A Barrier Potential Calculation for Tunneling Electrons at a Metal-Metal Interface

EUROPHYSICS LETTERS 1 January 1987

Europhys. Lett., 3 (1), pp. 101-106 (1987)

A Barrier Potential Calculation for Tunneling Electrons at a Metal-Metal Interface.

P. DE ANDRÉS (*), F. FLORES (*), P. M. ECHENIQUE (**) and R. H. RITCHIE (***)

(*) *Departamento de Física del Estado Sólido, Universidad Autónoma de Madrid, Cantoblanco*, 28049 *Madrid, Spain*
(**) *Cavendish Laboratory, Madingley Road, Cambridge*, CB3 OHE, *U.K.*
Euskal Herriko Unibersitatea, Quimicas, Donostia - Euzkadi, Spain
(***) *Health and Safety Research Division, Oak Ridge National Laboratory Oak Ridge*, TN-37830, *USA*

(received 12 May 1986; accepted in final form 28 August 1986)

PACS. 73.20. – Electronic surface states.
PACS. 73.40G – Tunnelling: general.
PACS. 73.40J – Metal-to-metal contacts.

Abstract. – The interface potential for tunneling electrons between two interface metals has been obtained as the sum of a local and a nonlocal contribution, the last one introducing image force effects. Our results show that the image potential is the dominant effect for interface distances between metal surfaces greater than 10 Å. For smaller distances, local effects control the barrier height. We have calculated this barrier height for distances between 5 and 10 Å and found its value ranging between 1.2 and 2.4 eV in good agreement with other independent evidence.

A complete theory of the scanning tunneling microscope [1] needs a full description of the barrier that electrons feel when they tunnel between the tip and the sample [2]. Although in some theoretical approaches [3] that barrier has been assumed to be independent of the distance between the two surfaces of the microscope, theoretical and experimental work [4, 5] have shown that the image force plays an important role lowering substantially the interface barrier height for intermediate distances between two metals ($\simeq(10.0 \div 15.0)$ Å). A theoretical analysis of this problem is still lacking: this is a cumbersome task, since a simple local formalism cannot be applied to it. Indeed, the image force is well known to be a nonlocal effect associated with the correlation energy of an electron leaving a surface. Although different approaches [6, 7] are available to calculate this image potential, local effects are not negligible for the distances of interest between the tip and the sample ($\simeq 10$ Å) in the microscope. The difficulty of calculating the barrier height is, then, associated with the necessity of including in the calculation, at the same time, local and nonlocal correlation effects. At present, there is a possibility of performing this calculation by using a local density formalism, supplemented with a prescription to describe the

nonlocal correlation energy for electrons moving away from a surface [8, 9]. This is a cumbersome self-consistent calculation, and in this paper we have followed a different approach by introducing some reasonable approximations in the general expression for the self-energy of an electron moving at the interface.

Figure 1 shows our model for a Au-W interface. We have simulated the two metals by means of a jellium model (for Au we take $r_s = 3.02$ and for W $r_s = 2.5$). The electronic charge

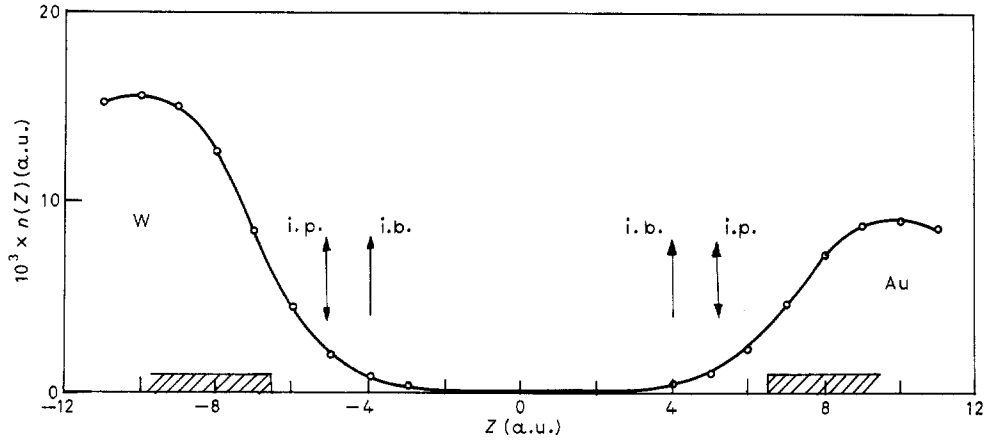

Fig. 1. – Jellium model for the Au-W interface showing the electronic density, the image planes (i.p.), the jellium edges and the infinite barriers (i.b.) for each surface.

