Contact resistance in the scanning tunneling microscope at very small distances

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A theoretical analysis of the contact resistance in the scanning tunneling microscope at very small distances is presented. For a single atom, we find that the resistance saturates at close contact, its value being $h/2e^2$. Our analysis of the recent experimental results of Gimzewski and Möller shows that the mechanical instability predicted by Pethica and co-workers appears for a distance of 1.5 Å between the tip and the sample.

The regime of close contact between the tip and the sample in the scanning tunneling microscope (STM)[1] is of high current interest. Gimzewski and Möller[2] have recently analyzed experimentally this limit and found important corrections to the simple exponential behavior[3] of the contact resistance as a function of distance. Their data also show a hysteresis pattern suggesting a transition from the tunneling to the point-contact regime.[4] This transition is related to the mechanical stability of the microscope: Pethica and co-workers[4,5] have shown that the tip and the sample jump together for very small separations, say, 1–2 Å.

The purpose of this communication is to analyze theoretically the contact resistance in the STM at very small distances. In our approach, we follow a tight-binding method whereby the main parameters of the model are obtained by means of a first-principle calculation using no adjustable parameters. We find that the tunneling current across a single tip atom presents a maximum at distances of a few Å's between the tip and the sample; the corresponding contact resistance is related to the quantum unit, h/e^2. We argue that this limit is obtained at distances that are close to the ones defining the mechanical instability of the microscope. Then, our theoretical analysis allows us to estimate the tip-sample distance at which that mechanical instability appears.

Figure 1 shows the interface geometry for two metals. We assume for simplicity that the tunneling current only flows through a single atom. We describe the tunneling problem using the following Hamiltonian:

$$\hat{H} = \hat{H}_l + \hat{H}_r + \hat{H}_{inter} , \tag{1}$$

where $\hat{H}_l$ is the left tight-binding Hamiltonian of the tip, $\hat{H}_r$ refers to the sample and

$$\hat{H}_{inter} = \sum_{k,\sigma} T_{lk} (\hat{c}_{k\sigma}^\dagger \hat{c}_{l\sigma} + \hat{c}_{l\sigma}^\dagger \hat{c}_{k\sigma}) , \tag{2}$$

where l is the atom at the tip's apex and k refers to the sample's eigenstates. We assume T_{lk} to be known; more about this point will be discussed below. We also assume that in the unperturbed system ($\hat{H}_{inter} = 0$) the Fermi energy of the left-hand electrode is $E_F + eV$ (V is the applied voltage), while it is E_F for the right-hand electrode.

This is a typical nonequilibrium system having a stationary state; its properties can be analyzed using Keldish method[6] as applied by Caroli, Combescot, Nozieres, and Saint-James[7] to the tunneling problem. First of all, notice that the total current, J, between the tip atom and the sample is given by

$$J = -\frac{ei}{\hbar} \sum_{k,\sigma} T_{lk} \{\langle \hat{c}_{l\sigma}^\dagger \hat{c}_{k\sigma} \rangle - \langle \hat{c}_{k\sigma}^\dagger \hat{c}_{l\sigma} \rangle \} , \tag{3}$$

where $\langle \rangle$ is the mean expectation value for the given operator in the stationary state of the whole system. Equation (3) can be written in terms of the Keldish-Green functions $G_{lk}^{+,-}$ (Ref. 6) in the following way:

$$J = -\frac{e}{\pi\hbar} \sum_k T_{lk} \int_{-\infty}^{\infty} \{G_{lk}^{+,-}(\omega) - G_{kl}^{+,-}(\omega)\} d\omega , \tag{4}$$

