

Scanning tunneling microscope as a structure-modifying tool

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We explore the possibility that surface charge induced by the scanning tunneling microscope will influence the structure of the surface under investigation. In general, we find that the emission currents limit the induced charge densities and preclude major structural modifications on the more stable surfaces. However, the possibility of modifying less stable structures or of reducing the transition temperatures for transformation between different surface phases does exist and is discussed in detail.

Recently, the scanning tunneling microscope (STM) has been used to investigate a variety of surfaces,¹⁻³ including the Si(111)(7×7),¹ to obtain a real-space map of the surface on an atomic scale. In doing so, a large field gradient (10⁶–10⁷ V/cm) is applied between a probe of atomic dimensions and the surface itself, and the resulting tunneling current is then monitored as the tip is rastered above the surface. Such field gradients are sufficiently large to perturb the charge density on the surface. A large increase in charge density, particularly for semiconductors, for example, may result in the filling of the unoccupied surface states and could lead to a change in the reconstruction of the surface. This possibility is based on the fact that, in general, the higher lying, unoccupied surface states on a semiconductor surface correspond to the antibonding states in diatomic or polyatomic molecules (Fig. 1). Filling such states can lead to sufficient repulsive energy to cause dissociation in molecules or, in the case of semiconductor surfaces, to actual reconstruction.

It is the purpose of this paper to inquire as to what conditions are necessary to produce significant changes in the charge density at the surface and to inquire as to whether or not such conditions can be achieved experimentally. This analysis requires the calculation of the steady-state induced surface charge. Therefore, we will first calculate this induced charge as a function of applied potential and then consider the charge transport processes (e.g., tunneling, field emission) which determine the maximum excess charge density which can be realized at the surface.

The potential between a grounded, conducting plane at $x = 0$ and a point charge q at some distance a from that plane is given by

$$V(x,y,z) = (q/4\pi\epsilon) \{ [(a-x)^2 + y^2 + z^2]^{-1/2} - [(a+x)^2 + y^2 + z^2]^{-1/2} \},$$

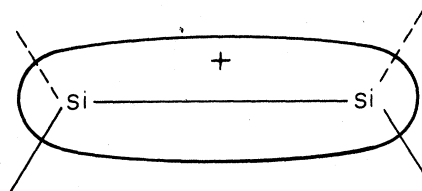
where ϵ is the dielectric constant of the medium between the point charge and the plane. If the point charge is replaced by a very small conducting sphere at some potential V_0 and radius b , then,

$$V(x,y,z) = V_0 b \{ [(a-x)^2 + y^2 + z^2]^{-1/2} - [(a+x)^2 + y^2 + z^2]^{-1/2} \}. \tag{1}$$

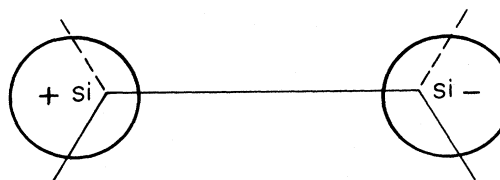
The charge density on that plane is given by

$$\sigma(\rho) = -2\epsilon V_0 b a / (a^2 + \rho^2)^{3/2}, \tag{2}$$

where $\rho^2 = y^2 + z^2$. In the case of the scanning tunneling microscope, for all practical purposes, $\epsilon = \epsilon_0$. Therefore, directly under the tip, the charge density is



(a) BONDING



(b) ANTIBONDING

FIG. 1. Schematic representation of the surface-state eigenfunctions at the Γ point of a silicon dimer for (a) the occupied and (b) the unoccupied surface states. Backbonding contributions have been neglected for simplicity.

$$\sigma(0) = -2\epsilon_0 V_0 b / a^2. \quad (3)$$

If we take $b = 9 \text{ \AA}$ and $a = 15 \text{ \AA}$ as representative values, then for $\epsilon_0 = 8.85 \times 10^{-14} \text{ C/V cm}$, $\sigma(0) = (-7.08 \times 10^{-7} \text{ C/V cm}^2) V_0$.

