Conductance of Ferro- and Antiferro-magnetic single-atom contacts: A first-principles study

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We present a first-principles study on the spin dependent conductance of five single-atom magnetic junctions consisting of a magnetic tip and an adatom adsorbed on a magnetic surface, i.e., the Co-Co/Co(001) and Ni-X/Ni(001) (X=Fe, Co, Ni, Cu) junctions. When their spin configuration changes from ferromagnetism to anti-ferromagnetism, the spin-up conductance increases while the spin-down one decreases. For the junctions with a magnetic adatom, there is nearly no spin valve effect as the decreased spin-down conductance counteracts the increased spin-up one. For the junction with a nonmagnetic adatom (Ni-Cu/Ni(001)), a spin valve effect is obtained with a variation of 22% in the total conductance. In addition, the change in spin configuration enhances the spin filter effect for the Ni-Fe/Ni(001) junction but suppresses it for the other junctions.

I. INTRODUCTION

Single-atom magnetic junctions (SAMJs) may serve as basic components for future electronic nanodevices. Therefore, the understanding of their electric transport property is of the fundamental interest, especially for their potential applications in spintronics[1]. So far, many experimental and theoretical studies have been devoted to quantify the conductance of SAMJs 2–21. For example, a number of studies were focused on investigating and understanding of the conductance of half conductance quantum, i.e., $e^2/h$, where $e$ is the proton charge and $h$ is the Planck’s constant 2–6, 8, 9, 11. It has been found that the spin-dependent conductance of a SAMJ is affected significantly by its contact atomic structure 16, 22 and its spin configuration 10, 14, 18, as well as by the magnetization direction relative to the crystallographic axes 12. The change of the spin configuration from ferromagnetism (FM) to anti-ferromagnetism (AFM) can cause a change in the total conductance and a spin valve effect which is a key topic in spintronics. Recently, a voltage-dependent spin valve effect was observed with a conductance variation of 40% for a SAMJ comprising a Cr-covered tip and a Co or Cr adatom on Fe nanoscale islands formed on a W(110) substrate 10. The variation of the total conductance was found to result mainly from the change of the spin-up conductance. For other SAMJs with different species and spin configurations, it is still an open and interesting problem whether this spin valve behavior also exists and how it is affected by the majority and minority electrons.

Here we present a first-principles investigation to show that there is no spin valve effect for several SAMJs with a magnetic adatom under zero bias when the spin configuration changes from FM to AFM. A spin valve effect with a large change in the total conductance is however observed for the junction with a nonmagnetic adatom. These results can be attributed to the different behavior of the majority and minority electrons caused by the change of spin configuration.

II. THEORETICAL MODELS AND METHODS

In this work, a SAMJ is modeled by a tip-adatom/surface junction. Five SAMJs having the similar atomic geometry are considered, i.e., the Co-Co/Co(001) and Ni-X/Ni(001) junctions, where X denotes a Fe, Co, Ni, or Cu adatom, respectively. The single adatom is adsorbed on the hollow site of the fcc (001) surface represented by a four-layer slab, with each layer containing 3 × 3 atoms as displayed in Fig1. The tip is modeled by a single apex atom adsorbed on a four-layer (001) slab. The tip-apex atom is placed above the adatom in the z direction. In transport calculations, these atoms construct the scattering region, and four additional (001) layers are added at the two ends of the scattering region, respectively, to mimic the left and right electrodes (leads). This kind of structure model has been proven to be reasonable in describing the spin transport properties of SAMJs in a previous work 11.

The atomic structure of the scattering region is optimized by the VASP code 23. The two bottom layers of the surface and the top layer of the tip are fixed during the structure optimization while the other atoms are fully relaxed until the maximum force is smaller than 0.01 eV/Å. Projector augmented-wave method 24 is used for the wave function expansion with an energy cutoff of 400eV. The PW91 version 25 of the generalized gradient approximation (GGA) is adopted for the electron exchange and correlation. The Brillouin zone is sampled with a $4 \times 4 \times 1$ grid of the Monkhorst-Pack k points 26.

For the quantum transport calculation, we adopt the first-principles nonequilibrium Green’s function (NEGF) approach 27, 28 which combines the NEGF formula for transport with ab initio density functional theory (DFT) calculation for electronic structure. A numerical double zeta plus polarization basis set (DZP) is used for the wavefunction expansion. Other computational details are the same as adopted in our previous work 11. The spin-polarization ratio (SPR) at Fermi energy

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The transport is along the z direction. The transport is along the z direction.