Now, $G^{+,-}$ can be calculated using[6] the following equation:

$$G^{+,-} = (1 + G'\Sigma')G_0^{+,-}(1 + \Sigma^a G^a) . \tag{5}$$

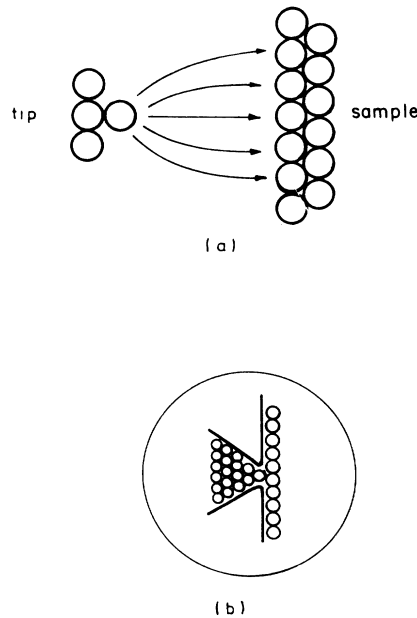This is a matrix equation, with $G_0^{+,-}$ being the Green

(a)

(b)

FIG. 1. Shows the interface geometry for two metal surfaces, (a) in the tunneling regime, (b) in close contact.

function of the uncoupled system, with $T_{lk} = 0$. G^r and G^a are retarded and advanced Green functions of the coupled system, and $\Sigma^r = \Sigma^a$ are given by the coupling T_{lk} between the atom l and the eigenstates k. The advanced and retarded Green functions, G^a and G^r, are obtained from the Dyson equation:

$$G^{r,a} = G_0^{r,a} + G_0^{r,a}\Sigma^{r,a}G^{r,a} . \qquad (6)$$

Equations (4), (5), and (6) yield the following result:

$$J = \frac{4\pi e}{\hbar}\sum_k \int_{E_F}^{E_F+eV} \frac{|T_{lk}|^2\rho_{ll}^0(\omega)\rho_k^0(\omega)}{\left|1 - \sum_k |T_{lk}|^2 G_{ll}^0(\omega)G_k^0(\omega)\right|^2} d\omega , \qquad (7)$$

where G_{ll}^0 and G_k^0 are the retarded Green-functions for the uncoupled tip and sample, respectively, while $\rho_{ll}^0(\omega)$ and $\rho_k^0(\omega)$ are the corresponding densities of states. In this equation, we assume the tip has its Fermi level at the energy E_F+eV.

Equation (7) is the basis of our analysis. The lowest order effect in T_{lk} is obtained replacing the denominator by 1. Higher-order terms necessary to calculate the case of short tip-sample distances are included in the denominator. For small voltages we can write the following equation for J:

$$J = \frac{4\pi e^2 V}{\hbar} \frac{\sum_k |T_{lk}|^2\rho_{ll}^0(E_F)\rho_k^0(E_F)}{\left|1 - \sum_k |T_{lk}|^2 G_{ll}^0(E_F)G_k^0(E_F)\right|^2} . \qquad (8)$$

We can go a step further by noticing that for half-occupied bands, the real parts of $G_{ll}^0(E_F)$ and $G_k^0(E_F)$ are small compared with their imaginary components [this is exact for symmetric densities of states, $\rho_{ll}^0(\omega)$ and $\rho_k^0(\omega)$, with respect to the Fermi energy]. Within this approximation we find

$$G_{ll}^0(E_F)G_k^0(E_F) \approx -\pi^2\rho_{ll}^0(E_F)\rho_k^0(E_F) , \qquad (9)$$

and Eq. (8) yields

$$J = \frac{4e^2 V}{\pi\hbar} \frac{\pi^2\sum_k |T_{lk}|^2\rho_{ll}^0(E_F)\rho_k^0(E_F)}{\left[1 + \pi^2\sum_k |T_{lk}|^2\rho_{ll}^0(E_F)\rho_k^0(E_F)\right]^2} . \qquad (10)$$

This equation shows that J is a function, $f(x)$, of $x = \pi^2\sum_k |T_{lk}|^2\rho_{ll}^0(E_F)\rho_k^0(E_F)$, with $f(x) = x/(1+x)^2$. This function has a maximum at $x = 1$; then

$$J = \frac{2e^2 V}{\hbar} \text{ for } \pi^2\sum_k |T_{lk}|^2\rho_{ll}^0(E_F)\rho_k^0(E_F) = 1 . \qquad (11)$$

We should comment that Eqs. (10) and (11) cannot be applied to a one-dimensional system. As shown by Landauer,[8] in this case the interface resistance is proportional to $T/(1-T)$ where T is the transmission coefficient. This effect changes Eq. (10) into

$$J = \frac{2e^2 V}{\hbar} \frac{4f(x)}{1-4f(x)} \qquad (12)$$

for a one-dimensional case, since $4f(x)$ appears to be the transmission coefficient of the interface. For the three-dimensional system we are interested in, we can neglect Landauer's effect. In the following, we disregard this

correction even for the one-dimensional systems, which are only discussed for the purpose of comparing with the three-dimensional cases.

