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Electronic transport through atomic size constrictions

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Abstract. We study the electronic transport properties of metallic nanocontacts, by means of ab-initio electronic-structure calculations. We use the screened Korringa-Kohn-Rostoker Green's function method to calculate the electronic structure while the conductance is obtained in the ballistic regime within the Landauer formalism. We present results for Pd constrictions and study the transport through different contact atoms connected to the Pd leads. For sp atoms, the transmission can be easily correlated to the local densities of states which is not the case for transition metal atoms.

1. Introduction

As the dimensions of electronic devices become smaller and smaller there is a growing interest in alternative design using new materials and concepts to achieve higher integration. For electronic components smaller than 10 nm we reach the limits of validity of the usual laws of diffusive electronic transport, and a full quantum mechanical treatment is necessary.

Recent advances in experimental techniques made possible the study of electronic transport properties through individual atoms or small molecules [1, 2]. In particular, in break junction experiments stress is applied to a nanometer size constriction while the current through the constriction is recorded as a function of time, until the junction breaks. In the last stage, just before breaking, the current flows through the few atoms of the constriction. In some cases the conductance quantum ($2e^2/\hbar$) can be clearly observed. Experiments are usually analyzed with conductance histograms using a series of break-junction experiments which record the last value of the conductance before the junction breaks. Clear peaks close to integer multiples of the conductance quantum unit are observed for the noble metals Cu, Ag, Au, but for transition metal constrictions the situation is more complicated and no clear peak is observed. Similar experiments have been carried out using metallic alloys and studying the conductance histograms by varying the alloy concentration [3].

Theoretically, several methods such as tight-binding and ab-initio, have been used to describe transport through a few-atoms constriction. An important conclusion is that the conductance of single atom contacts is related to the number of valence orbitals of the contact atom at the Fermi level [4, 5]

In this work we consider transmission through Pd constrictions and study the influence of different contact atoms on the transport properties. In particular we are interested in cases

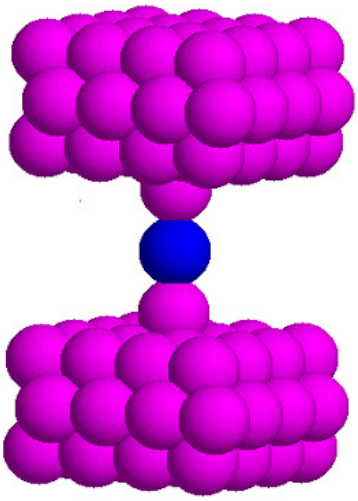

Figure 1. Atomic arrangement of the nanocontacts.

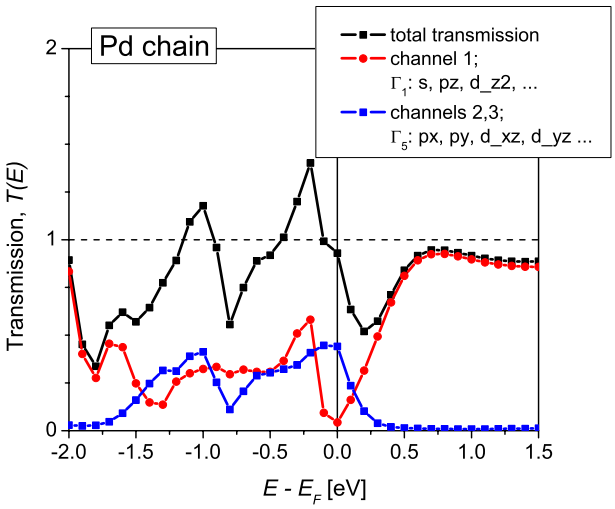

Figure 2. Energy variation of the transmission through a Pd nanocontact. The total transmission is decomposed according to the symmetry. Only three channels contribute; two of them are degenerate.

where transition metal atoms are involved and localized d orbitals dominate close to the Fermi level.

2. Method of Calculation

The electronic structure of the nanoconstrictions is calculated using the screened Korringa-Kohn-Rostoker Green's function method [6]. The method allows the description of the problem in steps. Firstly, we calculate the Green's function of the two semi-infinite Pd(001) leads separated by vacuum layers, and then we obtain the Green's function of the nanocontact region using a Dyson equation. A spherical, atomic sphere approximation is used for the potential but the non-sphericity of the charge density is fully taken into account. Transmission is calculated between two planes at the leads, using the Landauer formalism. Details about the calculation of the conductance can be found elsewhere [7, 8]. The transmission can be analyzed by considering a symmetry decomposition which allows the correlation of the conductance with the states of the contact atom. This is very helpful in high symmetry configurations as the ones we study in this work.

