

# Properties of vacuum tunneling currents: Anomalous barrier heights

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**A design of STM which does not use vacuum internal vibration isolation and may be cooled to liquid helium temperatures is described. Tunneling current characteristics underlying STM operations are discussed. A model is presented to explain the anomalously low (<1 eV) tunneling barrier heights often observed. On the basis of this model we suggest criteria for obtaining reliable STM images.**

## Introduction

The scanning tunneling microscope developed by Binnig and co-workers [1,2] represents a major addition to the techniques of surface science. This is not only because of its atomic-scale real space imaging, but also because of its sensitivity via tunneling spectroscopies to local electronic levels in a surface. The technique relies upon the ability to minutely control a vacuum gap and upon an understanding of the tunneling process itself.

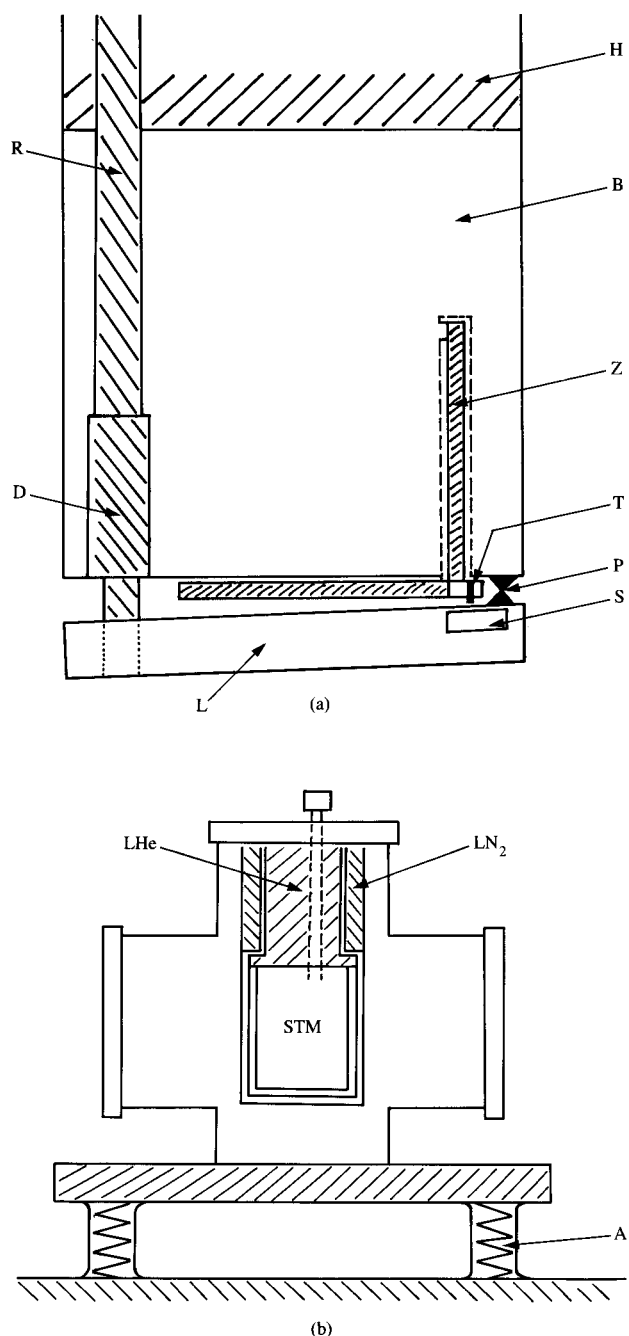
With the aim of understanding the processes involved in the tunneling current we have developed a "rigid" STM,

which can be cooled to helium temperatures and used in combination with other surface science techniques. Our results suggest that 1D theory fits the data quite well in most cases. Sometimes, however, anomalously low (<1 eV) tunneling barrier heights are seen. We present here an explanation for these anomalous barriers based on mechanical contact between tip and flat. Consideration of this model for low barriers allows us to suggest criteria for obtaining meaningful STM pictures.