at the interface can be calculated by using a local density formalism; the results of Smith and Ferrante [10] show that the electron density of that case is practically the superposition of the charges of the two independent surfaces. With this assumption, and using now the values calculated by LANG and KOHN [11] we can obtain the local charge and the barrier potential, $V_{xc}(z)$ for the interface. In fig. 2, 3 and 4 we show these potentials for three different distances between the two crystals; we take $d = 5.4$ Å, 7.6 Å and 9.7 Å, d being the distance between the image planes of both crystals [11]. Two comments are relevant at this point: i) first, notice that the barrier is substantially decreased by the overlapping of the metal electronic charges; this creates a deeper potential due to the local exchange and correlation energy. This result shows the importance of local effects in lowering the barrier height for tunneling electrons. ii) On the other hand, our calculations show that the distance between the points defined by the crossing of $V_{xc}(z)$ and the Fermi level is close to d as defined above. Indeed, for the three cases, we find the effective length of the barrier to be 5.7 Å, 8.1 Å and 10.1 Å, respectively.

In order to calculate the full potential seen by a tunneling electron, we start by introducing the nonlocal self-energy [12], $\Sigma(\boldsymbol{r}, \boldsymbol{r}'; w)$. We are interested in calculating this quantity at the Fermi energy, $w = E_F$. Now, we notice that, at the interface, the electronic density, $n(z)$, is rather low, and defines a local plasma frequency, $w_p(z)$, and a local Fermi momentum, $k_F(z)$. We find that the following condition is well satisfied: $w_p(z) \gg k_F^2(z)/2m$. This suggests to use Hedin's approximation [12] for $\Sigma(\boldsymbol{r}, \boldsymbol{r}'; E_F)$, and write

$$\Sigma(\boldsymbol{r}, \boldsymbol{r}'; E_F) \simeq \Sigma_{sx}(\boldsymbol{r}, \boldsymbol{r}') + \tfrac{1}{2}\Sigma_{Ch}(\boldsymbol{r} = \boldsymbol{r}'; w = 0)\,\delta(\boldsymbol{r} - \boldsymbol{r}') , \tag{1}$$

where $\Sigma_{sx}(\boldsymbol{r}, \boldsymbol{r}')$ is the screened exchange interaction, independent of w, and $\Sigma_{Ch}(\boldsymbol{r} = \boldsymbol{r}'; w = 0)$ the Coulomb-hole potential, given by the self-interaction of a static charge. Equation (1) holds if the time of response associated with the interface dielectric