3. Results discussion

We have used a lattice constant of 7.35 a.u. for bulk fcc Pd. The local densities of states (LDOS) are mainly d-like at the Fermi level for both the bulk and the Pd surface. In our calculations we have used a constriction as shown in Fig. 1. We consider different atoms in the middle of the junction as we will discuss later. The distance between the atoms is kept the same as in bulk Pd and no geometry optimization was performed. Here we should note that break-junction experiments do not measure an equilibrium atomic configuration in the constriction but rather record conductance dynamically, as the atoms move before breaking. For this reason we have chosen a representative atomic configuration for our study. According to the Landauer formula the conductance $G = 2e^2/\hbar \sum T(E_F)$ is essentially the transmission T at the Fermi level and the sum runs over all channels. The results of our ab-initio calculation

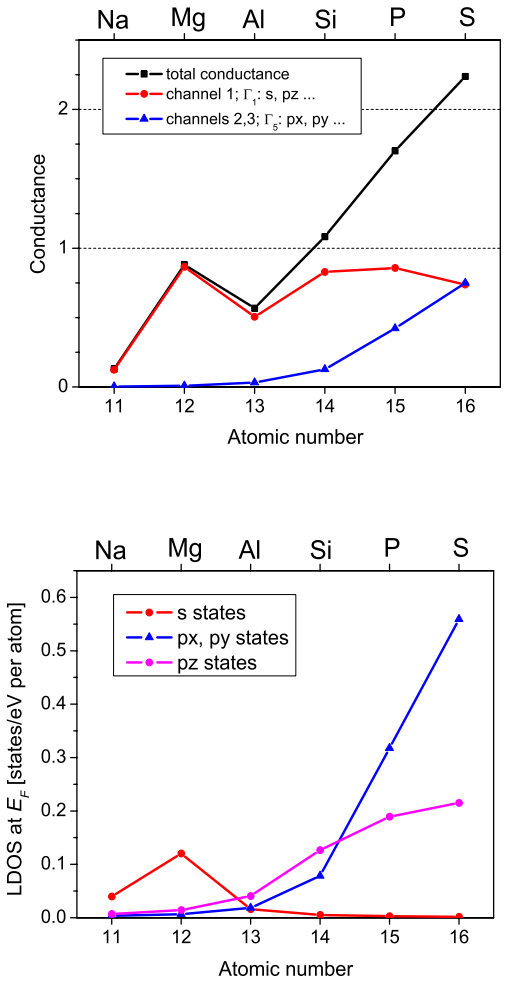

Figure 3. Conductance (upper panel) in units of $2e^2/\hbar$ together with LDOS at E_F (lower panel) for sp atoms in a Pd constriction, in the geometry of Fig. 1

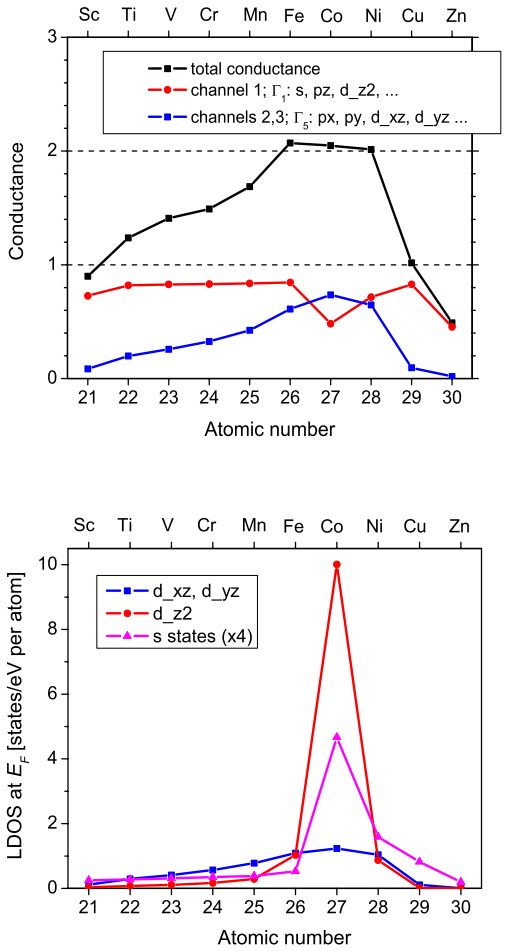

Figure 4. Conductance (upper panel) in units of $2e^2/\hbar$ together with LDOS at E_F (lower panel) for 3d atoms in a Pd constriction, in the geometry of Fig. 1