For the STM studies of the Si(111)(7×7) surface, the applied voltage V_{AP} was 2.9 V. This applied voltage is measured between the Fermi level of the sample and that of the STM probe. Therefore, $V_0 = V_{AP} + \phi - \phi_P$, where ϕ is the work function of the sample and ϕ_P is that of the probe (Fig. 2). Note that in semiconductors, band bending will affect the relative positions of the Fermi level at the surface and the vacuum level, and therefore affect ϕ , but will not affect the positions of such features as the valence-band maximum and the conduction-band minimum relative to the vacuum level. As the detailed nature of the STM tip is not known, we will assume a value of V_0 of $2.5 \pm 0.5 \text{ V}$. Substituting this value into Eq. (3) we find a surface charge density of $1.77 \times 10^{-6} \text{ C/cm}^2$ or about $1.11 \times 10^{13} e^-/\text{cm}^2$. As a complete filling of the unoccupied surface states on the unreconstructed Si(111) surface would require an excess charge density of about $7.9 \times 10^{14} e^-/\text{cm}^2$ above that required for charge neutrality, we see that these experimental conditions produce a nominal filling of about 1.4% of the unoccupied surface states.

For most surface structures, it is very unlikely that an excess charge density corresponding to filling even several percent of the unoccupied states would lead to any detectable reconstruction. Therefore, we can immediately conclude that, under its present operating conditions, the STM does not significantly perturb most surfaces. However, we are also led to the possibility that surface structural transitions could be induced by the deliberate application of larger field gradients. As can be seen in Eq. (2), the surface charge density is linear in V_0 . There-

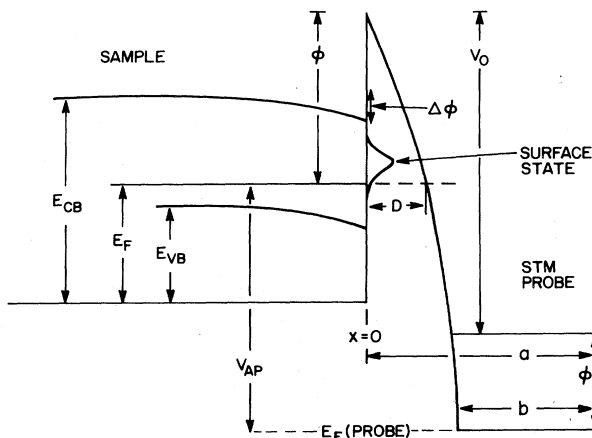


FIG. 2. Schematic energy-level diagram for a semiconductor surface adjacent to a STM probe. The zero of energy is taken at the bottom of the valence band within the sample. Here, it is assumed that the sample is p type and that its Fermi level is pinned at the surface in the bottom of the "unoccupied" surface state.

fore, it might seem to be straightforward to simply increase the applied voltage by approximately an order of magnitude to achieve substantial or even complete filling of the unoccupied surface states. However, there are several phenomena that severely limit the arbitrary increase of the field strength in real situations.

The most important limitation is the actual current density to be carried by both the sample and the probe tip. While the charge density is linear in $V_0 b / a^2$, the current density will increase much more rapidly as a function of this same parameter once the pure tunneling region is exceeded and the field-emission range is approached. We will consider several formalisms for estimating this current.

In 1928, Fowler and Nordheim developed a theory for field emission from a conducting surface in the presence of a strong electrical field induced by a planar probe.⁴ They found that the field emission current can be expressed as

$$I = A_{FN} E_F^{1/2} \phi^{1/2} (E_F + \phi)^{-1} (V_0/a)^2 \exp(-4\kappa\phi a/3V_0), \quad (4)$$

where E_F is the Fermi energy, ϕ the work function, and $\kappa = (2m\phi/\hbar^2)^{1/2}$. When ϕ and E_F are expressed in volts and V_0/a in V/cm, $A_{FN} = 6.2 \times 10^{-6} \text{ amps/V}$. This expression is not strictly applicable to the situation under consideration as it is derived for a case where the probe is planar as opposed to a tip of atomic dimensions. Furthermore, it is developed for a metallic surface where the consideration of band bending is quite immaterial. However, this formalism should provide an upper limit to the case where b is very large and $V_0 \gg \phi$.

