Electronic transport properties in copper nanowire

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ABSTRACT

In present work, we study the electronic transport properties of copper nanowire using the non-equilibrium Green's function technique on the density functional tight binding method for modelling the conductance under external bias voltage. We also carried out the calculations for the Au nanowire for comparison.

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1. Introduction

In recent years, a worldwide effort has been devoted to nanoelectronic devices transport properties both experimentally and theoretically [1] as the nanoscaled electronic systems represent the ultimate size limit of functional devices. The metal nanowires are mostly fabricated at quantum point contacts by the scanning tunnelling microscope and the mechanically controllable breaking junction [2,3]. As well-characterized experiments on nanoscale contacts remain challenging tasks, theoretical calculations play an important role for such an understanding. Although copper is a commonly used interconnect metal, fewer studies have been done on copper nanowires.

In this paper, the theoretical analysis has been performed on electronic transport properties of the copper and gold nanowires attached to the cognate (100) electrodes.

The paper is organized as follows: in Section 2 we describe the method and the model to study the system. The results are explained in Section 3, and a summary is given in Section 4.

2. Method of calculation

In order to study the electron transport properties, the copper nanowire sandwiched between crystalline electrodes in (100)

direction, is considered. The schematic view of the system under study, can be represented in the Fig. 1, is partitioned into three parts: two contacts, and the scattering region. The contacts are semi-infinite leads and it is assumed that their properties coincide with those of bulk system. The more realistic nanowire model is obtained by considering a part of the electrodes with several atomic layers in scattering region.

Calculations are performed using the non-equilibrium Green's function within the density functional tight binding method [4–7] and the Landauer–Büttiker theory [8,9] to obtain the differential conductance of the system. Interaction between the valence electrons is treated in the local density approximation (LDA) [10].

The tight binding Hamiltonian of the entire system takes the form:

$$H^0_{\mu\nu} = \begin{cases} \in^{\text{free-atom}}_{\mu}, & \mu = \nu \\ < \phi_{\mu}|T + v_{\text{eff}}(n^0_i + n^0_j)|\phi_{\nu} >, & \mu \in i, \nu \in j \end{cases} \qquad (1)$$

where φ_{μ} and φ_{ν} are the atomic orbitals localized around the atomic centres i and j; T is the kinetic energy operator, and v_{eff} is the effective one-particle potential which depends on the density of the two atomic centres i and j.

In experiments, the transport properties are measured by applying finite bias voltages between the electrodes. Since the applied bias changes the transport properties from those at the zero-bias limit, it is important to consider the effect of the applied bias in the theoretical studies. This is provided by the NEGF method introduced by Keldysh [11] to deal with non-equilibrium situation.
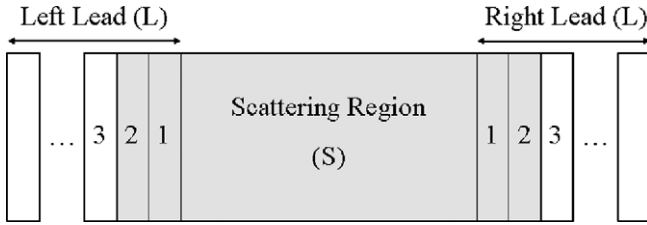
Fig. 1. Schematic setup of the system. It is divided into three regions: the scattering region (S), and the left (L) and the right lead (R). The numbering of the leads refers to the atomic layers considered into scattering region.

The density matrix needed for the density functional Hamiltonian can be described in terms of the NEGF:

$$\rho = \frac{1}{2\pi i} \int_{-\infty}^{+\infty} dE\, G^<(E) \qquad (2)$$

the Keldysh Green's functions, $G^<(E)$ and $G^>(E)$, are defined in terms of the retarded, the advanced Green's functions, and the non-equilibrium self energies $\sum^<$ and $\sum^>$.

$$G^{<,>} = G^r \sum^{<,>} G^a \qquad (3)$$

Within this formalism the current can be written with an expression formally equivalent to that of scattering theory by treating the coupling between the scattering region and the leads at perturbation [12–14].

$$I(V) = \frac{2e}{h} \int_{\mu_1}^{\mu_2} \text{Tr}\left[\sum_L^< G^> - \sum_L^> G^< \right] dE \qquad (4)$$

where $\sum_L^{<,>}$ are the self energy functions for the left contact. The limits of the integration, μ_1 and μ_2, are the electrodes chemical potentials.