FIG. 1: Atomic model for the transport calculations of the SAMJs. The transport is along the z direction.

is defined as \( P = (T_\uparrow - T_\downarrow)/(T_\uparrow + T_\downarrow) \), where \( T_\uparrow \) and \( T_\downarrow \) denote the transmission coefficients of the majority and minority spin, respectively. The conductance is scaled in units of \( e^2/h \).

III. RESULTS AND DISCUSSION

We first calculate the conductance of the SAMJs in FM configuration as a function of the tip height (the distance between the tip-apex atom and the surface atom before relaxation) and plot the result in Fig.2. In Fig.2(a), one can see clearly that as the tip height decreases the conductance increases and shows a faster change in the transition region, e.g., from 5.4 to 4.8 Å and then increases slowly in the contact region, e.g., below 4.6 Å. The conductance data in the transition and contact regions can be approximated by two straight lines, and their intersection point defines the contact conductance[8, 10]. According to this definition, we obtain the contact conductances of these SAMJs and find that the spin-up conductances of all the junctions are very close to each other, while the spin-down conductance varies largely between junctions (see Figs.2(a) and (c) vs. (b) and (d)). Specifically, the spin-up conductances of the Ni-Ni/Ni(001) and Co-Co/Co(001) junctions are almost the same (see Fig.2(a)) while the spin-down ones differ significantly (see Fig.2(b)). For the Ni-X/Ni(001) junctions, the same trend also exists (see Fig.2(c) vs. (d)). We note that the present result is consistent with our previous theoretical finding: For SAMJs with similar atomic geometry but different species, their spin-down conductance is sensitive to the species while the spin-up one is not [11]. In Fig.2 we can also find that for the Ni-Fe/Ni(001) junction the spin-up conductance is greater than the spin-down one, while for the other junctions the spin-down conductance becomes larger.

To investigate the influence of the spin configuration on conductance, we then calculate the contact conductance for the AFM configuration, in which the tip and right electrode are of the same spin alignment being opposite to that of the adatom/surface and the left electrode. The conductance as a function of the tip height is plotted in Figs.3 and the values of the determined contact conductance are listed in Table I together with those for the FM configuration. We find that, as compared to the FM configuration, there is nearly no change in the total conductance for the SAMJs with a magnetic adatom, i.e., the Co-Co/Co(001) and Ni-X/Ni(001) (X=Fe, Co, Ni) junctions, as can be seen clearly in Table I (The maximum change is only about 8%). In contrast, for the SAMJ with a non-magnetic adatom (Ni-Cu/Ni(001)), the change in the contact conductance is as large as 22% (see also Fig.3(c)).

To probe the origin of the different behavior for the two kinds of SAMJs (with a magnetic or a non-magnetic adatom), we study the two spin components of the total conductance, as plotted in Fig.4 for the Ni-Ni/Ni(001) and Ni-Cu/Ni(001) junctions as examples. We find that a general trend exists for all these SAMJs. That is, when the spin configuration of the junctions changes from FM to AFM, the spin-up conductance increases while the spin-down conductance decreases. This trend can be clearly seen in Figs.4 (a) and (c) vs. (b) and (d). For the junctions with a magnetic adatom, i.e., Co-Co/Co(001) and Ni-X/Ni(001) (X=Fe, Co, Ni), the increase of the spin-up conductance counteracts the decrease of the spin-down component, thereby leading to a very small change in the total conductance and nearly no spin valve effect. On the other hand, for the Ni-Cu/Ni(001) junction the increased spin-up conductance is less than the decreased spin-down counterpart, thus resulting in a spin valve effect with a variation of 22% in the total conductance.

To give a deeper understanding of this trend, we analyze the projected density of states (PDOS) of the tip-apex atom and the adatom, which determines the electron tunneling for a given tip height. In Fig.5 we give the PDOS of the Ni adatom and Ni tip-apex atom for the Ni-Ni/Ni(001) junction at the tip height of 3.8 Å. The first thing to note is that for the AFM configuration the spin-up and spin-down PDOS is basically symmetric as it should be because of the opposite spin polarization of the two atoms, while for the FM configuration the two PDOS become asymmetric, especially around the Fermi energy, due to the same spin polarization of the two atoms. As a result, when the junction changes from FM to AFM, the spin-up PDOS at the fermi energy is largely increased (see Fig.5(a)) while the spin-down PDOS is largely decreased (see Fig.5(b)). This explains the increase (decrease) of the spin-up (spin-down) conductance when the spin configuration of the junction changes from FM to AFM.