In strong contrast, both temporally and in terms of the detailed considerations, Tersoff and Hamann have developed a theory for vacuum tunneling between a real solid surface and a model probe with a locally spherical tip.⁵ Within their model, the tunneling current is given by

$$I = sV_0, \quad (5)$$

where

$$s = 32\pi^3 \phi^2 \hbar^{-1} e^2 D_t(E_F) b^2 \kappa^{-4} \exp(2\kappa b) \times \sum_{\nu} |\psi_{\nu}(v_0)|^2 \delta(E_{\nu} - E_F). \quad (6)$$

Here $D_t(E_F)$ is the density of states per unit volume of the probe tip, $\psi_{\nu}(v_0)$ is the surface eigenfunction at the tip, and again $\kappa = (2m\phi/\hbar^2)^{1/2}$ where ϕ is the work function which is assumed to be the same for both the probe and the surface. As before, b is the radius of the tip and a is the distance from its center of curvature to the surface. As Tersoff and Hamann note, $|\psi_{\nu}|^2 \propto \exp(-2\kappa a)$, therefore

$$I = A_{TH} V_0 \exp[-2\kappa(a-b)]. \quad (7)$$

This formalism clearly shows the exponential behavior of the tunneling current as a function of the distance between the probe and the surface. However, as it was developed for the case where the sample is metallic and, most importantly, where the applied voltage V_0 may be

significantly smaller than the barrier height ϕ , this approach is also not strictly applicable to the situation that we wish to consider. Despite this, even for semiconductors a similar functional form should be obtained in the limit of small applied voltages. Taking $\phi \cong 4.5$ eV, $a = 15$ Å, and $b = 9$ Å, then for $eV_0 \sim 2.5$ eV, we can roughly estimate $A_{TH} \sim 10^8$ A/V cm² for the Si(111)(7×7) case where 1 nA is drawn from an area of roughly 100 Å². It should be noted, of course, that this estimate of A_{TH} is strongly dependent upon the specific values of a , b , and ϕ .

We now seek an expression for the emission current from a planar surface to a point probe (as opposed to the planar probe modeled by Fowler and Nordheim) and at higher field strengths (in contrast to the Tersoff-Hamann derivation). It is not our purpose to define the dependence of the emission current upon the details of the surface electronic states, but rather to determine the gross dependence upon the applied voltage and tip radius and distance to the surface.

As previously discussed, the potential induced by a very small spherical probe may be expressed classically as

$$V(r) = V_0 b \{ [(a-x)^2 + \rho^2]^{-1/2} - [(a+x)^2 + \rho^2]^{-1/2} \}. \quad (8)$$

In the vicinity of the surface, for $(x/a)^2 \ll 1$, $V(r) \cong V(x) = 2V_0 b x / a^2$. Therefore, Schrödinger's equation has the form $\nabla^2 \psi(x, \rho) = \alpha - \beta x$, where $\alpha = 2m(C - W)/\hbar^2$ and $\beta = 4meV_0 b / a^2 \hbar^2$. Here, $C = E_F + \phi$, where E_F is the Fermi energy and ϕ is the work function. Here, the effect of band bending is contained in the term ϕ which will differ from the "bulk"

work function ϕ_B by $\Delta\phi$ (see Fig. 2). As is shown in the Appendix, $\psi(x, \rho)$ can be expressed in the form

$$\psi(x, \rho) = R(x, \rho) X(x), \quad (9)$$

where $R(x, \rho)$ is a slowly varying function of x and $X(x)$ and is a Bessel function within the tunneling region and a Hankel function beyond that region.⁴ As is also shown in the Appendix, the transmission coefficient for tunneling through the barrier is given by

$$T(W) = 4C^{-1} [W(C - W)]^{1/2} \exp[-4(\alpha')^{3/2}/3\beta], \quad (10)$$

where $\alpha' = \alpha - 3/4d^2$ and $d \geq a$.