## Experiment

The essential features of an STM must include rigidity, isolation from disturbing vibrations, and linkage with standard surface-science techniques. Operation at cryogenic temperatures is also desirable for studying low-temperature and inelastic tunneling phenomena. Of the first two requirements, rigidity is the most important, because a reliable roll-off response of 6 dB/octave to external vibrations is achieved below the lowest resonant frequency  $\omega_0$  of the structure. One arranges for  $\omega_0$  to be as high as possible. Vibration isolation of the tunneling apparatus ideally produces a complementary roll-off against higher frequencies but is relatively easily short-circuited. An example of this is the relatively efficient propagation of acoustic waves along the springs of a spring suspension system. As a result, one can finish up with a complex multicomponent isolation system, each part dealing with a different frequency range. It is, therefore, most effective to concentrate on making the tunneling unit as rigid as possible.

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**Figure 1**

Schematic diagrams of an STM: (a) shows lever system for tip-surface approach, with helium block H, base block B, piezoelectric drive Z, tip assembly T, pivot P, sample assembly S, lever L, differential screw D, and rotary motion drive R; (b) shows cryostat and chamber mounted on air suspension A. The whole system is in a sound-proofed room.

**Figure 1(a)** shows a schematic of the current version of our apparatus. An earlier version is described in [3]. It differs

from that of Binnig et al. [1,2] in two respects. First, vibration isolation is external to the vacuum system [Figure 1(b)]. The system is enclosed in an acoustically isolated room and lifted up on air mounts, the latter for low-frequency isolation. Second, coarse motion of the sample is effected by a differential screw and reduction lever assembly which eliminates the need for the "louse" and is highly reliable in operation. One turn corresponds to about 10  $\mu\text{m}$  gap movement. The specimen can be removed complete with its heater, eventually allowing transfer to other positions in the UHV chamber. In this design cooling to low temperatures is easy. Our present machine is able to reach about 20 K. It is supported and shielded by a large copper block [Figure 1(b)] which is cooled by liquid helium. Thermal drift is very small due to the large thermal mass of the whole STM assembly. Creep of less than 0.5  $\text{\AA}$  per minute is commonly obtained.

The electronics used [3] is similar to that described by Binnig et al. [1, 2]. The tunneling current amplifier, mounted on the vacuum feedthroughs, is an AD545M FET amplifier connected as a virtual ground current amplifier. Inside the vacuum chamber the tip wire has a coaxial guard shield which extends to within a few mm of the tip. This amplifier has a roll-off frequency of  $\approx 20$  kHz at optimum response, and an inherent noise figure of 10 fA/ $\sqrt{\text{Hz}}$  at 1 kHz. This is sufficient for simple inelastic tunneling spectroscopy. However, it transpires that the noise on the vacuum tunneling current is considerably greater than the shot noise limit. Sometimes the noise is sinusoidal and clearly associated with vibrational modes of the apparatus. Another type of noise resembles very sharp steps in the current, either up or down, with a rise time limited only by the head amplifier. This "switching" noise has recently been observed at specific sites in  $\text{SiO}_2$  by Welland and Koch [4] and explained in terms of occupation and emptying of electron traps in the barrier. We have also seen this type of noise on metal surfaces and at temperatures down to 20 K; it may be connected with defects in the surface. Experiments to determine the origin of this noise on metals are in progress but at present, "switching" and small vibrational noise are too large to allow inelastic tunneling spectroscopy at practical speeds.

#### • Tunneling current characteristics

We have shown in a previous paper [5] that the one-dimensional theory of Simmons [6] gives a good fit to the observed behavior in both low-voltage and field-emission regimes. In the low-voltage region this is broadly as expected, since in theories of STM operation [7,8] the effects of tip radius  $R$  only appear in the pre-exponential term for the current density  $J$ ,

$$J \propto Vf(R) \exp(-A\phi^{1/2}s),$$

where  $V$  is the applied voltage,  $A$  a constant,  $\phi$  the barrier height, and  $s$  the gap width. While tip displacement  $\Delta s$  can