In order to show the behavior of J as a function of the tip-sample distance, we have calculated Eq. (10) using two different models: (i) in one case, we consider a one-dimensional chain for both the tip and the sample; (ii) in a second case, we have analyzed a Ag-Ag interface (see Fig. 1) with tight-binding parameters for each crystal taken from Ref. 9. The hopping interaction, T_{lj}, between orbitals l and j of the tip and the sample, respectively, is calculated using the following equation:[10]

$$T_{lj} = \frac{\hbar^2}{2m} \int_{\sigma_{lj}} (\psi_l^*\nabla\psi_j - \psi_j^*\nabla\psi_l)dS , \qquad (13)$$

where σ_{lj} is a surface between the orbitals l and j. In Ref (11), it is argued that the best approximation to T_{lj} is obtained by choosing σ_{lj} to satisfy the condition

$$\tfrac{1}{2}\int_\Omega \psi_l^*\psi_j\,d\mathbf{r} = \int_{\Omega_l}\psi_l^*\psi_j\,d\mathbf{r} = \int_{\Omega_j}\psi_l^*\psi_j\,d\mathbf{r} , \qquad (14)$$

where the whole space Ω is split into the two subspaces Ω_l and Ω_j by the surface σ_{lj}: $\Omega = \Omega_l + \Omega_j$. Wave functions ψ_l and ψ_j are taken from the Herman-Skillman tables[12] for atomic wave functions.

Figure 2 shows $\log_{10}J$ as a function of the distance between the tip atom and the surface layer of the sample. In the three-dimensional calculation, it has been assumed that the tunneling intensity crosses the interface from the single tip atom to the five nearest neighbors of the sample [the tip atom is on a top position of the (100)-surface layer of the sample], and that the main contribution to the intensity comes from the s orbitals. These results show clearly how the intensity saturates at small tip-sample distances. Notice that the three-dimensional and the one-dimensional models yield very similar results. In our calculation, J reaches its maximum value, with $R \sim h/2e^2$, for $d_m \sim 2.5$ Å; as stated before, this distance is defined by
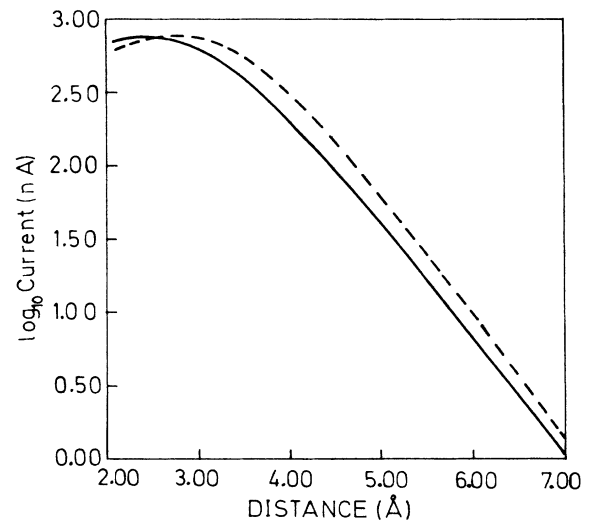

FIG. 2. Shows $\log_{10}J$ vs d for the one-dimensional model with a band width of 8 eV (dashed line) and for the three-dimensional case (full line). In both cases, $V = 20$ meV.

Eq. (11) (Landauer's effect shows that the one-dimensional resistance of this case is zero). It is interesting to notice that using this equation and the one-dimensional model for both the tip and the sample, we find that Eq. (11) yields the condition

$$T_{12}^2 = T_{11}T_{22},\tag{15}$$

where T_{12} is the hopping interaction between the last atoms of the one-dimensional crystals 1 and 2, while T_{11} and T_{22} are the hopping parameters of the one-dimensional models used for the two metals.