It is assumed that the voltage drops across the scattering region, this assumption results in the contact self-energy functions $\sum_{L(R)}^{<(>)}$ reducing to

$$\sum_{L(R)}^< = -2if_{L(R)}\text{Im}\left(\sum_{L(R)}^r \right)$$
$$\sum_{L(R)}^> = 2i(1 - f_{L(R)})\text{Im}\left(\sum_{L(R)}^r \right) \qquad (5)$$

where $f_{L(R)}$ is the Fermi distribution function and $\text{Im}(\sum_{L(R)}^r)$ is the imaginary component of the retarded self-energy in the respective contact.

Based on the Landauer's scattering approach to electron transport, and assuming that transport is ballistic for finite bias voltages, the current can be established by noting that the transmission matrix $t(\varepsilon)$ as

$$t(\varepsilon) = [\Gamma_R(\varepsilon)]^{1/2} G^r(\varepsilon)[\Gamma_L(\varepsilon)]^{1/2} \qquad (6)$$

where the $\Gamma_{L(R)}(\varepsilon)$ is given by

$$\Gamma_{L(R)}(\varepsilon) = i\left(\sum_{L(R)}^r(\varepsilon) - \left[\sum_{L(R)}^r(\varepsilon) \right] \right) \qquad (7)$$

By substituting the transmission matrix into Eq. (4) the current is obtained as follows

$$I(V) = \frac{2e}{h} \int \text{Tr}[\Gamma_R G^r \Gamma_L G^a](f_R(E) - f_L(E))dE \qquad (8)$$

where $\text{Tr}[\Gamma_R G^r \Gamma_L G^a]$ gives the transmission coefficients.

The differential conductance can be obtained from the current flowing through the system by taking the derivative of current with respect to bias voltage [15–17].

In the adiabatic approximation, the zero-bias voltage conductance at zero temperature can be written as $G = G_0 T$, where $G_0 = 2e^2/h$ is quantum conductance and the factor T represents the average probability that an electron injected at one end of the conductor will transmit to the other end.

3. Results and discussion

The transmission coefficients of the copper nanowire depicted in Fig. 1 for external bias voltages of 0–2 V have been calculated. The total transmission spectra with respect to the electron incident energy in zero and 1.0 applied bias voltages are shown in Fig. 2a and b, respectively. The results indicate that the fluctuation amplitudes of transmission spectra decrease by increasing the applied bias voltage and the whole transmission spectra shifts to lower energies in the presence of applied bias voltage.

The electronic transport properties of gold nanowire with the structure similar to the copper nanowire are presented for comparison. The calculated I–V characteristics of each nanowire up to a bias voltage of 2.0 V as non-linear behaviour are shown in Fig. 3.
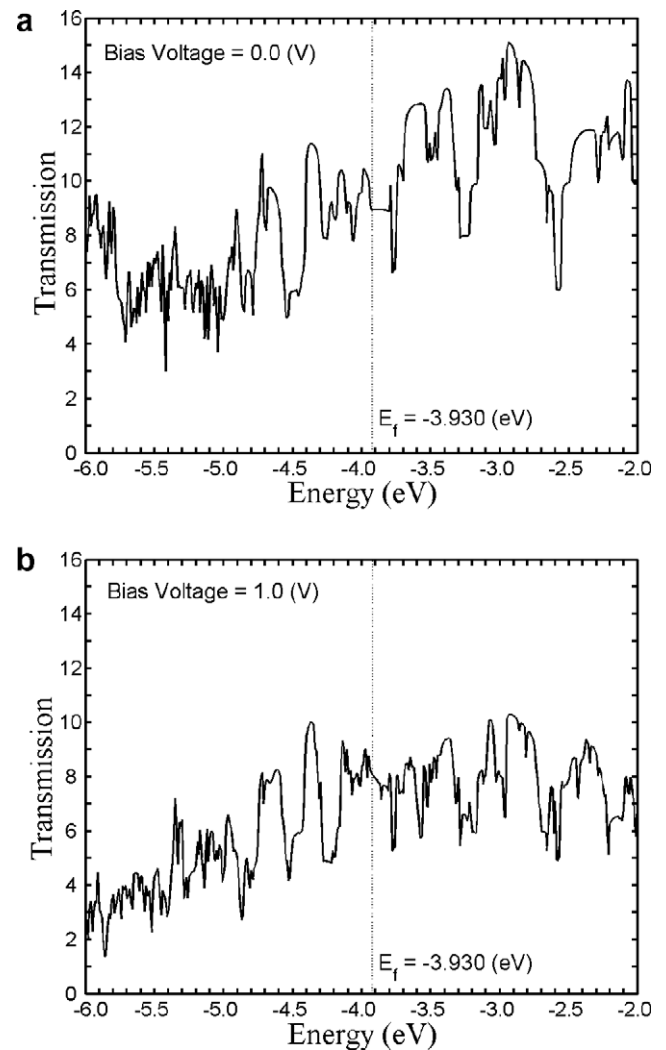