The current through the barrier is given by the integral of the transmission coefficient with the number of electrons with energy W available for tunneling per unit time as

$$I(V_0) = e \int_0^\infty T(W) N(W) dW. \quad (11)$$

This may be broken down into a bulk component, with contributions from both the valence band and the conduction band, and a component from the surface states as $I = I_v + I_c + I_{SS}$. The valence-band contribution will have a form very similar to the Fowler-Nordheim (FN) formalism as

$$I_v = A_{FN}(E_v)^{1/2} (\phi + E_F - E_v)^{1/2} (E_F + \phi)^{-1} \times (2V_0 b / a^2) \exp[-4(\alpha'')^{3/2}/3\beta], \quad (12)$$

where $\alpha'' = (E_F - E_v + \phi)(2m/\hbar^2)$. Note that here band bending will have an effect due to its influence on the relative position of the Fermi level and the valence-band maximum. The contribution from the conduction band will similarly be sensitive to band bending and to its control of carrier concentrations in the band at the surface. However, as long as the charge density in the conduction band is negligible, its contribution to the field-emission current can be neglected.

Here, it has been assumed that the Fermi level is pinned by the surface states and that the density of these states is large enough to screen the bulk (i.e., that essentially all of the induced charge is in the surface states). Under these conditions, when there is a relatively small change in the occupation of the surface states, there will be little or no change in the bulk band bending. If, however, there are few unoccupied surface states in the gap (e.g., $\leq 1 \times 10^{13}/\text{cm}^2$), then a strong field gradient will induce charge which may fill these states, and can have a significant effect on band bending. A low density of unoccupied states within the gap will usually reflect the absence of intrinsic surface states and will be associated with the presence of isolated defects and/or impurities. To the extent that such centers are isolated, the accompanying surface states will not have even the two-dimensional conductivity that is often found with the high-density surface states associated with reconstruction. Therefore, the current limiting process may be the transport of carriers to these isolated surface states. This will be strongly influenced by band bending which, in turn, may be very sensitive to the applied field because of relatively weak screening. However, even the complete occupation of such a low density

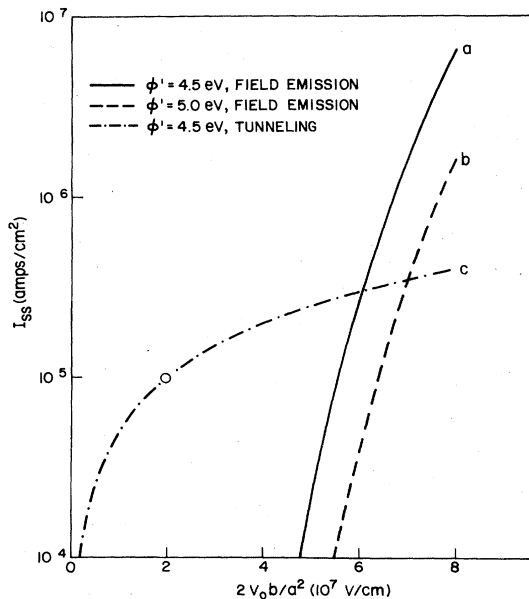


FIG. 3. Emission current is shown as a function of the normalized field gradient $2V_0 b / a^2$ for field emission where for (a) and (b) $\phi' = 4.5$ and 5.0 eV, respectively, and for (c) tunneling where $\phi' = 4.5$ eV.

of states is unlikely to affect surface reconstruction.

If, as on the Si(100)(2×1) surface, the Fermi level is pinned at the surface by the surface states, and if those states are fairly narrowly localized in energy space, we can write

$$I_{SS} = e \int_0^\infty T(W) N_0(W) \delta(E_F - W) dW. \quad (13)$$

This approach ignores the detailed nature of the surface states and is not applicable when appreciable dispersion occurs in the occupied portion of those states. Furthermore, we have neglected lower-lying fully occupied surface states, although they may be treated in the same fashion with the above provisions, as, at least at lower field strengths, emission from the highest state will predominate. Similarly, in considering only Eq. (13), we neglect tunneling from the valence band (because of its larger barrier height under most circumstances) and from the conduction band (because of its lower carrier concentration).

