

APPARENT BARRIER HEIGHT FOR TUNNELING ELECTRONS IN STM

J.M. PITARKE

*Fisika Teorikoa Saila, Zientzi Fakultatea, Euskal Herriko Unibertsitatea, 644 Posta Kutxatila,
48080 Bilbo, Basque Country, Spain*

P.M. ECHENIQUE

*Materialen Fisika Saila, Kimika Fakultatea, Euskal Herriko Unibertsitatea, 1072 Posta Kutxatila,
20080 Donostia, Basque Country, Spain*

and

F. FLORES

*Departamento de Física de la Materia Condensada (C-12), Universidad Autónoma de Madrid,
E-28049 Madrid, Spain*

Received 16 December 1988; accepted for publication 22 February 1989

An analysis of the apparent barrier height at a metal–vacuum–metal interface, as a function of separation, is presented for different model potentials. A parametrized model, consistent with recent theoretical work on the barrier potential which takes into account both non-local and local exchange and correlation effects is studied in detail.

1. Introduction

The scanning tunneling microscope [1] (STM) has proved to be a useful tool not only to obtain topographic images of surfaces [2] but also to provide a measure of the barrier height the electrons see when tunneling between two crystals [3]. A main problem, as regards this last point, is to understand why the apparent barrier height, as measured with the microscope, is practically independent of the tip–sample separation, and equal to the average work function of the two crystals, when the image potential and the exchange and correlation effects tend to reduce drastically the interface barrier [4]. On very general grounds one can write the microscope tunneling current intensity, at small bias, as follows [5]:

$$I = V_a K(s) e^{-2\sqrt{2\phi}s}, \quad (1)$$

where V_a is the applied voltage, s the tip-sample distance, Φ the mean tunneling barrier, and $K(s)$ a function of s . Unless otherwise stated, we use atomic units throughout.

Eq. (1) suggests that an apparent barrier height can be defined as follows:

$$\Phi_{ap} = \frac{1}{8} [d(\ln I)/ds]^2 V_a, \quad (2)$$

so that it should coincide with the mean tunneling barrier if the dependence on s of Φ and the pre-exponential factor in eq. (1), could be neglected.

Eq. (2) has been defined for the $V_a = \text{constant}$ mode but, alternatively, one could introduce Φ_{ap} using the current-stabilized mode ($I = \text{constant}$) and write [6]:

$$\Phi_{ap} = \frac{1}{8} [d(\ln V_a)/ds]^2 I. \quad (3)$$

Nevertheless, if V_a is assumed to be small enough, eqs. (2) and (3) yield the same value for the apparent barrier height, as it has been shown by Coombs et al. [7]. Accordingly, we will only discuss, for small bias, eq. (2) and its relationship with the actual barrier height.

The purpose of this paper is two-fold. First we want to give new arguments showing why the apparent barrier height, Φ_{ap} , is so much constant over such a long range of tip-sample distances as experiments show. Second, we present specific results for the apparent barrier height, calculated using an interface potential consistent with that given in a previous calculation [4]. The advantage of this interface potential is that it introduces both image forces and exchange and correlation effects, and gives an appropriate description of the actual barrier height that electrons see when tunneling between two metals.

2. General considerations

In this section, we shall discuss eq. (2), using a WKB approximation to calculate the tunneling current. More general results will be presented in section 3. The calculations presented in this paper have been obtained for two planar parallel metallic electrodes having Fermi energies of 8.0 and 5.5 eV and work functions of 4.8 eV, and a given interface potential $V(z)$ (z is the direction perpendicular to the surfaces).

