

Conductance simulation through single atom junctions at the scanning tunnelling microscope

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Abstract

Using a Keldish–Green Function formalism we simulate the current flowing through transition and noble metal atoms wires. Such a kind of wire is nowadays experimentally studied with several methods involving mechanically controllable break junction or a scanning tunnelling microscope operating in close contact regime. Our aim is to reproduce the experimental differences found between several materials. Results for Pt, Ni and Au and their comparison with the experiments are discussed.

Keywords: Conductance; Tunelling

1. Introduction

Using the scanning tunnelling microscope, different experimental groups have recently shown that the total conductance of the metal–tip junction presents different quantizations close to a multiple of the quantum conductance unit $2e^2/h$ [1–3]. In these experiments, the metal tip is pressed against a sample of the same material and, in the next step, the tip is pulled off until it becomes separated from the sample. In this process, a microscopic wire is formed and the conductance of the wire is measured. This conductance shows different jumps along the pulling process, and the last jump before zero current defines a conductance that probably corresponds to the case of a single atom connecting the tip and the sample. This characteristic quantum conductance has a different value depending on the material considered.

Some molecular-dynamics calculations have already shown how the tip–sample interface evolves as a function of the pulling process [4]; in particular, atoms rearrange along the interface wire and, in the final process, a simple atom makes the contact between the two sides of the interface (Fig. 1).

In spite of those complicated simulation calculations, no complete description has yet been presented for obtaining the conductance of the wire formed at the interface. In the most complete calculations [4], a single-

orbital has been associated with each atom and the conductance has been obtained using a tight-binding approach.

Our aim in this paper is to analyze the quantum conductance of a single atom linking the tip and the sample, using a description of the system that takes into account all the different orbitals contributing to the conductance. Although the case of noble metals Au, Ag or Cu, can be expected to be well described by a single s-orbital, other cases, like Ni and Pt, need a description that involves the contribution coming from d-orbitals, since these electrons are well-known to contribute to the metal conductance. As the interface conductance depends on the number of effective channels contributing to the conductivity, an appropriate description of the single atom case we are considering here should include the atomic d-levels.

2. Model and method of calculation

In our model, we have analyzed different cases with a single atom linked to different geometries. Figs. 2(a), 2(b) and 2(c) show the three cases we have considered: in Fig. 2(a) a single atom sees the local geometries of two (100) surfaces; in Fig. 2(b) the atom sees the local geometries of the (111)-surfaces; in Fig. 2(c) we have considered that two atoms form a short wire between the (100) faces of the tip and the sample. In our calculations we have assumed that the small clusters

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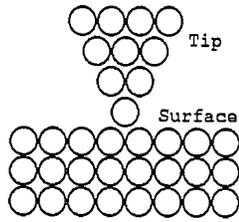


Fig. 1. Single atom junction formed by the tip-sample system.

simulating the tip and the sample are joined to Bethe-lattices simulating the bulk density of states of the metal. In our model we use a tight-binding approach with the parameters taken from Ref. [3]. We have introduced self-consistency in our problem by imposing a local charge neutrality condition at each atom. This is a crucial step for it compensates for the effect of band narrowing produced at the junction, where the coordination is reduced; (self-consistency pushes the narrowed bands up, avoiding an unrealistic decrease of the density of states at the Fermi level, and therefore of the total current itself.) The d and s levels can also change their relative energies owing to the low coordination of the interface atoms. This was taken into account by interpolating between the levels of the bulk [5] and those of the isolated atom [6] as a function of the atomic local environment.

In our specific approach we follow Refs. [7,8] and start with the Hamiltonian:

$$\hat{H} = \hat{H}_1 + \hat{H}_2 + \hat{H}_{12} \quad (1)$$

where \hat{H}_1 and \hat{H}_2 define the unperturbed Hamiltonian of the tip and the sample, with the atom at the interface arbitrarily associated to the tip-geometry. In Eq. (1) \hat{H}_{12} couples both sides and defines, in our approach, the perturbative Hamiltonian.

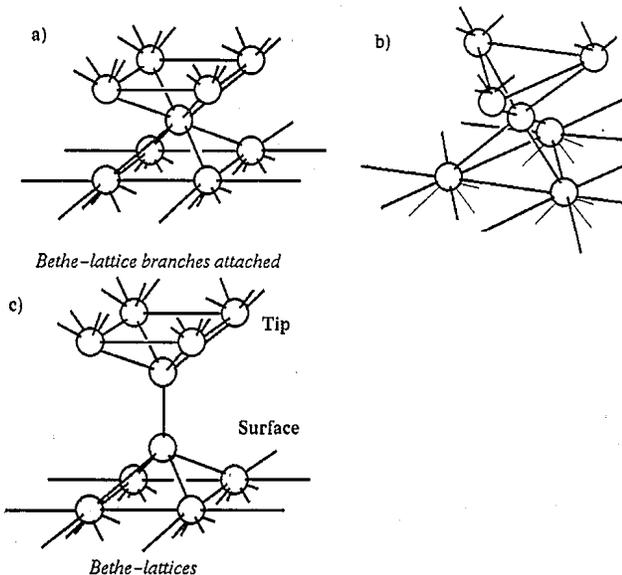


Fig. 2. (a) (100) single atom junction; (b) (111) single atom junction; (c) (100) two-atoms wire.

Using a localized basis, we write \hat{H}_{12} as follows:

$$\hat{H}_{12} = \sum_{ts\sigma} T_{ts} (C_{t\sigma}^+ C_{s\sigma} + C_{s\sigma}^+ C_{t\sigma}) \quad (2)$$

where t and s represent orbitals in the tip and the sample respectively, and T_{ts} defines the hopping matrix elements.

