Ballistic resistivity in Al nanocontacts(*)

Anwar Hasmy
Centro de Física, IVIC, Apdo. 21827, Caracas 1020A, Venezuela
anwar@ivic.ve

Today, where manipulation of atoms is readily accessible, the lack of knowledge about the real efficiency of the electronic ballistic/non-dissipative transport in nanodevices limits future innovations. The few detailed studies available in the literature relate to single-atom contacts[1]. It has been evidenced that the only electronic channel available for a single-atom gold contact has a better transmission performance than any single electronic channel, of the possible three, of the aluminum atom[1,2]. A fact which proves that more channels is no guarantee of better transport at the atomic scale.

In this work we show that the efficiency of ballistic conductivity can be quantitatively estimated through a transport parameter that, on average, is independent of contact neck thickness, for neck sizes smaller than the mean free path of electrons. We perform Molecular Dynamics simulations of aluminum nanocontact ruptures simultaneously computing the evolution of the cross-section and the full quantum conductance[3], for a representative series of breakages. The average $<G>$ and the value for the maximum G_{max} of the resulting conductance distribution are plotted in Figure 1, as a function of the number of atom contacts S_n.

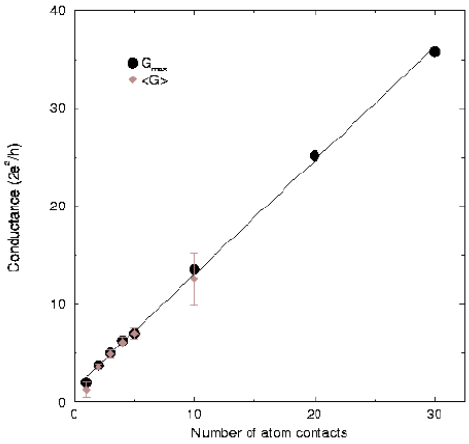

Fig. 1. Conductance average (gray symbols) and its maximum value of the distribution curve (black symbols) as a function of the number of atom contacts.

(*) The work has been done in collaboration with J.J. Palacios (U. Alicante, Spain), M. Díaz and E. Medina from IVIC, Venezuela, and P. García-Mochales, P.A. Serena and J.L. Costa-Krämer from CSIC, Spain.

A linear fit of the data shows that $<G>=S_n/\rho_b$, where ρ_b defines a transport parameter which we call the *ballistic resistivity* for the energetically preferred aluminum nanocontact configurations[4,5].

From the slope of Figure 1, we obtain ρ_b = 0.86 for the aluminum nanocontacts. Comparison of this quantity with that of monovalent metals as gold, silver or copper (as can be obtained from previous published results[2,6]), leads to the conclusion that, in contrast to the macroscale, aluminum nanocontacts are better conductors than those corresponding to monovalent noble-metals.

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