Mechanical, Electrical, And Magnetic Properties Of Ni Nanocontacts

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***Abstract*—The dynamic deformation upon stretching of Ni nanowires as those formed with mechanically controllable break junctions or with a scanning tunneling microscope is studied both experimentally and theoretically. Molecular dynamics simulations of the breaking process are performed. In addition, and in order to compare with experiments, we also compute the transport properties in the last stages before failure using the first-principles implementation of Landauer's formalism included in our transport package ALACANT.**

Keywords; nanocontacts, conductance, ab initio, spintronics.

I. INTRODUCTION

While a large amount of experimental and theoretical work has been reported for nanocontacts of many metals [1,2], a deep theoretical understanding is still lacking in the case of magnetic nanocontacts, which exhibit a very rich and complex behavior [3]. Modeling their mechanical, electrical, and magnetic properties with accuracy is a challenge from which we expect to learn important lessons on our way towards reliable theoretical descriptions of more sophisticated systems of relevance in present and future spin-based devices. We present here a comparison between theoretical results of the mechanical, magnetic, and conduction properties of Ni nanocontacts, and experiments carried out in our labs.

II. SCANNING TUNNELING MICROSCOPE HISTOGRAMS

For the experiments we used a high-stability scanning tunneling microscope (STM) at low temperatures (4.2K) and under cryogenic vacuum conditions. For both, tip and sample, we used Ni wire 99.99+% pure. The wire was cleaned by sonication in an acetone bath and scratched to remove contamination attached to the surface. The conductance properties of the contacts formed in between tip and sample were measured in a typical two probe configuration. A constant bias voltage (typically 10-100mV) was applied between tip and sample and the current was measured using a home-made current amplifier in the range of tens of μA.

We recorded traces of conductance as function of the relative tip-sample distance as the two electrodes were brought together and separated. In every trace we made a deep tip-sample indentation in order to prevent the repetition of the same atomistic configurations and to assure the clearness of the contacts. Afterwards the traces were collected to build a Conductance histogram like the one shown in Fig. 1.

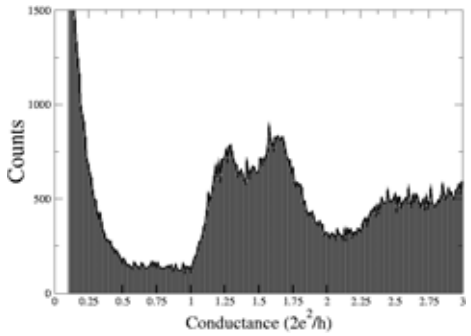

Figure 1: Experimental conductance histogram for Ni nanocontacs recorded at a bias voltage of 100 mV and a temperature of 4.2 K where two low conductance peaks are clearly visible.

Histograms for the first stages of conduction in Ni nanocontacts have been studied before[2][4][5]. A broad peak around 1.6 G_0, where $G_0 = 2e^2/h$ is the quantum of conductance, has been reported as the first peak after vacuum tunneling. This peak is attributed to the cases in which the contact consists of a single atom. For values of conductance below the one-atom peak we can notice a large amount of data coming from tunneling. This effect is stronger in Ni than in other metals, like Au, since for Ni some of the traces show a smooth transition from tunneling to contact, without a jump[6].

Here we have studied in detail this lowest conductance peak and noticed that indeed it is not a single broad peak but the superposition of two at around 1.2 G_0 and 1.5 G_0. The position of these peaks slightly changes for different contacts and this may be the reason why they have not always been clearly resolved. We have performed separated conductance histograms from the traces for the cases of either forming or breaking the contacts. There we find a different ratio in the height of the peaks, being in the case of breaking traces the peak at 1.2 G_0, in general, higher than the one at 1.5 G_0 and vice versa in the case of making the contacts. Finally we noticed a dependence of the position of the peaks with the bias voltage, with a variation of even 0.3 G_0 in a voltage range of 300 mV.