If the WKB approximation is used to evaluate the electron transmission probabilities, the tunneling current density can be written (measured in $\text{\AA cm}^{-2}$) approximately, for small bias, as [8]

$$J = 8.48 \times 10^{12} V_a \Delta s^{-1} \bar{\Phi}^{1/2} (1 - 1/\sqrt{2\bar{\Phi}} \Delta s) e^{-2\sqrt{2\bar{\Phi}} \Delta s}, \quad (4)$$

where $\bar{\Phi}$ represents the mean barrier height:

$$\bar{\Phi} = \frac{1}{\Delta s} \int_{s_1}^{s_2} [V(z) - E_F] dz, \quad (5)$$

and

$$\Delta s = s_2 - s_1 \quad (6)$$

is the distance between the classical turning points s_1 and s_2 of the $V(z)$ potential at the Fermi level, E_F , which is assumed to be the same for the two metals in the case of small applied bias.

Binnig et al.'s argument [3] neglected the dependence on s of the whole pre-exponential factor in eq. (4). Then, they consider the behaviour of the exponent as a function of s , and assume:

$$\Delta s = s, \quad (7a)$$

and the image potential reduced mean barrier:

$$\bar{\Phi} = \phi_0 - (\ln 2)/s, \quad (7b)$$

where ϕ_0 represents the average work function, that is,

$$\phi_0 = \frac{1}{2}(\phi_L + \phi_R),$$

with ϕ_L and ϕ_R representing the work functions of the tip and the sample, respectively.

For $(\ln 2)/s$ smaller than $\phi_0/2$, it is a good approximation to write:

$$(\bar{\Phi})^{1/2} \approx \phi_0^{1/2} - \frac{1}{2}(\ln 2)/s\phi_0^{1/2} + O(1/s^2), \quad (8)$$

showing that:

$$2\sqrt{2\bar{\Phi}} \Delta s \approx 2\sqrt{2\phi_0}s - (\ln 2\sqrt{2})/\phi_0^{1/2} + O(1/s). \quad (9)$$

This equation, eq. (2) and the assumption made about the pre-exponential factor, yield the following result:

$$\Phi_{ap} = \phi_0 + O(1/s^2), \quad (10)$$

which obviously differs from the mean barrier height given by eq. (7b), but coincides with the barrier height, ϕ_0 , in the limit $s \rightarrow \infty$.

In this section, we explore the effect of introducing in J the full behaviour given by eq. (4). To this end, we use Simmons approximation [8]:

$$V(z) - E_F = \phi_0 - (1.15 \ln 2 s)/4z(s - z), \quad (11)$$

and find

$$\Delta s = s[1 - (1.15 \ln 2)/\phi_0 s]^{1/2}, \quad (12a)$$

$$\bar{\Phi} = \phi_0 - f(s)/\Delta s, \quad (12b)$$

where

$$f(s) = \frac{1.15 \ln 2}{2} \ln \frac{s + \Delta s}{s - \Delta s}. \quad (12c)$$

Eqs. (12), (2) and (4) yield the following result:

$$\Phi_{ap} = \phi_0 + \frac{1}{2}(\sqrt{2\phi_0} - 1.15 \ln 2)(1/s) + O(1/s^2), \quad (13)$$

showing that the pre-exponential factor in (4) introduces, up to second order in $1/s$, the correction

$$\sqrt{2\phi_0}/2s.$$

For typical work functions ($\phi_0 = 4.8$ eV) and $s = 10$ Å, the first order term in (13) is approximately -0.15 eV, in such a way that this correction turns out to be comparatively rather small, so that the apparent barrier height remains, for gap widths large enough for second and higher order terms in $1/s$ to be negligible, nearly equal to the average work function, as the results of section 3 will show.

We should mention at this point that Coombs et al. [7] have neglected the

$$1 - 1/\sqrt{2\phi_0} \Delta s$$

pre-exponential factor in eq. (4). On the other hand, the value of the apparent barrier height deduced from (2) as a function of gap distance when the tunneling current is calculated by (4), is in agreement with the calculations of Payne and Inkson [6] obtained either in the $V_a = \text{constant}$ mode or in the current-stabilized mode.