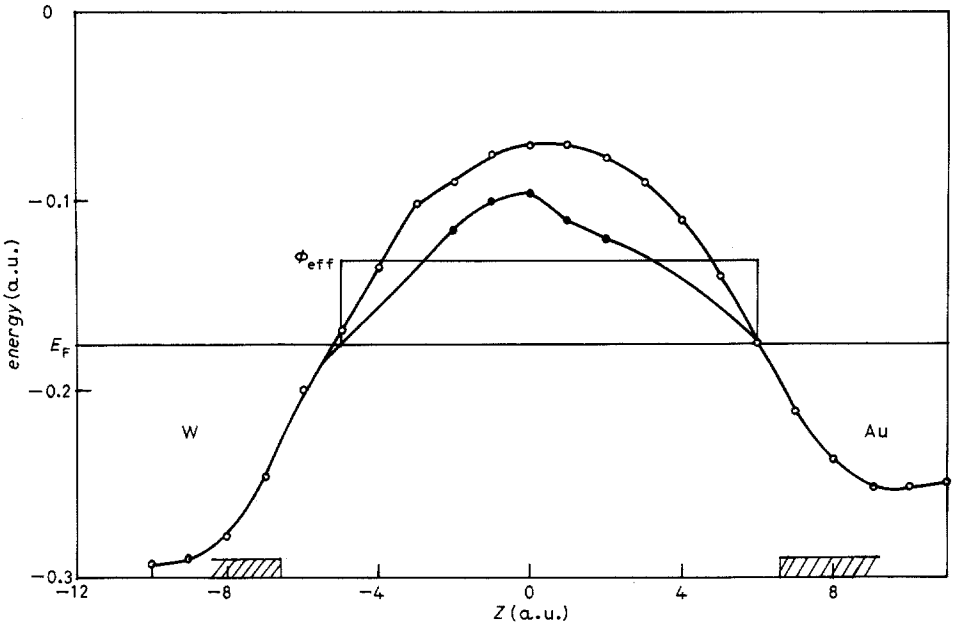

Fig. 2. – Potential barrier in the Au-W interface for a distance between the image planes equal to 5.4 Å. Open dots: local exchange and correlation potential. Full dots: total potential including local and nonlocal contribution (dots correspond to the calculated points).

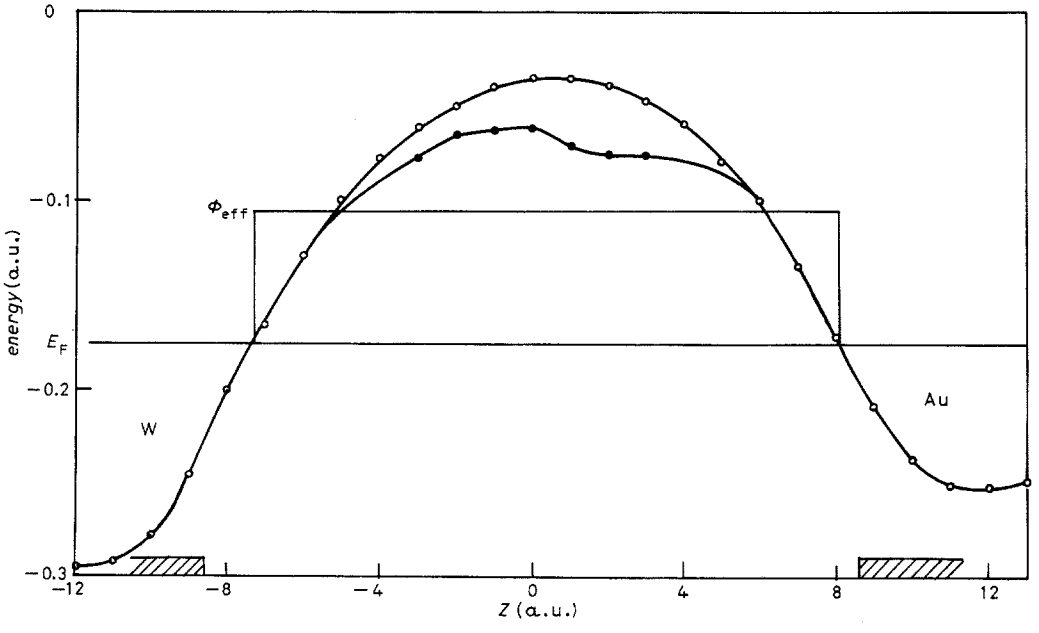

Fig. 3. – Potential barrier in the Au-W interface for a distance between the image planes equal to 7.6 Å. As fig. 2 for the differents curves.