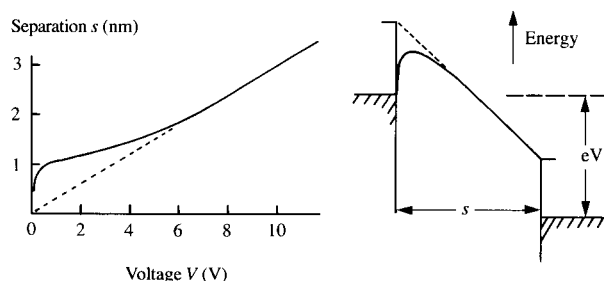
be measured in an STM, it is not so easy to determine the absolute value of separation. As a result, it is not easy to study effects such as tip radius variations which do not directly affect the vacuum decay length  $(4\phi)^{-1/2}$ . The only means currently available to estimate the absolute tip-to-flat separation is field-emission data. As seen in Figure 2, which shows  $V$  vs.  $s$  (from [5]) at constant tunneling current  $I$ , extrapolating the constant field line back to  $V = 0$  gives an estimate of the point  $s = 0$ . Some precautionary comments must be made about this simple picture:

1. The absolute value of the work function must be known; as is discussed shortly, this is not a simple matter to determine. Further, the potential diagram of Figure 2 is simplistic; there is no guarantee that the barrier region will bend so as to give  $s = 0$  as the  $V = 0$  limit of the constant field line.
2. It is assumed that 3D effects are unimportant, in particular that a sharp tip radius will not give a field enhancement. Clearly, this effect will depend on the local macroscopic tip shape. Also, it is likely that contributions to the current will come from a larger area as the voltage rises further into the field-emission region; that is,  $J$  changes at constant  $I$ .
3. In practice, the application of 10 V and greater often irreversibly modifies the structure of the tip and hence renders comparison with earlier data meaningless. This process is often used in tip-preparation procedures.

The uncertainty in absolute gap width has consequences not only in studying possible effects of tip geometry, but also in the assessment of the effect of image forces in lowering the tunneling barrier. The barrier height  $\phi$  is normally measured by varying  $V$  or  $I$  and observing the corresponding change in  $s$  [1, 5]. Binnig et al. [9] have shown that the first-order term in the image potential actually cancels out in this type of experiment and the measured barrier height will be the nonimage-reduced value even when image forces are acting. The only way in which the effect of image forces may be directly seen is in the dependence of conductance on absolute separation. Neither of these is well-defined in the STM.

A possible approach to studying the image force barrier reduction has been pointed out by Payne and Inkson [10]. They show that for a simple classical image potential the measurements  $(\partial \ln I / \partial s)_V$  and  $(\partial \ln V / \partial s)_I$  will yield different apparent barrier heights, the difference being also a function of the current density. This type of measurement could be used to determine the form of the image potential and possibly also the current density and hence the tunneling area.

There is, however, a difficulty in applying the above theory to STM because very often extremely low apparent barrier heights have been reported [1, 11];  $\ln I$  vs.  $s$



**Figure 2**

Variation of gap width  $s$  with applied voltage  $V$  at constant current. Inset shows potential barrier in field-emission region.

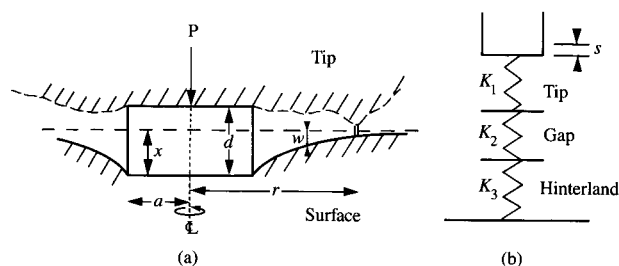
measurements can at times yield values of the order of a few hundred millielectron volts. Clearly, such anomalous barrier heights cannot be physically real, since such low work functions are never observed in other experiments. In the next section we present an explanation for these anomalous values which suggests that great care needs to be taken in performing experiments to measure refined changes of tunnel barriers.