3. Exact results

In order to illustrate the discussion of section 2, in fig. 1 we show the apparent barrier height, Φ_{ap} , for two interface potentials. In one case we take:

$$V(z) - E_F = \phi_0 - (\ln 2)/s, \quad (14a)$$

while in the second, we use Simmons approximation:

$$V(z) - E_F = \phi_0 - (1.15 \ln 2 s)/4z(s - z). \quad (14b)$$

The transmission probabilities have been calculated by connecting the exact solutions of the Schrödinger equation through the barrier in question in the first case, and using numerical methods in the second, thus obtaining the exact result for the tunneling current density, by integrating over all allowed energies. As fig. 1 shows, when the image potential reduced barrier is supposed to be constant and equal to its maximum value (eq. (14a)), Φ_{ap} is, for $s > 2$ Å, larger than ϕ_0 , while it is somewhat smaller than ϕ_0 when the more appropriate potential of eq. (14b) is considered, in agreement with the discussion of section 2. It is clear from this figure the important role that the image potential plays in lowering the apparent barrier height, even though it is, for all gaps widths, higher than the maximum barrier height (dash-dotted line). It

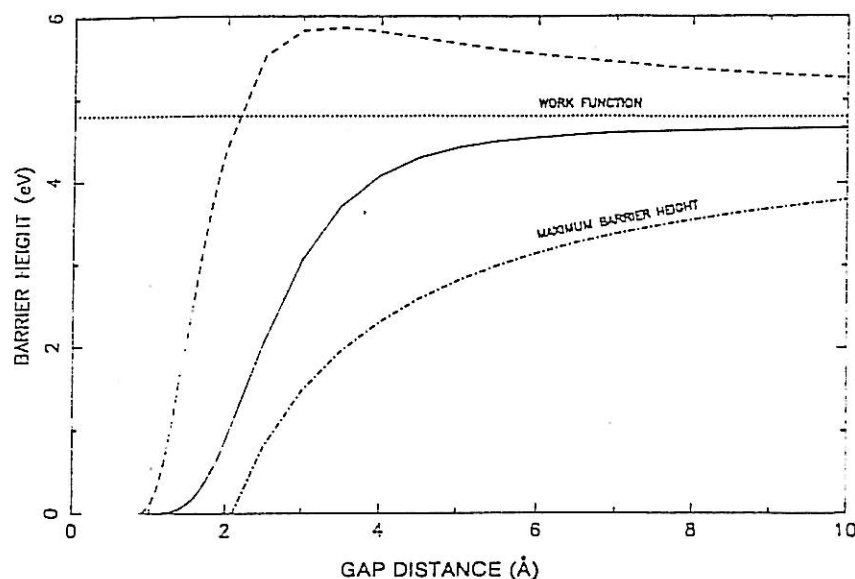


Fig. 1. Apparent barrier height as a function of gap distance when the Schrödinger equation is solved for the interface potentials of eq. (14a) (dashed curve) and eq. (14b) (solid curve). The average work function, ϕ_0 (dotted curve), and the maximum barrier height (dash-dotted curve) are given for comparison.

is also interesting to notice that Φ_{ap} is, for the more appropriate potential of eq. (14b), rather constant and close to ϕ_0 for distances larger than 5 or 6 Å. On the other hand, let us comment that in these calculations Φ_{ap} goes to zero for $s \approx 1$ Å; this is a shortcoming of the potential models introduced in eqs. (14), which at very small distances do not describe the barrier that electrons feel when they tunnel between the tip and the sample. Indeed, as shown by Lang [9] and Ferrer et al. [10], Φ_{ap} goes to zero for $s = 0$.