This result suggests that the maximum value for J in three-dimensions [Eq. (11)], or the zero resistance in the one-dimensional case, must appear when both crystals are in close physical contact, i.e., at the equilibrium distance between the tip atom and the sample. At that moment [see Fig. 1(b)] we can expect to have a minimum contact resistance, its value being $R = h/2e^2$ (one half of the quantum unit of resistance), in good agreement with other theoretical independent estimations.[13]

We should comment that the results of Fig. 2 are meaningless for distances smaller than the one for which the conductance shows a maximum (d_m): In that regime, the elastic deformations of both the tip and the sample crystals are important and the assumption of having the two crystals undeformed while the tip-sample distance is reduced has no validity. That is the reason why the results of Fig. 2 can be taken as significant only for $d > d_m$. At shorter distances, strong deformations will produce that more atoms will take contact, and the contact resistance will drop.

We will proceed to discuss these results in the perspective of the experiments of Gimzewski and Möller.[2] First of all, we notice that these authors see a mechanical instability[4,5] at $R \sim 4 \times 10^4$ Ω, a value somewhat larger than $h/2e^2 \sim 1.3 \times 10^4$ Ω, the resistance for the close contact for a single atom. On the other hand, we notice that Pethica's and Sutton's work[5] suggests that the mechanical instability of the microscope appears when the distance between the tip and the sample is 1–2 Å larger than the close contact between the two crystals. Accordingly, we propose that a minimum value in the resistance (close to $h/2e^2$) should be obtained in the microscope if no mechanical instability had appeared when approaching the tip to the sample. In Fig. 3 we show the results of Gimzewski and Möller,[2] and a plausible extension of the
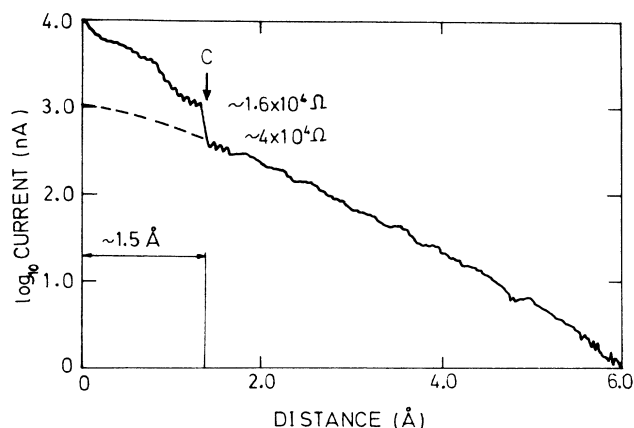

FIG. 3. Shows the results of Gimzewski and Möller (Ref. 2) extended to shorter distances between the tip and the sample (see text).

values obtained by these people before the instability to shorter tip-sample distances (the inaccessible region of Pethica and Sutton[5]). Notice that we assume that the minimum resistance of the extended curve is defined by the value of the measured resistance after the jump: At this point, $R \sim 1.6 \times 10^4$ Ω, close, although a little larger than $h/2e^2 \sim 1.3 \times 10^4$ Ω. This suggests that after the mechanical instability, the sample and the tip are in contact only through a single atom; the small difference between the experimental value and $h/2e^2$ can be related to the assumptions of the theoretical analysis: For a nonsymmetric density of states at the tip or the sample (in the experiments of Ref. 2, the tip is Ir), the resistance would increase slightly with respect to the ideal value calculated in this paper. On the other hand, Fig. 3 shows how the extended curve for the contact resistance suggests that the jump between the tip and the sample at the instability appears for distances of 1.5 Å, in very good agreement with the discussion of Pethica and Sutton.[5]

In conclusion, we have presented a theoretical calculation of the contact resistance for STM at variable short tip-sample distances. Our results are in good agreement with the experimental evidence of Gimzewski and Möller[2] and show how to deduce the experimental tip-sample distance for which the microscope mechanical instability[4,5] appears.

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