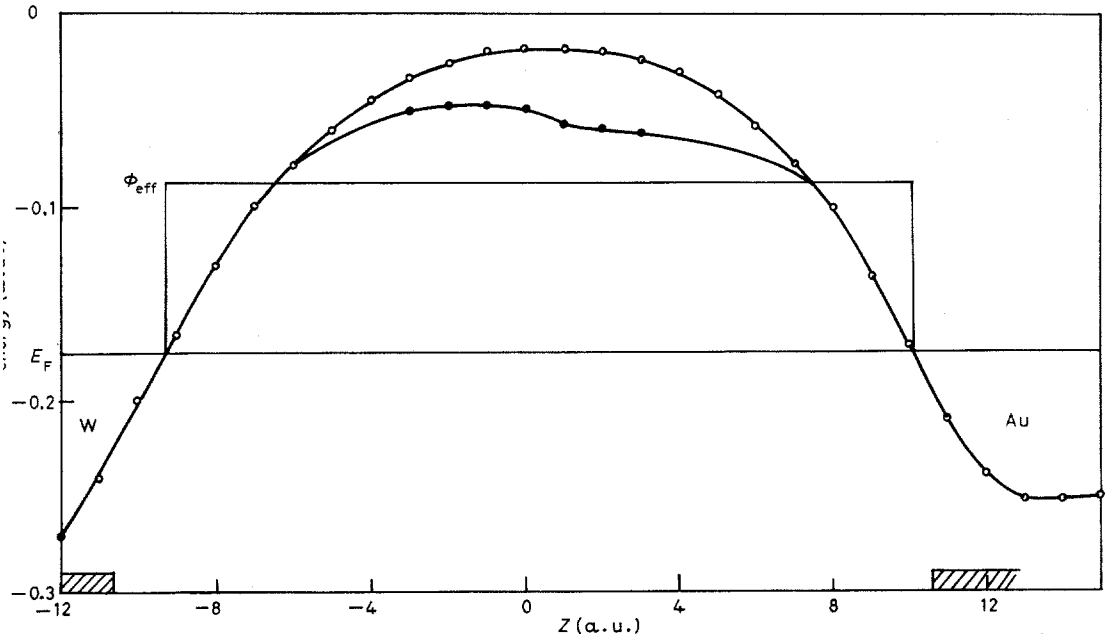

Fig. 4. – Potential barrier in the Au-W interface for a distance between the image planes equal to 9.7 Å. As fig. 2 for the differents curves.

function is short compared with the time an electron takes to travel an inter-electronic distance. Two typical frequencies appear in the interface dielectric function: the surface plasma frequency, w_s, and the local plasma frequency, $w_p(z)$; on the other hand, in the tunneling region an electron crosses the interface with a velocity given by [13] $\sim\sqrt{2m\varphi}$, where φ is the tunneling barrier height. Conditions for using eq. (1) can be written as follows:

$$w_p(z) \quad \text{or} \quad w_s \gg \sqrt{(2m\varphi)}/r_s \quad \text{or} \quad k_F^2(z)/2m \,.$$

These equations are equivalent to the condition $r_s(z) \ll 40$ for $\varphi \simeq (1 \div 2)$ eV, which is well satisfied if $d \leqslant (10 \div 15)$ Å. At larger distances, however, local effects start to be negligible, the only significant frequency is w_s, and eq. (1) is a good approximation to the self-energy.

Notice that the screened exchange self-energy is a very localized interaction. This suggests to write eq. (1) as follows:

$$\Sigma(\boldsymbol{r}, \boldsymbol{r}'; E_F) \simeq \Sigma_{sx}(\boldsymbol{r}, \boldsymbol{r}') + \tfrac{1}{2}\Sigma_{Ch}(\boldsymbol{r} = \boldsymbol{r}'; w = 0, n(z))\,\delta(\boldsymbol{r} - \boldsymbol{r}') + \\ + \{\tfrac{1}{2}\Sigma_{Ch}(\boldsymbol{r} = \boldsymbol{r}'; w = 0) - \tfrac{1}{2}\Sigma_{Ch}(\boldsymbol{r} = \boldsymbol{r}'; w = 0, n(z))\}\,\delta(\boldsymbol{r} - \boldsymbol{r}') \,, \qquad (2)$$

where we have introduced the Coulomb-hole interaction associated with the local density $n(z)$. The first two terms of eq. (2) are the local expression of the self-energy for an electron gas having the homogeneous density $n(z)$. This local contribution is a good approximation to the local potential calculated by using the local density formalism. Accordingly, the last two terms given by eq. (2) represent the specific contribution associated with the nonlocal self-energy. This means that the results calculated above for the local potential have to be corrected by the following nonlocal form:

$$V^{nl}(z) = \tfrac{1}{2}\{\Sigma_{Ch}(z' = z; w = 0) - \Sigma_{Ch}(z' = z; w = 0, n(z))\} \,. \qquad (3)$$