#### • Anomously low barrier heights

Two aspects of these anomalously low ( $<1$  eV) barrier height measurements are important. Firstly, they are inferred from  $\ln(\text{voltage})$  or  $\ln(\text{current})$  vs. distance plots, where typically a displacement of  $\approx 10$  Å gives a three-order-of-magnitude current or voltage change. This precludes any explanation based on electronic polarization at very sharply curved tips, or effects due to image forces, since these could not give the drastic apparent barrier height lowering over such "large" distances. Indeed, Binnig et al. [9] predict lowering of only a volt or so down to 4 Å separation. A second aspect is that the transition to field-emission behavior (Figure 2) always occurs at a voltage of around 4 V even when the  $I$  or  $V$  vs.  $s$  behavior is showing extremely small apparent barriers.

We propose that when the very low barrier heights are observed, the tip and sample are in contact somewhere. If, as is shown below, this contact behaves in a linear elastic fashion, then the effect is to change the calibration of displacement—that is, the gap movement is some fixed fraction of the piezoelectric element movement. This preserves the exponential dependence of current on separation but, since the actual tunneling gap is moving less than the positioning piezoelectric elements, a lower apparent barrier is observed. Further, the transition to field emission is unaffected and still occurs at reasonable voltages. We now discuss some possible contact geometries and show that they can lead to the necessary distance rescaling.

The situation of Figure 3(a) shows a particle, perhaps oxide or dust, represented for simplicity as a disk of radius  $a$



**Figure 3**

Displacements when a contact is made in the tip-flat gap: (a) shows displacements (symbols in text) as function of position. Vertical scale enhanced and tip hinterland compression omitted for clarity. Tunneling region at right. (b) shows simplified spring constants  $K_1$  for tip and mounting structure,  $K_2$  for gap particle, and  $K_3$  for near-particle hinterland material.

and thickness  $d$ . The piezoelectric element drive produces a given strain  $s$ , **Figure 3(b)**; this strain is then distributed among the (simplified) components of the system, viz., tip structure, particle in gap, and hinterland material adjacent to the particle, according to the values of their spring compliances  $K$  as shown. If we take the tip structure as a wire  $\approx 0.2$  mm in diameter and 3 mm long with  $E = 3 \times 10^{11}$  N-m $^{-2}$ , we obtain  $K_1 = EA/l \approx 10^6$  N-m $^{-1}$ , where  $A$  is the cross-sectional area of the wire and  $l$  is its length. Similarly, for a particle of area  $(1000 \text{ \AA})^2$  and thickness 30  $\text{\AA}$ ,  $K_2 \approx 10^6$  N-m $^{-1}$ . Thus the compressibilities of tip and oxide are of the same order, and this alone may give substantial effects. However, more important is the compression of the hinterland material: Take the formula for distance  $x$  traveled under load  $P$  into a medium by a rigid punch radius  $a$  [12]:

$$x = P(1 - \nu^2)/2aE. \quad (1)$$

Thus,  $K_3 = P/x \approx 2 \times 10^4$  N-m $^{-1}$  for  $a \approx 500 \text{ \AA}$  as in the particle shown here. The term  $K_3$  is much smaller than the others, and so most of the piezoelectric element strain is taken up by the near-particle hinterland. Note that in Figure 3(b) we have ignored, for diagrammatic clarity, the tip hinterland compression, for which a term similar to  $K_3$  will apply.

Clearly, if the tunneling is through the oxide, the relatively low compressibility of the oxide ( $K \approx 10^6$  N/m) compared to that of the hinterland ( $K \approx 10^4$  N/m) may lead to exceedingly low apparent work functions. More realistically, consider the tunneling to be occurring through vacuum, a little way away from the particle at a point which happens, because of pre-existing surface irregularities, to be at the correct separation for tunneling [Figure 3(a)]. The nearby particle in contact is taken as not contributing to the tunneling current, but will influence the surface

displacements  $w$  at the tunneling point, which is a distance  $r$  from its center. The value of  $w$  [Figure 3(a)] is given by a set of elliptic integrals [12], but with sufficient accuracy for our purposes, by the expression