Fig. 2. Transmission spectra as a function of incident electron energy. Diagrams (a) and (b) show the total transmission spectra at the 0 and 1 bias voltages, for copper nanowire, respectively.
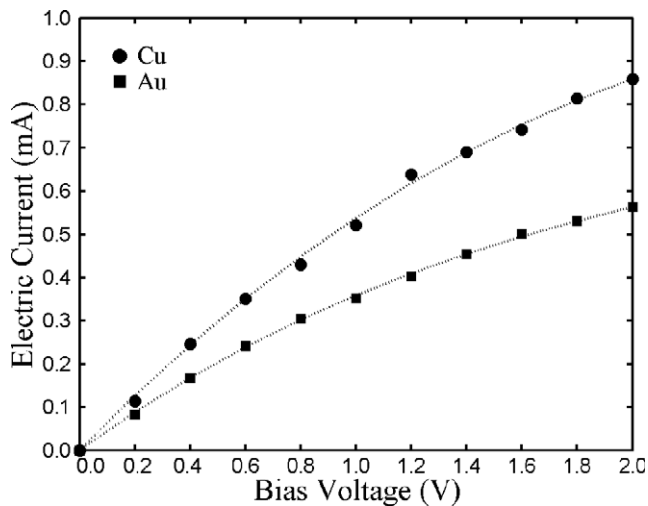
Fig. 3. Total current as a function of the applied bias voltage. Dotted lines are the fitting characteristics.
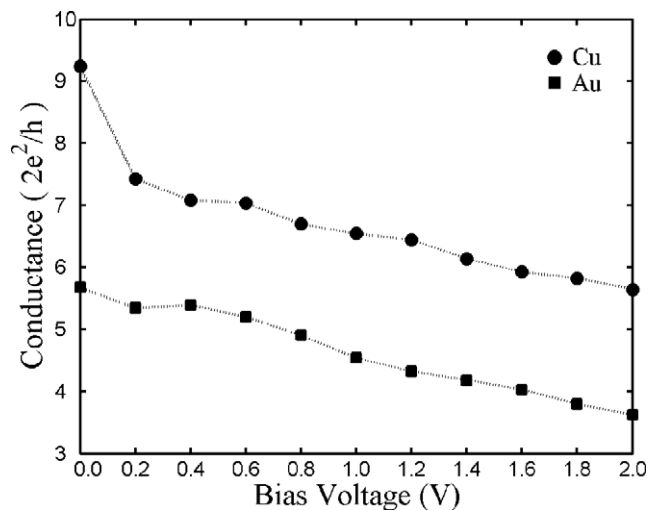

Fig. 4. Conductance as a function of external bias voltage for Cu and Au nanowires.

One can see that the theoretical data of the current can be approximately fit into a cubic function of bias voltage shown by dotted lines in Fig. 3.

The numerical integration of Eq. (8), giving the total current, is carried out in order to obtain the differential conductance by taking the integration step $\Delta E = 0.01$. Based on these calculations, the conductance of Cu and Au nanowires shown in Fig. 4 depends on the applied bias voltage and exhibits non-linearity response for both Cu and Au nanowires. The variation of the conductance is different for the two elements, which in Cu, $G(V)$ varies by $9.24-5.64$ and in Au varies by $5.68-3.62$ in units of quantum conductance when the bias voltage increases.

4. Conclusions

In summary, a theoretical analysis of the electronic transport properties of copper and gold nanowires sandwiched between crystalline electrodes in (100) directions has been performed by applying finite voltages, based on the non-equilibrium Green's function within the density functional tight binding calculations. We have shown the dependency of the total transmission fluctuations on the incident electron energy and the applied bias voltages. The current–voltage characteristics of each system could be explained as a non-linear function and for the differential conductance in terms of the applied bias voltage the linear response is not valid. In comparison with copper nanowire, gold nanowire exhibits smaller electron conduction.

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