash curves. The work function Φ for the sample electrode by itself is shown for comparison. The tip-sample separation (defined in the text) is denoted by s. (1 bohr = 0.529 Å.)

Figure 4 gives contour maps of the actual barrier potential for several distances s. It shows the contour $v_{\rm eff}(r)=\varepsilon_F$ (this is the one closest to the atom), as well as a number of other contours for values above ε_F; thus the contour-filled areas represent regions where a Fermi-level electron encounters a potential barrier. At $s=5$ bohrs, for example, the electrons moving from the single-atom tip to the sample electrode encounter essentially no barrier whatsoever, while at $s=11$ bohrs, there is a barrier for electrons tunneling along all directions.

For $s=9$ bohrs, e.g., electrons tunneling along most directions encounter a barrier, but, in fact, even along directions close to the surface normal through the atom, there will be an effective barrier. The reason for this is that though there is a small opening in the barrier, whose transverse size we denote by a, electrons moving through this opening will, by the uncertainty principle, have a minimum transverse momentum of $O(\hbar/a)$. This in turn decreases the energy available for motion along the direction of the surface normal, and thus a Fermi-level electron

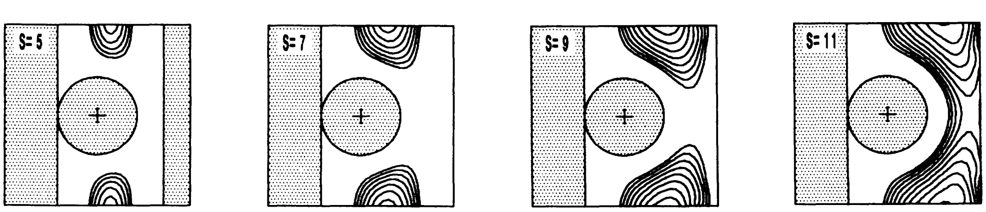

FIG. 4. Contour maps of the potential $v_{\rm eff}$ for two-electrode case with an adsorbed Na atom (tip). The presence of the atom is represented by a shaded circle with a cross at the position of the nucleus; the positive background regions of both tip and sample electrodes are shaded also. Maps are shown for four values of s (given in bohr), which is the distance between the nucleus of the tip atom and the positive background edge of the sample electrode. The nucleus is at the center of each box, so that the sample electrode in fact lies outside of the box for all but the smallest of the s values shown ($s=5$ bohr). The contour closest to the atom in each case is that for $v_{\rm eff}=\varepsilon_F$; the contours shown for higher energy values are spaced by $\frac{1}{4}$ eV, starting at ε_F. (1 bohr = 0.529 Å.)

will in fact have to tunnel through a barrier even in the region of this opening.[23,24]

We have seen in this paper that some of the familiar ideas of macroscopic surface physics break down at the short distances involved in scanning tunneling microscopy. The barrier height, both calculated as $v_{\mathrm{eff}}(r)-\varepsilon_F$, and measured in terms of ϕ_A, can fall well below the actual work function of the sample for separations commonly encountered experimentally.

I am delighted to thank J. Tersoff for a number of helpful discussions, and to express my gratitude to him and to J. E. Demuth, R. M. Feenstra, and R. J. Hamers for many useful comments on the manuscript.

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[1] See, e.g., J. G. Simmons, J. Appl. Phys. **34**, 1793 (1963).

[2] G. Binnig and H. Rohrer, Surf. Sci. **126**, 236 (1983).

[3] M. S. Khaikin and A. M. Troyanovskii, Sov. Tech. Phys. Lett. **11**, 511 (1985).

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[5] B. Marchon, P. Bernhardt, M. E. Bussell, G. A. Somorjai, M. Salmeron, and W. Siekhaus, Phys. Rev. Lett. **60**, 1166 (1988).

[6] N. D. Lang, in *Theory of the Inhomogeneous Electron Gas*, edited by S. Lundqvist and N. H. March (Plenum, New York, 1983), p. 309.

[7] $(4/3)\pi r_s^3 \equiv \bar{n}^{-1}$, where $\bar{n}$ is the mean bulk electron density.