In order to give a more realistic description of the barrier, we have improved on these results, by using the following parametrized potential barrier [11]:

$$V(z) = \begin{cases} \frac{U_L}{A_L e^{B_L z} + 1}, & z \leq 0, \\ -\frac{1}{4} \left[\frac{1 - e^{-\lambda_L z}}{z} + \frac{1 - e^{-\lambda_R(d-z)}}{d-z} \right] \\ + \frac{\mu}{4d} \left[2\gamma + \Psi\left(1 + \frac{z}{d}\right) + \Psi\left(2 - \frac{z}{d}\right) \right], & 0 \leq z \leq d, \\ \frac{U_R}{A_R e^{B_R z} + 1}, & d \leq z. \end{cases} \quad (15)$$

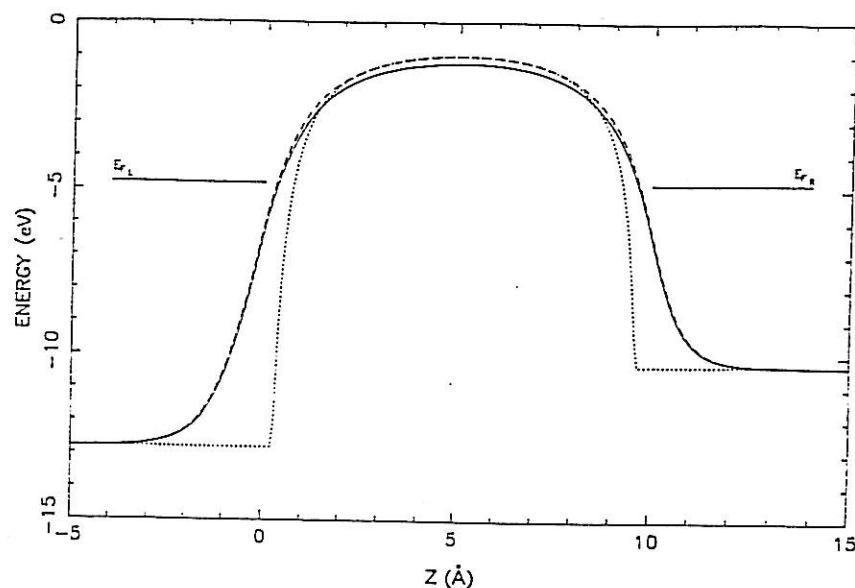


Fig. 2. Model barrier of eq. (15) with $\lambda_L = \lambda_R = 0.9a_0^{-1}$ ($a_0 = 0.529 \text{ Å}$), and $\mu = 0.5$ (solid curve) or $\mu = 1.0$ (dashed curve), for $d = 10 \text{ Å}$. Notice that in the tunneling region, far outside the image planes, this barrier converges to the classical image reduced potential barrier (dotted curve) when $\mu = 1.0$; however, for distances smaller than 4 or 5 Å it does not longer converge to the classical barrier.

In this expression the potential is referenced to the tip vacuum level. A_L , B_L , A_R and B_R are determined by matching $V(z)$ and its derivative at $z = 0$ and $z = d$, the gap distance, which is defined to be the distance between the image planes of the two metals, U_L and U_R represent the values of the bulk inner potentials of the tip and the sample, respectively, γ is the Euler number, and Ψ , the digamma function [12]. The μ quantity tells us about the dependence of the barrier height on d , and the quantities λ_L and λ_R determine the range of transition from the vacuum potential to its value in the bulks.

In fig. 2 we show the model potential of eq. (15). In figs. 3 and 4, Φ_{ap} is exhibited as a function of d , for the special case $\phi_L = \phi_R = 4.8 \text{ eV}$ and for significantly different values of ϕ_L and ϕ_R ($\phi_L = 3 \text{ eV}$ and $\phi_R = 6 \text{ eV}$), when the potential barrier parameters λ and μ of eq. (15) are considered to have the values represented in tables 1 and 2, respectively, which fit the potential of de Andrés et al [4]. These results also show that the apparent barrier height is rather constant and quite close to ϕ_0 for $d > 6 \text{ Å}$, although they differ, at short distances, substantially from the ones calculated from eq. (14b). In particular, the apparent barrier height, Φ_{ap} , as calculated from eq. (15), goes to zero for $d = 0$, in agreement with refs. [9,10].

