BALLISTIC SPIN-VALVES WITH Ni NANOCONTACTS

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The strong sensitivity of the current flow between two ferromagnetic metals (FM's) separated by a non-magnetic region to the relative orientation of their magnetization vectors is a fundammental physical phenomenon with a huge impact in the magneto-electronics industry[1]. The quantity characterizing this phenomenon is the so-called magneto-resistance (MR) which is defined as the difference in resistance between antiparallel (AP) and parallel (P) relative magnetic orientations of the FM's normalized to the maximal or minimal resistance of the two orientations. Recently a number of groups [2-4] have studied MR in break junction systems, where two sections of a Ni wire are connected through an atomic-size contact. In this arrangement the intermediate region connecting the two bulk FM's has a different geometry but the same chemical composition, in contrast to GMR [5] and TMR [6] systems. Some groups have obtained extremely high values of MR compared to GMR[2] while others obtain moderate or even *negative* values[3,4]. Mainly, two different mechanisms have been proposed so far to account for the large values of MR, when observed: Ballistic domain-wall (DW) scattering [7] and magnetostriction[4]. Previous theoretical works present mutually conflicting results with methodologies that either used an oversimplified description of Ni electronic structure [8] or idealized geometries [9]. Thus the fundamental question of whether MR is dramatically enhanced in atomic sized ferromanetic contacts due to the presence of a DW remains open and is the subject of this work.

We present transport calcuations [10] of Ni nanocontacts describing the electronic, magnetic, and atomic structure with *ab-initio* calculations (Fig. 1 and Fig. 2) using both LSDA and the hybrid functional B3LYP. Our results lead us to conclude that *intrinsic* ballistic MR is certainly *not* large in Ni nanocontacts [11]. Finally, we report on *ab-initio* calculations of oxidized Ni nanocontacts where an oxygen atom forms an atomic bridge between the two Ni tip atoms. Our calculations indicate that the Ni-O-Ni bridge acts as an insulating barrier which strongly suppresses the current via the Ni s-orbitals. This nanoscale tunneling union should exhibit enhanced MR compared to the pure Ni nanocontact and could thus serve as a nanoscopic ballistic spin valve.

References:

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[10] The *ab-initio* transport calculations on Ni nanocontacts were done with our new *ALACANT* code which is a further development in Fortran90 of our previous Gaussian Embedded Cluster Method (see J. J. Palacios et al., Phys. Rev. B **64**, 115411 (2001)). The code and documentation will be available soon at this web-site: http://www.dfa.ua.es.
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Figures:

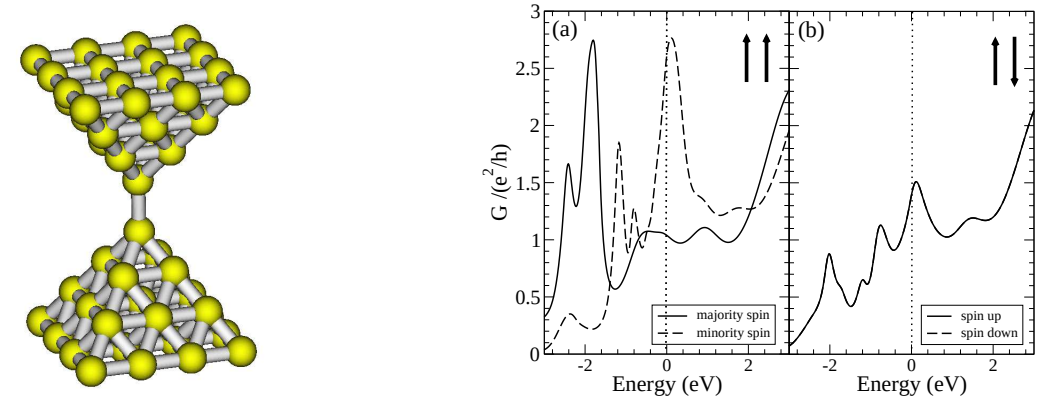

Figure 1: Left: Ni nanocontact consisting of two pyramids formed along the (001) direction having bulk atomic distances and perfect crystalline order and with the two tip atoms being 2.6 Å apart. Right: Conductance for P (a) and AP (b) alignment of the electrodes' magnetizations for the idealized geometry on the left calculated with LSDA.

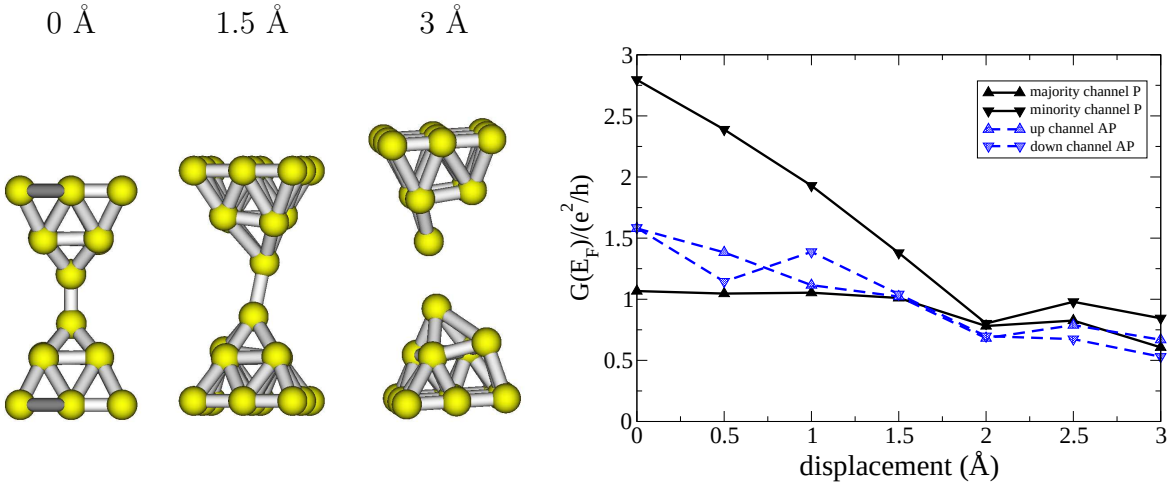

Figure 2: Left: *Ab-initio* simulation of the breaking of a Ni nanocontact. We start with a slightly compressed contact compared to Fig. 1 and displace the outer planes in steps of 0.5 Å and perform *ab-initio* structural relaxations of the inner atoms at each step. Right: The conductances of the two spin channels for the P and AP alignement of the electrodes' magnetizations as a function of the stretching of the Ni nanocontact.