[8] The work function of the tip electrode is the same as that of the sample here because the work function of a macroscopic electrode is not changed by the presence on it of a single atom. The dipole moment of this atom of course changes the local electrostatic potential, which enters our calculation via the self-consistently computed wave functions.

[9] G. Binnig, N. Garcia, H. Rohrer, J. M. Soler, and F. Flores, Phys. Rev. B **30**, 4816 (1984).

[10] See also J. H. Coombs, M. E. Welland, and J. B. Pethica, Surf. Sci. (to be published); M. C. Payne and J. C. Inkson, *ibid.* **159**, 485 (1985).

[11] Cf. N. D. Lang, Phys. Rev. Lett. **46**, 842 (1981).

[12] N. D. Lang, Phys. Rev. B **36**, 8173 (1987).

[13] Curves of $\phi_{\max}$ have also been given by J. Ferrante and J. R. Smith, Phys. Rev. B **31**, 3427 (1985).

[14] By construction of the jellium model, the positive background edge is half of an interplanar spacing outside of the outermost lattice plane. The image plane and classical turning points are, respectively, $\sim 1\frac{1}{2}$ and $\sim 2\frac{1}{2}$ bohrs outside of the background edge (for $r_s = 2$ bohrs).

[15] Note that for the simpler case of a square barrier, the s-dependent part of the preexponential factor omitted from Eq. (2) is just s^{-1} for large s, which gives $\phi_A \approx \Phi(1+1.95 s^{-1}\Phi^{-1/2})$, where s is in Å and Φ is in eV. This shows the way in which ϕ_A approaches Φ from above for very large s.

[16] W. Kohn and L. J. Sham, Phys. Rev. **140**, A1133 (1965).

[17] Cf. discussion in N. D. Lang and A. R. Williams, Phys. Rev. B **25**, 2940 (1982).

[18] A possible unrelated source of low apparent barrier heights in some of the experiments is the compression of impurity particles by the tip, with a consequent change in the calibration of displacement, as discussed by J. H. Coombs and J. B. Pethica, IBM J. Res. Dev. **30**, 455 (1986).

[19] We keep the tip atom at the equilibrium distance from its electrode calculated in the absence of the sample.

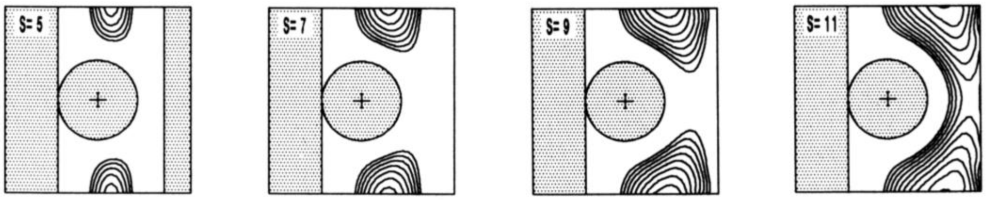
[20] We take the covalent radius of the substrate atoms to have the typical value of ~ 1.3 Å. Note also that as $A \to \infty$, the ϕ_A curve of course tends toward that shown in Fig. 1 (note the different origin for the distance scale there).

[21] This is the region of near contact, which has been explored experimentally by J. K. Gimzewski and R. Möller [Phys. Rev. B **36**, 1284 (1987)], and theoretically in Ref. 12.

[22] It is surmised that this variability in the data is related to the chemical identity of the actual tip atom. If it is a loosely bound impurity atom then it may jump toward the sample as the tip is moved in before the plateau has a chance to develop; if, on the other hand, it is strongly bound, then the plateau does have a chance to develop before any substantial movement of the tip atom occurs.

[23] I would like to thank Jerry Tersoff for pointing this out.

[24] The potential at the saddle point in this opening is just 0.4 eV below the Fermi level ($s = 9$ bohrs). If the potential parallel to the surface through this saddle point is fit with a parabola, the minimum transverse kinetic energy is found to be ~ 1.9 eV, so the effective barrier is at least ~ 1.5 eV.



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