The number of electrons in the surface state that are available for tunneling per unit time is proportional to the charge density in that state and is given by

$$N_0(E_F) = \frac{1}{4} v_F (\bar{\sigma}/D), \quad (14)$$

where v_F is the velocity of the electrons in the surface state at the Fermi level, $\bar{\sigma}$ is the average charge density beneath the tip, and D is the thickness of the barrier at E_F and is determined by the condition $\phi - (2V_0b/a^2)D = 0$. Taking $\bar{\sigma}$ to be approximately $2\epsilon_0 V_0b/a^2$, we have

$$N_0(E_F) = \frac{1}{4} \epsilon_0 v_F (2V_0b/a^2)^2 \phi. \quad (15)$$

Using our previously derived expression for $T(W)$, we find that

$$I_{SS} = B(2V_0b/a^2)^2 \times \exp[-4(2m/\hbar^2)^{1/2}(\phi')^{3/2}/3(2V_0b/a^2)] \quad (16)$$

where $B = \epsilon_0 v_F [E_F^{1/2}/\phi^{1/2}(E_F + \phi)]$ and $\phi' = \phi - (\hbar^2/2m)(3/4d^2)$.

This expression is quite similar to the Fowler-Nordheim expression. The major differences are that the field gradient $F = V_0/a$ is replaced by a normalized field gradient $2V_0b/a^2$ and that the work function ϕ is modified by the term $(\hbar^2/2m)(3/4d^2)$. Both of these variations will serve to enhance the field-emission current density for a spherical probe relative to that for a planar probe. For silicon, relative to the bottom of the valence band the Fermi energy is about 12.5 eV. Therefore, assuming an effective mass of unity, the velocity of the electrons in the surface state at the Fermi level $v_F = 2.1 \times 10^8$ cm/sec. Taking a value for the work function of 4.9 eV, $B = 3.6 \times 10^{-6}$ A/V² and $\phi' = 4.5$ eV for $d^2 = 2a^2$, where $a = 15$ Å. (It should be noted that, for a given case, the values of E_F and ϕ will depend upon the doping of the sample.)

Shown in Fig. 3 is the tunneling current predicted by the Tersoff and Hamann formalism (normalized to 10^5 A/cm² at $V_0 = 2.5$ V or $2V_0b/a^2 = 2 \times 10^7$ V/cm), and the field-emission current predicted by Eq. (16). As expected, in the region where the applied voltage V_0 is

less than or comparable with the barrier height ϕ , the total current is dominated by the tunneling component. However, when V_0 exceeds ϕ , the situation is reversed and the field-emission component rapidly increases with the applied potential. As can be seen, current densities in excess of 10^6 A/cm² are to be expected for values of $2V_0b/a^2$ less than 10^8 V/cm. Such current densities would strain the very fabric of both the sample and the tip itself irrespective of the latter's composition and geometry. In addition, particularly for semiconductors, the rate at which current can be supplied to the surface may become a limiting factor.

On the basis of these considerations, it is obvious that the essentially exponential increase in current with the normalized field gradient $2V_0b/a^2$ is strongly limiting in terms of how much excess charge density can be induced on a surface. Referring back to Eq. (3), it may be shown that filling more than about 5% of the unoccupied states on the unreconstructed Si(111) surface, for example, is quite unlikely. Therefore, for relatively simple, stable surfaces it is highly doubtful that the STM can either adventurously or inadvertently perturb the system under investigation. However, there are situations where even such a small excess of surface charge density could be influential.

Consider, for example, the Si(100)(2×1) surface. It is known that this surface can be annealed at 600°C.⁶ This annealing involves the breaking and remaking of dimer bonds at the surface, and it is probable that the spontaneous dissociation of these dimers is the rate-limiting step in this process.⁷ Therefore, the annealing temperature is directly dependent upon the dimer-bond energy which, in turn, should be strongly influenced by the degree of occupation of the "antibonding" surface states in the gap. Similar considerations will be important both for order-order transitions [e.g., Si(111)(2×1) → Si(111)(7×7)] and for order-disorder transitions [e.g., Si(111)(7×7) → Si(111)(1×1)]. Furthermore, the partial occupation of these nominally unoccupied surface states would not only weaken, for example, dimer bonds on the Si(100) surface, but would also lengthen them, though it is rather doubtful that this effect could be observed using the STM.