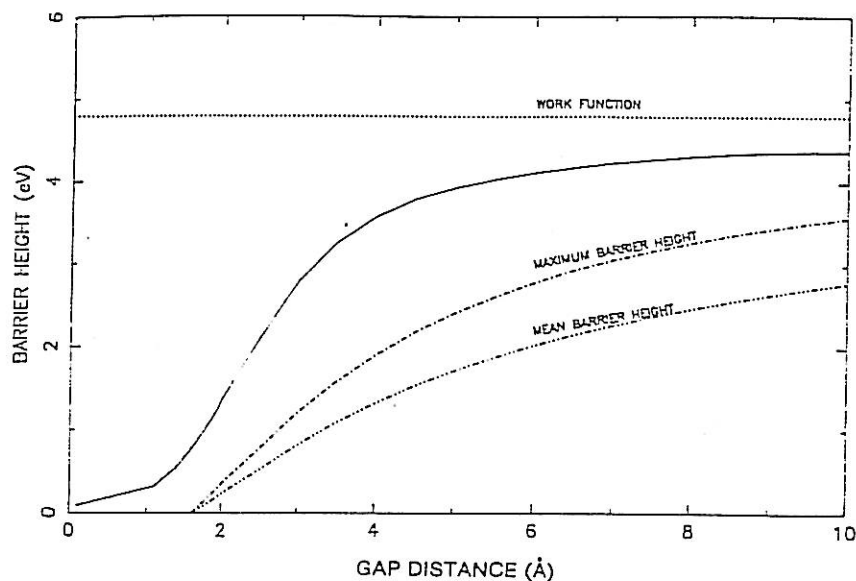


Fig. 3. As in fig. 1, but when the model barrier of eq. (15) is considered, with $\phi_L = \phi_R = 4.8$ eV and the parameters λ and μ represented in table 1. Also shown is the mean barrier height, as defined by (5) (dash-dot-dot-dot curve).

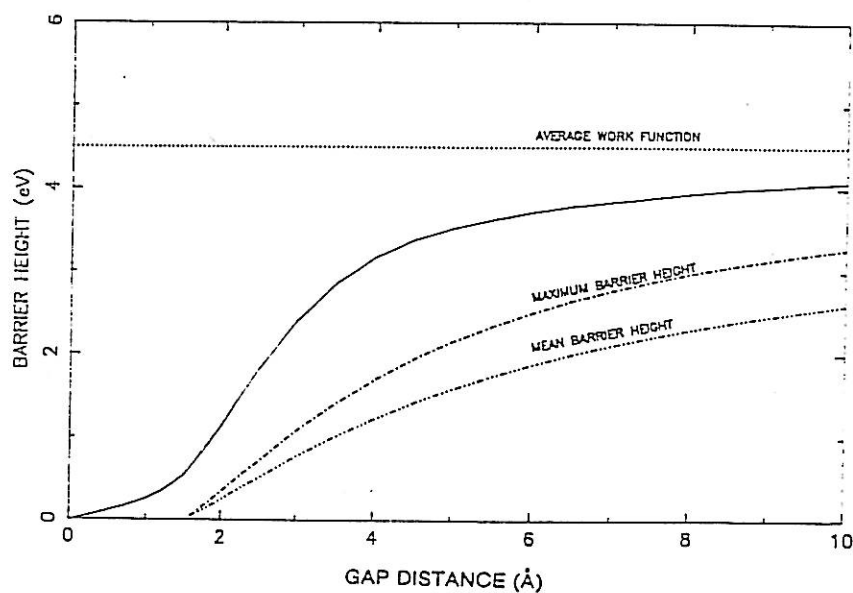


Fig. 4. As in fig. 3, but with $\phi_L = 3$ eV and $\phi_R = 6$ eV, and the parameters λ and μ represented in table 2.