With eq. (3), the problem of calculating the nonlocal potential at the interface is reduced to obtaining the self-interaction of a static charge. Obviously, in the limit $d \to \infty$, the local terms are negligible and $\frac{1}{2}\Sigma_{Ch}(z' = z;\, w = 0)$ goes to the classical image potential. $\Sigma_{Ch}(z' = z;\, w = 0)$ has been calculated using an infinite barrier model [14, 15] for each metal, and by introducing a small uniform charge at the interface, trying to simulate the screening effect associated with the tails of the electronic states (see fig. 5). The infinite barrier for each metal has been located imposing the condition that its image plane coincides with the known image plane of the metal [11]. On the other hand, the small uniform electronic charge has been chosen to be the same as the one locally seen by the external charge. We have used the model shown in fig. 5 to calculate the self-energy, $\Sigma_{Ch}(z = z';\, w = 0)$, of a static charge at

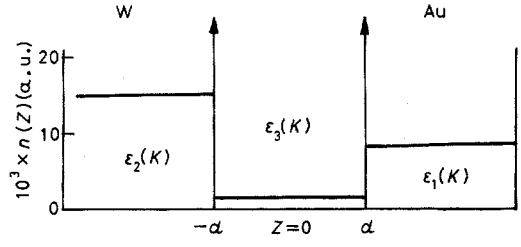

Fig. 5. – Model used to calculate the dielectric response in the Au-W interface. Different media are characterised by the bulk dielectric functions, $\varepsilon_1(k)$, $\varepsilon_2(k)$ and $\varepsilon_3(k)$.

a given position z; this is equivalent to calculating the electrostatic potential induced by a unit charge at z on itself. This has been performed by using, for metal 1 and 2, the infinite-barrier model of ref. [14], and for medium 3 a semi-classical infinite barrier model with the Lindhard dielectric function corresponding to the electronic density at the point z. We remark that, in this calculation, we extend the different region 1, 2 and 3 of fig. 5 to infinite uniform media, each one having fictitious charges adjusted to give the adequate electrostatic boundary conditions at each interface (details will be published elsewhere; see also ref. [7], chapter 5).

We mention that we can only expect the simple model used here to be a good approximation for points not to close to the metal surfaces. In our calculation, we have only obtained the nonlocal contribution at the points of the central region as shown in fig. 2, 3 and 4; then, we have joined smoothly the calculated total potential to the local potential near the two surfaces (note that for z approaching a surface, $\Sigma_{Ch}(z' = z;\, w = 0)$ goes to $\Sigma_{Ch}(z' = z;\, w = 0,\, n(z))$ and the nonlocal contribution goes to zero).

The results of our calculations are shown in fig. 2, 3 and 4. In these figures we show the local interface potential, and the total potential, obtained by adding to the local potential the nonlocal contribution. Notice that in the three cases presented in this paper, we find a small wiggle in the total potential near the middle of the interface; this is an effect which in our model is due to the assymetry of the interface, since W and Au have been modelled by different electronic densities. In particular, we find the nonlocal correction to the total potential to be more important at regions of low electronic densities: this appears not exactly at the middle of the interface, but a little shifted toward the Au surface. A word of caution should be added: these wiggles will be considerably reduced and may disappear if a self-consistent calculation is performed. The main results coming out of our calculation are the following: i) the nonlocal contribution is always negative and reduces the barrier height; ii) this nonlocal potential is a small fraction of the correction due to the local potential for $d = 5.4$ Å. Nonlocal effects do not change very much in the range of values of d taken in this paper; however, as local effects decrease with d, nonlocal effects become more important,

dominating the interface potential for large d. In particular, for $d = 9.7$ Å, nonlocal effects overcome the local ones. iii) Finally, our results show that the barrier height is very much reduced for the distances considered in this paper.