for the transmission through a Pd constriction for an energy range close to the Fermi level are shown in Fig. 2. As we can see, the conductance is close to $2e^2/\hbar$ but we also observe a strong variation of the transmission with energy. The energy variation can be understood if we consider the decomposition of the total transmission into channels using the symmetry of the junction. The junction has the C_{4v} symmetry, but essentially only 3 channels contribute to the transmission. A channel which projects onto s, p_z, d_{z^2} orbitals of the contact atom, and a doubly degenerate channel which projects onto p_x, p_y, d_{xz}, d_{yz} orbitals. The other channels are found to have negligible contributions. From Fig. 2 we observe that the total transmission has two pronounced peaks at -1 eV and at -0.2 eV below the Fermi level. The symmetry decomposition shows that the lower peak is mainly d_{z^2}-like and it can be correlated with a corresponding peak at the d_{z^2} LDOS of the Pd atom in the middle of the junction (not shown). The second peak at -0.2 eV below E_F is due to degenerate d_{xz}, d_{yz} orbitals and can be also traced at the LDOS in this energy range. It is interesting that the conductance of the junction is close to $2e^2/\hbar$

but the transmission varies strongly if we move away from E_F. Thus the conductance is very sensitive to the exact geometrical arrangement of the atoms during the breaking of the junctions in the experiment. This is due to the dependence of the peaks in transmission on the energetic position of the d orbitals which will change if we consider a small atomic rearrangement. This is in accordance with the experimental finding for Pd and can be generalized to other transition metals as well [1].

Let us now discuss the influence of different contact atoms on the transmission through the junction. Experiments with different atoms can be realized using a STM tip to probe conductance through an atom, or using alloys in a break-junction experiment [3]. We have performed a systematic study by considering both sp and d transition metal contact atoms in a Pd constriction in order to understand the general trends and our results are shown in Figs. 3, 4. In Fig. 3 in the top panel we present the conductance together with the channel decomposition and compare it to the LDOS of the contact atom, at the Fermi level (bottom panel). For sp atoms the change in the conductance with the atomic number follows the variation of the LDOS. For low valences (Na and Mg) states have essentially s character at E_F, but the transmission is low since the coupling to the Pd states is weak. The transmission is essentially due to the channel of Γ_1 symmetry which projects onto s, p_z states. By increasing the atomic number, more electrons move to lower energies with respect to E_F and the transmission increases for Mg. As we move up to Al the s states are filled up with 2 electrons, and the reduction of the s LDOS at E_F results in the small drop in the conductance for Al. For Si, P, and S our results are well understood since the p virtual bound state becomes more occupied and the LDOS at E_F increases for p_x, p_y and p_z states. As a result the conductance increases up to a value of 2.3 for S while both p_z and p_x, p_y channels contribute equally. The direct correlation of the channel transmission to the orbital LDOS of the contact atom can be clearly seen from Fig 3. Moreover as we go to the end of the p series, the p states are filled resulting to a drop of the conductance.

In the case of transition-metal atoms the situation is slightly different. This is mainly due to the fact that these atoms have localized states with small velocities. This makes the formation of highly transmissive channels more difficult. Our results are shown in Fig. 4. The conductance is close to $2e^2/\hbar$ for Sc and is mainly due to the s-like channel, which is almost open along the 3d series. The conductance increases mainly due to contributions from the doubly degenerate d_{xz}, d_{yz} channel and reaches a peak for Ni. On the contrary the increase in the d_{z^2} and s LDOS is accompanied by a small reduction of the transmission of the corresponding channel because these states are localized at the contact atom. For Cu and Zn both d and s states move lower in energy away from the Fermi level and the conductance drops. Thus if transition metal atoms are involved, high LDOS does not necessarily mean increased transmission.

In conclusion we studied the electronic transport through different contact atoms connected to Pd electrodes. Transmission can be easily correlated to the LDOS of the contact atom in the case of sp atoms but not when d states are involved in the transmission.

4. References

[1] Agraït N, Levy Yeyati A and van Ruitenbeek J M 2003 *Phys. Rep.* **337** 81
[2] Ohnishi H, Kondo Y and Takayanagi K 1998 *Nature* **395** 780
[3] Enomoto A, Kurokawa S and Sakai A 2002 *Phys Rev B* **65** 125410
[4] Cuevas J C, Yeyati A L and Martín-Rodero 1998 *Phys. Rev. Lett.* **80** 1066
[5] Scheer E, Agraït N, Cuevas J C, Levy Yeyati A, Ludoph B, Martín-Rodero A, Rubio Bollinger G, van Ruitenbeek J M and Urbina C 1998 *Nature* **394** 154
[6] Papanikolaou N, Zeller R and Dederichs P H 2002 *J. Phys.: Condens. Matter* **14** 2799
[7] Mavropoulos Ph, Papanikolaou N and Dederichs P H 2004 *Phys. Rev. B* **69** 125104
[8] Bagrets A, Papanikolaou N and Mertig I 2004 *Phys Rev B* **70** 064410