QUANTUM CONDUCTANCE PROPERTIES OF ATOMIC-SIZE METAL WIRES

Daniel Ugarte^{1,2}

¹Lab. Nac. de Luz Síncrotron (LNLS), C.P. 6192, 13084-971 Campinas - SP, Brasil ²Instituto de Física Gleb Wataghin, UNICAMP, C.P. 6165, 13081-970 Campinas - SP, Brazil E-mail: ugarte@lnls.br

Electrical transport properties of metallic nanowires (NWs) have received huge attention due to the quantum conductance behavior. Atomic-scale metal wires may be generated by elongating metal contacts; during the elongation and just before rupture, the NW conductance shows flat plateaus and abrupt jumps of approximately a conductance quantum ($G_0 = 2e^2/h$, where *e* is the electron charge and *h* Planck's constant). In these experiments, NW atomic arrangement and conductance change simultaneously, making difficult to discriminate electronic and atomic structure effects.

In this work, the atomic arrangement of NWs was studied by time-resolved high resolution transmission electron microscope (HRTEM), while their electrical properties using an UHV ($< 10^{-10}$ mbar) mechanically controllable break junction (MCBJ) operated at room temperature. From the analysis of many HRTEM images and video recordings, we have deduced that metal (Au, Ag, Pt, Cu, etc.) junctions generated by tensile deformation are crystalline and free of defects. The neck structure is strongly dependent on the surface properties of the analyzed metal, this was checked comparing different metals (Au, Ag, Cu), which have similar atomic structure (FCC) and different surface energies (faceting patterns). The correlation between the observed structural and transport properties of NW points out that the quantum conductance behavior is mainly defined by the preferred atomic atructures at the narrowest constriction.

In spite of a large amount of experimental and theoretical work on metal nanowires, it is surprising that wires made from magnetic materials have not yet been intensively studied. We have observed that the atom chain structure made of Co shows a conductance of half the conductance quantum as should be expected when a fully spin polarized current is allowed to travel through the nanowire. A similar effect has been observed for other 3d ferromagnetic metals such as Fe and Ni, Pd (4d) and Pt (5d). Then, our results suggest that this phenomenon occurs spontaneously for one-atom-thick ferromagnetic metal wires in zero magnetic field and at room temperature. These results open new opportunities for spin control in nanostructures.

We have observed by HRTEM that suspended chains of atoms are formed for different metals (Au, Ag, Cu, Pt, Pd, Co, etc.) and, also with very long interatomic distances (0.30-0.36 nm). The physical origin of these extremely long bonds is at the origin of an intense debate, and the presence of spurious atoms which may not be detected in HRTEM images (ex. light atoms H, C, O, etc.) have been proposed to account for the long bonds. Ab-initio calculations show that C atoms represent the most suitable candidate to form contaminated metal chains within experimental conditions. An extensive study of gold atom chain structure reveals that even if the presence of contaminant atoms is assumed to be true, the existence of clean metal-metal bonds as long as 0.33 nm can still be derived from the present available experimental data.