We have also calculated the effective barrier by means of the following equation:

$$\int_a^b \varphi^{\frac{1}{2}}(z)\,\mathrm{d}z = (b-a)\,\varphi_{\mathrm{eff}}^{\frac{1}{2}}\,, \tag{4}$$

where $\varphi(z)$ is the interface potential, and b and a are defined by the crossing of $\varphi(z)$ and the Fermi level. We have obtained for φ_{eff} the following values: 1.2 eV, 1.9 eV and 2.4 eV for $d = 5.4$ Å, 7.6 Å and 9.7 Å, respectively. These barriers are in very good agreement with the ones given in the fig. 2 of ref. [4] if we assume that the barrier collapses for $d_0 \simeq 3.5$ Å (in ref. [4] it was found $d_0 \simeq 3.4$ Å).

In conclusion, we have given a simple method to calculate the interface potential for tunneling electrons between two surface metals. Our results show the importance of introducing local and nonlocal effects to obtain the interface barrier. Image potential is the dominant effect for distances between metal surfaces greater than 10 Å. For smaller distances local effects control the interface barrier.

* * *

Partial financial support of this work is gratefully acknowledged to the USA-Spain Joint Committee for Scientific and Technological Cooperation and the C.A.I.C.Y.T. One of us (PME) gratefully acknowledges help and support from Iberduero SA and the March Foundation.

REFERENCES

[1] BINNING G., ROHRER H., GERBER CH. and WEIBEL E., *Appl. Phys. Lett.*, **40** (1982) 178; *Phys. Rev. Lett.*, **49** (1982) 57.
[2] BINNIG G., FRANK K. H., FUCHS H., GARCÍA N., REIHL B., ROHRER H., SALVAN F. and WILLIAMS A. R., *Phys. Rev. Lett.*, **55** (1985) 991; ECHENIQUE P. M., FLORES F. and SOLS F., *Phys. Rev. Lett.*, **55** (1985) 2348.
[3] TERSOFF J. and HAMMAN D. R., *Phys. Rev. Lett.*, **50** (1983) 1999.
[4] BINNIG G., GARCÍA N., ROHRER H., SOLER J. M. and FLORES F., *Phys. Rev. B*, **30** (1984) 4816.
[5] GARCÍA N., OCAL C. and FLORES F., *Phys. Rev. Lett.*, **50** (1983) 2002.
[6] RITCHIE R. H., *Phys. Lett. A*, **38** (1972) 189; ECHENIQUE P. M., RITCHIE R. H., BARBERAN N. and INKSON J., *Phys. Rev. B*, **23** (1981) 6468; MANSON J. R. and RITCHIE R. H., *Phys. Rev. B*, **24** (1981) 4867.
[7] GARCÍA-MOLINER F. and FLORES F., *Introduction to the Theory of Solid Surfaces* (Cambridge University Press, Cambridge) 1979.
[8] GUNNARSSON O. and JONES R. O., *Phys. Scr.*, **21** (1980) 394; ALVARELLOS J. E., TARAZONA P. and CHACÓN E., *Phys. Rev. B*, to appear.
[9] OSSICINI S., BERTONI C. M. and GIES P., *Europhys. Lett.*, to appear.
[10] FERRANTE J. and SMITH J. R., *Phys. Rev. B*, **31** (1985) 3427.
[11] LANG N. D., *Solid State Physics*, Vol. **28** (Academic Press, New York, N. Y.) 1973.
[12] HEDIN L. and LUNDQVIST S. O., *Solid State Physics*, Vol. **23** (Academic Press, New York, N. Y.) 1969, pp. 1-43.
[13] BÜTTIKER M. and LANDAUER R., *Phys. Rev. Lett.*, **49** (1982) 1739.
[14] GARRIDO L. M., FLORES F. and GARCÍA-MOLINER F., *J. Phys. F*, **9** (1979) 1097.
[15] RITCHIE R. H. and MARUSAK A., *Surf. Sci.*, 4 (1966) 234.