Our next step is to calculate the current intensity J between the tip and the sample for a given bias V . This has been calculated using a Keldish formalism [9,10] that yields nonequilibrium Green functions, $G^+ - (\omega)$; in this approach J is given by:

$$J = \frac{e}{\pi\hbar} \sum_{ts\sigma} \int_{-\infty}^{\infty} d\omega [T_{ts} G_{st}^+ - (\omega) - T_{st} G_{ts}^+ - (\omega)] \quad (3)$$

In contrast, Green functions $G^+ -$ are given by the Dyson-like equations [9,10]:

$$G^+ - = (I + G^R T^+) G_0^+ - (I + T G^A) \quad (4)$$

$$G^{R(A)} = G_0^{R(A)} + G_0^{R(A)} T G^{R(A)} \quad (5)$$

where $G^{R(A)}$ is the retarded(advanced) Green-function's matrix, the subscript 0 refers to the uncoupled system, and T defines the tip-sample coupling.

Eqs.(3)–(5) yield the following result for the tunnelling current [11]:

$$J = \frac{4\pi e}{\hbar} \int_{-\infty}^{\infty} d\omega \text{Tr} [\hat{T}_{ts} \rho_{ss}^0(\omega) D_{ss}^R(\omega) \hat{T}_{st}^+ \rho_{tt}^0(\omega) D_{tt}^A(\omega)] \times [f_t(\omega) - f_s(\omega)] \quad (6)$$

$$D_{tt}^A(\omega) = [\hat{I} - \hat{T}_{ts} G_{ss}^{A(0)} \hat{T}_{st}^+ G_{tt}^{A(0)}]^{-1} \quad (7)$$

$$D_{ss}^R(\omega) = [\hat{I} - \hat{T}_{st} G_{tt}^{R(0)} \hat{T}_{ts}^+ G_{ss}^{R(0)}]^{-1} \quad (8)$$

where f is the Fermi distribution function of each side of the interface. This is the equation we have used to calculate the tip-sample conductance. For small bias, Eq. (6) yields

$$\sigma = \frac{J}{V} = \frac{4e^2}{\hbar} \text{Tr} [\hat{T}_{ts} \rho_{ss}^0 D_{ss}^R \hat{T}_{st}^+ \rho_{tt}^0 D_{tt}^A]_{\omega = E_F} \quad (9)$$

In our calculations we obtain $G^{R(0)}$ and $G^{A(0)}$ for the uncoupled system and calculate the conductance using Eq. (9).

3. Results

Numerical calculations have been performed for three different transition metals: Pt, Ni and Au. Our results are presented in Fig. 3; they show that for each geometry, the highest conductance always occurs for Pt; Ni gives a slightly lower value, while for Au the conductance has, in each case, the lowest figure.

This behaviour is in agreement with recent experimental work [1–3], and it can be explained by the differences in the electronic structures of the different metals.

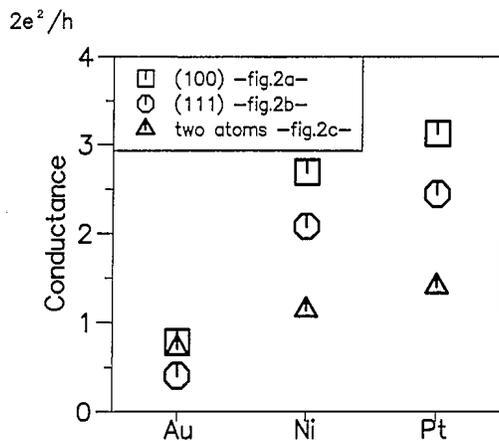


Fig. 3. Conductance calculated for the different transition metals and structures considered. The values are expressed in conductance quantum units ($2e^2/h$).

For Au the d-bands are located deeply below the Fermi level and, accordingly, the tunnelling through these orbitals does not give any contribution to the total current. In contrast, p-bands appear mostly above the Fermi level, and the tunnelling through these orbitals is not significant either; thus, the main conductance is due to the tunnelling via s-orbitals (single channel tunnelling). Similar conditions appear for the other noble metals, like Cu and Ag. In all these cases (i.e. Au, Ag, Cu) only the s-orbital is contributing to the tunnelling current and, consequently, the conductance is near one quantum unit, being smaller than one in any case.

A basically different case appears for Pt and Ni, where d bands are located around the Fermi level. Then, besides the s-contribution the total conductance also has a strong contribution from the d-orbitals. As a result the conductance for Pt and Ni is significantly greater than one quantum unit and, depending on the structure considered, it takes values between 1 and 3 (several channels contributing to the interface conductance).

Our results also show that the junction geometry also strongly influences the value of the conductance, in agreement with the experimental evidence that shows fluctuations [2] probably due to changes in the geometry.

4. Conclusions

Our approach seems to be an appropriate way to face the problem of the conductance through narrow wires. It has the quality of dealing very directly with the particular electronic character of each material, en-

abling us to understand the qualitative differences between materials. In particular, we have shown that for some transition metals, like Ni and Pt, the tunnelling current through the d orbitals yields an important contribution to the total current intensity, leading to a many channel conductance. In the case of Au only the s orbital is playing a role, with a consequent lower conductance.

The model presented here does not exhibit any limitation for being improved. The first step to be taken in order to obtain accurate quantitative results, would be to introduce a complete treatment of the chemical interactions taking place around the atoms of the interface. This would be achieved in a way similar to the treatment of chemisorption on surfaces [12]. It would also be desirable to develop a molecular dynamics calculation of the interface structure [4], in order to avoid the arbitrary choice of the tip-sample geometry. In fact we conclude that the specific shape of the structure plays an important role in the final interface conductance.

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