In highly complex surface structures, such as the Si(111)(7×7), it is probable that some elements of the surface structure are less stable than others. Small changes in the surface charge density would most likely leave unchanged the larger features, such as the holes at the apices of the unit cell,^{1,8} and the periodicity of the superlattice itself. On the other hand, other features will be more vulnerable to reconstruction or relaxation. For example, in the model proposed by McRae,⁸ there are two kinds of surface dimers within the unit cell whose bonds should be significantly weaker than those in bulk Si because of back-bonding strain. In this model, there are nine dimers in the surface layer itself, six in contact with, and three not in contact with, the corner holes. Within this model,⁸ the 49 surface atoms for the unreconstructed surface are reduced to 30 which should have 4.8×10^{14} surface states per cm² of which about 2.4×10^{14} will be filled (assuming charge neutrality) in the absence of externally applied electrical fields.

Let us now consider the three dimer pairs not associat-

ed with the corner holes. While the local density of states corresponding to these dimer bonds may overlap that from other portions of the surface structure, it is expected to be relatively narrow and to have a relatively small binding energy. Similarly, the unoccupied antibonding local density of states corresponding to the dimers is also expected to be relatively narrow and to fall either at or near the bottom of the unoccupied band. Therefore, if there was an actual gap between the occupied and the unoccupied surface states, any additional surface charge density induced by an externally applied electrical field might be expected to predominantly populate those unoccupied levels that correspond to dimer antibonding orbitals. This would weaken or possibly even disrupt these bonds which is equivalent to a partial reconstruction of the surface. Experimentally, "metallic" surface states are observed on the Si(111)(7×7) (Ref. 9) surface that may indicate that these antibonding states are partially occupied even in the absence of an externally applied field. In this case, the possibility for partial reconstruction is even better as the maximum induced charge density of 3 to $4 \times 10^{13} e^-/\text{cm}^2$ would be augmented by the existing charge and could exceed the $4.8 \times 10^{13} e^-/\text{cm}^2$ required to completely fill the noncorner dimer antibonding states. (It should be noted that the "metallic" surface state might also indicate a charge deficit in the bonding states and that completing the occupation of these states might either further stabilize the surface or, at a remote chance, cause additional reconstruction.)

Finally, it is of interest to consider the case where the surface states are nonconducting in the surface plane, or where such conductivity is severely diminished with decreasing temperature. Here the transport of carriers to or from the surface will occur via interactions with the bulk valence and/or conduction bands and may represent the current limiting process. The surface Fermi-level position will determine the free-electron and hole concentration, as well as the energy of the highest occupied surface state. It would therefore affect the kinetics of carrier exchange between the surface states and the bands. Thus, in principle, variation of temperature and current direction may be used to study the surface density of states and Fermi-level position. Illumination of the surface during the measurement might yield additional information. (Actual heating of the sample by the tunneling or field-emission current is not expected to be a significant factor. While the current density is quite large, it passes through a sufficiently small area such that the total heat produced is very small

and is easily dissipated by thermal diffusion.)

In conclusion, we find that an excess surface charge density is induced by the applied electrical field gradients used in scanning tunneling microscopy, but that under "usual" operating conditions this surface charge density is inadequate to cause the reconstruction of relatively stable surface structures. However, we also find that under certain conditions, such as near a phase transition or in complex structures with "vulnerable" bonding units, there is a possibility that reconstruction might be induced by operating the STM in an atypical, high-field mode. In addition, when the density of those surface states pinning the Fermi level is sufficiently low to preclude surface conductivity, then the temperature dependence of the forward and reverse currents may, in principle, be used to gain information on their number and energy position within the gap. We hope that the next series of experiments will be able to address these questions and provide definitive answers as to the possibility of using the STM to influence surface structures and phase transitions.