We note that a spin-valve effect was found experimen-
|                | Co-Co/Co(001) | Ni-Ni/Ni(001) | Ni-Fe/Ni(001) | Ni-Co/Ni(001) | Ni-Cu/Ni(001) |
|----------------|---------------|---------------|---------------|---------------|---------------|
| **FM**         | 3.22          | 3.54          | 1.96          | 2.50          | 2.66          |
| **↑**          | 1.38          | 0.97          | 1.17          | 1.04          | 1.01          |
| **↓**          | 1.84          | 2.57          | 0.79          | 1.46          | 1.65          |
| **SPR**        | -14.29%       | -45.19%       | 19.39%        | -17.13%       | -24.06%       |
| **AFM**        | 3.26          | 3.44          | 2.12          | 2.64          | 2.08          |
| **↑**          | 1.64          | 1.73          | 1.71          | 1.63          | 1.22          |
| **↓**          | 1.62          | 1.71          | 0.41          | 1.01          | 0.86          |
| **SPR**        | 0.61%         | 0.58%         | 61.32%        | 23.48%        | 17.31%        |

**TABLE I**: Contact conductances and the two spin components (in units of $e^2/h$), as well as the SPR of the five SAMJs in the FM and AFM configurations, respectively.

**FIG. 3**: Conductance as a function of the tip height for the SAMJs in the FM and AFM configurations, respectively.

Finally, let us look at the spin filter effect and how it is influenced by the change of the spin configuration of the SAMJs. Tab. 1 lists the SPR of the five junctions in the FM and AFM configurations, respectively. One can see that for the FM configuration the absolute value of SPR ranges from 15% to 45%, showing a considerable spin filter effect. Among the five junctions, only the Ni-Fe/Ni(001) junction has a positive value of SPR while other junctions have negative ones. This is because the spin-up channel dominates in the former while the spin-down channel is less significant in the latter. When the junctions change from FM to AFM, the values of SPR become all positive, since the spin-up conductance increases and becomes larger than the spin-down one. As a result, the absolute values of SPR are reduced significantly because now the contributions from the spin-up and spin-down channels become closer to each other except for the Ni-Fe/Ni(001) junction. In the case of the Ni-Fe/Ni(001) junction, the total conductance for the FM configuration already has the main contribution from the spin-up channel, when the junction changes from FM to AFM its spin-up conductance is further increased. Consequently, its SPR is enhanced from 19% to 61%.

**FIG. 4**: Spin-dependent conductance as a function of the tip height for (a), (b) Ni-Ni/Ni(001) and (c), (d) Ni-Cu/Ni(001) junctions in the FM and AFM configurations, respectively. The up and down arrows indicate the spin-up and spin-down components, respectively.

**IV. CONCLUSION**

In conclusion, by performing first-principles quantum transport calculations we have investigated the spin-dependent conductance of five SAMJs in the FM and AFM spin configurations, respectively. When the junctions change from FM to AFM, their spin-up conductance increases while the spin-down one decreases. For the Co-Co/Co(001) and Ni-X/Ni(001) (X=Fe, Co, Ni) junctions the increase of the spin-up conductance counteracts with the decrease of the spin-down component, thereby showing no spin valve effect. For the Ni-Cu/Ni(001) junction, a spin valve effect is observed with a variation of 22% in the total conductance. In addition,
FIG. 5: (a) Spin-up and (b) spin-down PDOS of the Ni tip-apex atom and the Ni adatom of the Ni-Ni/Ni(001) junction at the tip height of 3.8Å for the FM and AFM configuration, respectively.

the spin filter effect of the Ni-Fe/Ni(001) junction is largely enhanced since the spin-up electrons contribute more than the spin-down ones to the total conductance. In contrast, the spin filter effect of the other junctions is suppressed, as their conductance has the main contribution from the spin-down electrons. Our results show a general behavior of spin-dependent conductance for these SAMJs under the change of the spin configuration, and the resulting influences on the spin valve effect, as well as on the spin filter effect.

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