III. MECHANICAL PROPERTIES

We have performed molecular dynamics simulations for this systems. The interatomic potential for Ni developed by Mishin *et al* [7] was used in these calculations. The initial cross sections of these simulations were taken between 1.5 and

$3.5a_0$, where a_0 is the lattice parameter, a_0= 3.52 Å. A tension is applied perpendicular to the [001] plane by displacing the outer two layers of atoms on each side of the simulation box a fixed distance every 1000 simulation steps, similar to what is done by other authors[8]. The simulation temperature was kept at 4.2K.

Figure 2 shows a histogram of minimum cross section obtained from 25 independent calculations and for the larger case studied, with an initial cross section of $3.5a_0$. From this histogram we can clearly observe 5 peaks. The first peak is the formation of a single atom contact, whose width has been arbitrarily assigned as $0.5a_0$. The last peak is the initial configuration. Peaks 2, 3, and 4 are related to cross sections with 2 atoms, 3 atoms, and 4 or 5 atoms respectively..

Two structures have been identified before break-up: a single atom acts as a bridge between the two contacts, and a dimer, where two atoms aligned form a bridge between the two sides of the wire. These two configurations are shown in the insets of Fig. 4, (a) being the monomer and (b) the dimer. From all the cases computed (125), 76% form a dimer before failure while only 24% break from the monomer. In the cases studied in detail, the monomer is formed before the dimer, but in a few cases the contact breaks before forming the dimer.

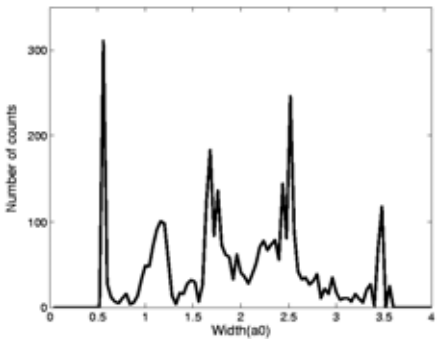

Figure 2: Histogram of minimum cross sections from 25 independent simulations

IV. TRANSPORT PROPERTIES.

The basics to calculate the zero-bias, zero-temperature conductance, *G*, in a metallic nanocontact are contained in Landauer's formalism where *G* is proportional to the quantum mechanical transmission probability of the electrons at the Fermi energy, E_F:

$$G = \frac{e^2}{h}\left[T_\uparrow(E_F) + T_\downarrow(E_F)\right] \qquad (1)$$

The detailed electronic and magnetic structure of the nanocontact is important and, in order to achieve a quantitative level of agreement with experiments, one has to rely on first-principles or *ab initio* calculations. These calculations are performed with our code ALACANT[9]. Using as input data two representative atomic configurations as those shown in Fig. 4, the transmission spectrum of these two structures has been calculated at the local spin density approximation (LSDA) level. As expected for Ni, majority conduction is smooth as a function of energy due to the s-like nature of this channel while minority conduction is strongly fluctuating close to the Fermi energy due to the d-like character of this channel [10]. Interestingly, the average value of the conductance around the Fermi level for both examples lies somewhere in the vicinity of 1.6 $\frac{2e^2}{h}$, which agrees fairly well with the value of the highest conductance peak in the histogram (see Fig. 1). As far as the origin of the low-conductance peak, one could possibly attribute it to the presence of a domain wall at the narrowest section. More experimental and theoretical work is, however, needed in this direction before this hypothesis can be confirmed.

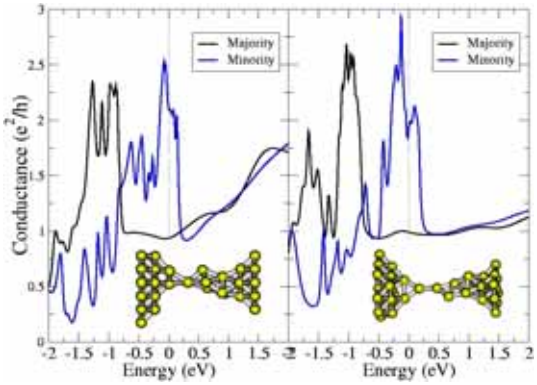

Figure 4: (Left panel) Transmission for both spin species as a function of energy for the monomer configuration (shown in the inset) before failure. (Right panel) The same, but for a dimer configuration before failure.

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