ACKNOWLEDGMENTS

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APPENDIX

In the tunneling region $0 < x < D$, the wave function should decrease radially from the central axis between the tip and the surface. In addition, it is damped (and at lower applied potentials strongly damped), on going from the surface to the tip. At the surface, we know that

$$x = 0, \quad |\psi(0, \rho)|^2 = \sigma(\rho)/t = 2C/(a^2 + \rho^2)^{3/2}, \quad (\text{A1})$$

where t is the "thickness" of the surface layer and $C = \epsilon_0 V_0 b a / t$. Therefore, the wave function in the tunneling region may be approximated as

$$\psi(x, \rho) = C^{1/2} R(x, \rho) X(x), \quad (\text{A2})$$

where $R(x, \rho)$ is a slowly varying function of x of the form

$$R(x, \rho) = [(a+x)^2 + \rho^2]^{-3/4}. \quad (\text{A3})$$

From the Schrödinger equation, $\nabla^2 \psi(x, \rho) = (\alpha - \beta x) \psi(x, \rho)$, where $\alpha = 2m(C - W)/\hbar^2$ and $\beta = (2m/\hbar^2)(2V_0 b/a^2)$. Therefore,

$$R^{-1} \left[\frac{\partial^2 R}{\partial \rho^2} + \rho^{-1} \frac{\partial R}{\partial \rho} + \frac{\partial^2 R}{\partial x^2} \right] + X^{-1} \frac{\partial^2 X}{\partial x^2} + R^{-1} X^{-1} \frac{\partial R}{\partial x} \frac{\partial X}{\partial x} = \alpha - \beta x. \quad (\text{A4})$$

Now

$$R^{-1} \nabla^2 R = 3/4 [(a+x)^2 + \rho^2] = 3/4 d^2, \quad (\text{A5})$$

where $d^2 = (a+x)^2 + \rho^2$. This term roughly accounts for

the decrease in the transmission current with ρ for those portions of the sample that are not directly under the tip. Properly speaking, this ρ dependence should be accounted for in $X(x)$ but, as the solution is not exact, it will suffice to replace ρ and x in d^2 by nominal values. The term

$$R^{-1} \frac{\partial R}{\partial X} \cong -3x/(a^2 + \rho^2) \lesssim -3x/a^2, \quad (\text{A6})$$

which may be neglected for $a \gg x$. Therefore, we have

$$\frac{\partial^2 X(x)}{\partial x^2} = (\alpha' - \beta x)X(x), \quad (\text{A7})$$

where $\alpha' = \alpha - 3/4d^2$. Following Nordheim and Fowler,⁴ this leads to a solution for $X(x)$ of the form of a Bessel function of the $\frac{1}{3}$ order in the tunneling region

$$0 < x < D, \quad X(\xi) = \xi^{1/2} J_{1/3}(2\xi^{3/2}/3), \quad (\text{A8})$$

and a Hankel function

$$D < x, \quad X(\xi) = \xi^{1/2} H_{1/3}^{(1)}(2\xi^{3/2}/3) \quad (\text{A9})$$

beyond the barrier, where $\xi \equiv [(\alpha'/\beta) - x] \beta^{1/3}$. This functionality, in turn, leads to a transmission coefficient

through the barrier of the form

$$T(W) = C^{-1} [W(C - W)]^{1/2} \exp[-4(\alpha')^{3/2}/3\beta], \quad (\text{A10})$$

where the argument of the exponential is

$$\begin{aligned} 4(\alpha')^{3/2}/3\beta &= (4/3)(2m/\hbar^2)^{1/2} \\ &\times [(C - W) - 3\hbar^2/8md^2]^{3/2}/(2V_0 b/a^2) \\ &= (a/2b)(4/3)(2m/\hbar^2)^{1/2} \\ &\times [(C - W) - 3\hbar^2/8md^2]^{3/2}(V_0/a). \end{aligned} \quad (\text{A11})$$

Note that this differs from the Fowler-Nordheim expression by the inclusion of the term $a/2b$, which is a measure of the relative diameter of the tip, and by the term $3\hbar^2/8md^2 = 3\hbar^2/8m(a^2 + \rho^2)$ which will be less than 1 eV.

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