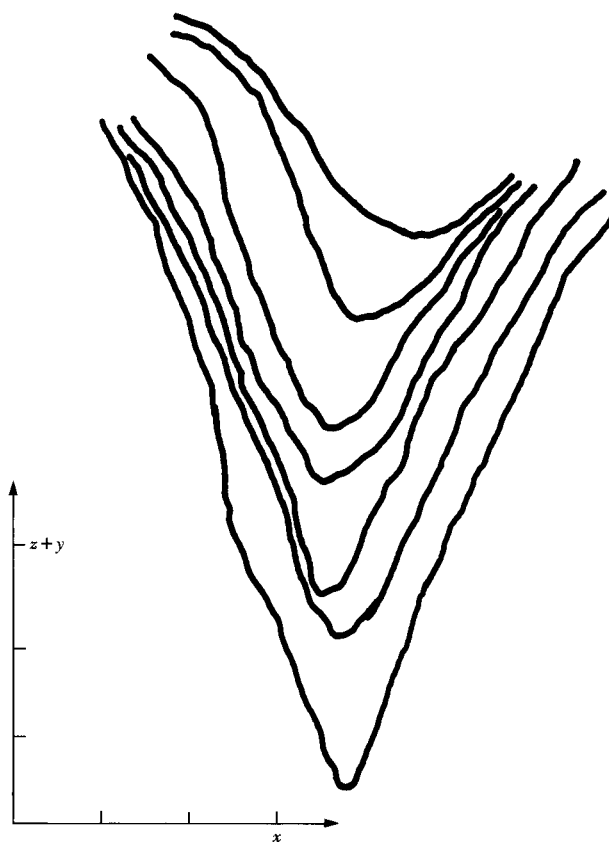
$$w = P(1 - \nu^2)/2rE. \quad (2)$$

Now the gap displacement differs from the piezoelectric element displacement  $s$  by the amount  $w$ . We may also take  $s \approx x$  since  $K_3$  is far the smallest spring constant in the system. Using (1) and (2) we find that the apparent barrier height  $\phi_a$  is given by

$$\phi_a = \phi_0 \left( \frac{s - w}{s} \right)^2 = \phi_0 \left( 1 - \frac{a}{r} \right)^2.$$

Thus an arbitrary value of  $\phi_a$  can be obtained by adjusting  $r$ .

It could be argued that a real microcontact might not behave in the simple elastic fashion described above. In particular, plastic (irreversible) deformation will occur upon application of a loading force. However, as we have shown elsewhere [13], the deformation that occurs upon subsequent



**Figure 4**

Image taken on Pt(110) showing deep valley. Scale marks at 0.4-nm intervals.

unloading is elastic. That is, provided the initial load is not exceeded, subsequent reloadings in the same place are purely elastic; no hysteresis need be seen. More complex contact models could be developed, but do not add to the essential features of the model described here.

Some consequences of tip-flat contact in the STM are as follows:

1. The lateral and vertical calibration of pictures may be affected. This may be involved in the strange images sometimes seen, such as that in **Figure 4**. If such a deep groove is physical, then the tip must be a cone of apical angle  $<15^\circ$ , tens of Å long, and with a single atom on the end. Although such high-aspect-ratio "whiskers" have been observed on a large scale [14], it seems a little unlikely that they can be only two or three atoms wide over such a considerable length. Other workers have seen features such as large, near-vertical-sided steps, with or without hysteresis in position. If physical contact is involved, then the true topography of the surface need not be as abrupt as the images imply, and such sharp tips need not be invoked. Alternatively, the two valley sides of the image may correspond to tunneling from different areas on the tip, and the "sharpness" of the image need not imply a sharp tip.
2. A particle between tip and flat may lead to very stable, vibration-free tunneling currents, due to the obvious gap-width stabilization. This effect has been observed by Hansma and coworkers in their squeezable tunneling junctions [15]. We have also observed this in our STM operating in air. Caution should thus be exercised when looking for stable tunneling currents during tip treatment.
3. Attempts to perform lithography when insulating layers are present may lead to scratching as the primary method of track generation.

In summary, if the above model is applicable, then it is essential that  $I$ ,  $V$  vs.  $s$  barrier heights should be large (a few volts) for images to be treated as real. This is particularly important as the STM is now advancing to the imaging of structures not determinable by other techniques, that is, where one does not know in advance what one is looking for.

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