Table 1

Potential barrier parameters μ , λ_L and λ_R considered in our calculations of fig. 3, as a function of gap distance

d (Å)	μ	$\lambda_L = \lambda_R (a_0^{-1})$	d (Å)	μ	$\lambda_L = \lambda_R (a_0^{-1})$
0.1	0.01	0.49	1.0	0.50	0.76
0.3	0.09	0.57	3.0	0.50	0.81
0.5	0.22	0.65	5.0	0.50	0.85
0.7	0.35	0.71	7.0	0.50	0.86
0.9	0.46	0.75	9.0	0.50	0.87

Table 2

Potential barrier parameters μ , λ_L and λ_R considered in our calculations of fig. 4, as a function of gap distance

d (Å)	μ	$\lambda_L (a_0^{-1})$	$\lambda_R (a_0^{-1})$	d (Å)	μ	$\lambda_L (a_0^{-1})$	$\lambda_R (a_0^{-1})$
0.1	0.01	-1.59	2.99	1.0	0.50	0.44	1.04
0.3	0.09	-0.19	1.43	3.0	0.50	0.55	1.00
0.5	0.22	0.16	1.16	5.0	0.50	0.58	1.02
0.7	0.35	0.33	1.08	7.0	0.50	0.60	1.04
0.9	0.46	0.42	1.05	9.0	0.50	0.61	1.05

In figs. 3 and 4 we show, as well, the mean barrier, $\bar{\Phi}$, as calculated from eq. (5) using the potential model of eq. (15). The comparison of the two barriers, Φ_{ap} and $\bar{\Phi}$, show the large difference between the apparent and the mean barrier for the actual potential of the interface. On the other hand, notice that the apparent barrier height is always smaller than ϕ_0 : this is the main difference between the results of this paper and Lang's calculation [13] (that otherwise show a reasonable agreement with our results at short distances). The reason of this discrepancy can be traced back to the non-local effects (image potential), not included in the calculations of ref. [13], which play an important role in lowering the apparent barrier height, as it has been shown above.

Acknowledgements

The authors gratefully acknowledge Gipuzkoako Foru Aldundia, Eusko Jaurlaritza and the spanish CAYCIT. Two of the authors (P.M.E. and F.F.) thank Iberduero S.A. for help and support.

References

- [1] G. Binnig, H. Rohrer, Ch. Gerber and E. Weibel, Appl. Phys. Letters 40 (1982) 178; Phys. Rev. Letters 49 (1982) 57.

- [2] G. Binnig and H. Rohrer, *Helv. Phys. Acta* 55 (1982) 726.
- [3] G. Binnig, N. Garcia, H. Rohrer, J.M. Soler and F. Flores, *Phys. Rev. B* 30 (1984) 4816.
- [4] P. de Andrés, F. Flores, P.M. Echenique and R.H. Ritchie, *Eurphys. Letters* 3 (1987) 101.
- [5] N. Garcia, C. Ocal and F. Flores, *Phys. Rev. Letters* 50 (1983) 2002.
- [6] M.C. Payne and J.C. Inkson, *Surface Sci.* 159 (1985) 485.
- [7] J.H. Coombs, M.E. Welland and J.B. Pethica, *Surface Sci.* 198 (1988) L353.
- [8] J.G. Simmons, *J. Appl. Phys.* 34 (1963) 1793.
- [9] N.D. Lang, *Phys. Rev. B* 36 (1987) 8173.
- [10] J. Ferrer, A. Martín-Rodero and F. Flores, *Phys. Rev. B* 38 (1988) 10113.
- [11] J.M. Pitarke, F. Flores and P.M. Echenique, to be published.
- [12] M. Abramowitz and I.A. Stegun, *Handbook of Mathematical Functions* (Dover, New York, 1965).
- [13] N.D. Lang, *Phys. Rev. B* 37 (1988) 10395.