Fully relaxed magnetic structure of transition metal nanowires: First-principles calculations

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We present fully relaxed magnetic structures of domain walls in magnetic transition metal nanocontacts (Ni, Co, and Fe) calculated from first principles. The domain wall is pinned in a monatomic nanowire, which is suspended between two semi-infinite leads. We show that the magnetization profile of the domain wall differs from the known Bloch and Néel walls. In particular, a "separation angle" between the directions of the moments of the outermost atoms and a clustering of the inner moments is observed. In addition, we calculate the conductance using the Landauer approach generalized to noncollinear magnetic structures. It is shown that the noncollinear magnetic order has considerable effect on the transport properties of the nanowires.

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I. INTRODUCTION

The enormous progress in nanotechnology during the past two decades stimulated interest in ferromagnetic nanocontacts. Unlike other typical objects of spin electronics consisting of two electrodes separated by a thin layer of different metallic or insulating materials, in these systems the electrodes are connected by a few-atom long wire of the same material. Large, up to 300%, ballistic magnetoresistance (MR) in Ni (Refs. 1 and 2) and Co (Ref. 3) nanocontacts was measured. More recently, even larger, up to 700%, MR values in Ni nanocontacts were reported.[4] Significant, though one order of magnitude smaller, MR values were found in Fe nanocontacts.[5] There are indications that the very large MR values are artifacts of the measurement.[6,7] However, a geometrically constrained domain wall (DW) can cause the MR effect. It was argued[8,9] that in the systems consisting of a thin isthmus between two regions of much wider cross section, magnetized antiparallel to each other, the thickness of the DW is determined by the size of the constriction. For an adequate description of the DW resistance in this system, the knowledge of an exact atomic and magnetic structure of a nanocontact is of primary importance. While the DW resistance in bulk materials is already well understood from first principles,[10–12] *ab initio* descriptions of a DW in nanocontacts are still under investigation. The theoretical study of the magnetic structure of the nanoconstriction has been done mainly within a model approach based on either a continuum[9,13] or a discrete[14] approximation. Reported model considerations of ballistic transport in the nanocontacts are based on a predefined simplified structure of a DW.[8,15] Bagrets *et al.*[16] calculated from first principles the magnetoresistance of a three-atom chain of Co suspended between two semi-infinite Co leads. Although based on the self-consistent electronic structure, this study is restricted to collinear magnetic configurations. Velev and Butler[17] presented ballistic conductance trough Ni, Co, and Fe nanocontacts calculated within a tight-binding approach. The magnetic structure of the constriction was modeled by a Bloch wall. For the atoms in the wall, they used bulk potentials properly transformed in the spin subspace. Burton *et al.*[18] reported DW resistance in Ni wires based on *ab initio* electronic structure calculations. The nanoconstriction was modeled by freestanding monatomic wires and wires with a cross section of 5×4 atoms. The DW was simulated by one-, three-, and five-monolayer long spiral-like regions. The magnitude of the magnetic moments was calculated self-consistently, and the effect of the reduced moments (softening) on conductance was discussed. The magnetic structure of the DW remained still unrelaxed in this work.

In this paper, we present the magnetic structure of a pinned DW in Ni, Co, and Fe nanocontacts obtained by *ab initio* electronic structure calculations with fully relaxed magnetic moments. Full relaxation in this context means that both magnitude and direction of the local moments are determined self-consistently. The effect of the realistic magnetic structure on ballistic transport is discussed as well.

II. METHOD AND SYSTEM

Our self-consistent calculations were done by means of the screened Korringa-Kohn-Rostoker (SKKR) Green's function method within the local spin-density approximation of the density functional theory.[19] We have developed a modification of the KKR method to noncollinear magnetic systems.[20,21] While in our previous publications noncollinear structures with predefined orientations of the local moments were investigated, the magnetic structure is now fully relaxed in a self-consistent manner. Details of the method are presented elsewhere.[22] We calculate both diagonal and off-diagonal elements of the spin-density matrix, and in this way, obtain information about the direction of the local magnetization. Within the SKKR method, the Green's function of the entire system (nanowire between two semi-infinite leads) is obtained in two steps. First, the Green's function of the "reference" system consisting of two semi-infinite leads separated by a vacuum spacer is calculated. In the second step, the nanowire is embedded between the leads, and the Dyson equation connecting the required Green's function with the one of the reference system is solved self-consistently. By means of this technique, we are able to treat the leads and the atomic contact on the same footing without adjustable parameters and without a supercell approach.

We consider structures where the semi-infinite leads and the monatomic nanowire (see Fig. 1) are made of the same material, i.e., magnetic transition metals Ni, Co, and Fe. We

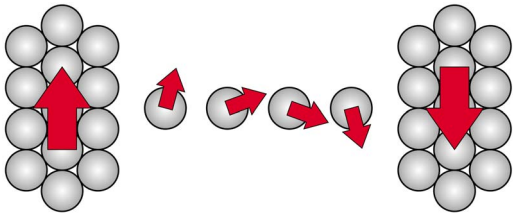

FIG. 1. (Color online) Considered structure of a domain wall in a freestanding monatomic nanowire suspended between two semi-infinite macroscopic leads. Wire and leads consist of the same material, i.e., magnetic transition metals Ni, Co, and Fe.

use the following values of the bulk lattice constants: $a=3.52$ Å for fcc Ni, $a=3.55$ Å for fcc Co, and $a=2.87$ Å for bcc Fe. As interatomic distances in the wire, we choose the nearest neighbor distances of the corresponding bulk lattice. In detail, $a_{wire}^{fcc}=a_{bulk}/\sqrt{2}$ and $a_{wire}^{bcc}=a_{bulk}\sqrt{3}/2$. We calculated the fully relaxed magnetic structure in the wires for parallel and antiparallel alignments of the lead magnetization. The direction of the magnetization axes of the leads were fixed as boundary condition.[23] However, the potentials were not fixed to take the charge relaxation into the leads correctly into account.

III. RESULTS AND DISCUSSION

For parallel alignment, the collinear magnetic configuration of the system is always energetically preferable due to ferromagnetic coupling between the atoms. In the antiparallel magnetic configuration, a DW is formed. Because of the strong ferromagnetic coupling in the leads, the DW is pinned in the constriction. The self-consistently calculated magnetic structure of the DW in Ni, Co, and Fe nanocontacts with the wire length varied from three to five atoms is shown in Fig. 2. Since the spin-orbit coupling was not included in our calculations, only the relative angle between the local magnetization axes matters. We observe that both angle and magnitude of the magnetic moments along the wire differ from the uniform distribution. All the discussed systems show the following trend: for the atoms next to the surface of the electrodes, on both sides of the wire, the moment is aligned nearly parallel to the lead magnetization, while the moments of the other atoms, excluding the two outermost ones, tend to form a bunch mainly oriented around the bisectrix of the angle between the lead magnetizations. The magnitude of the inner moments is increased relative to the bulk values. The origin of this behavior can be attributed to the different coordination numbers for the outermost and inner atoms of the wire, respectively. An outermost atom has four

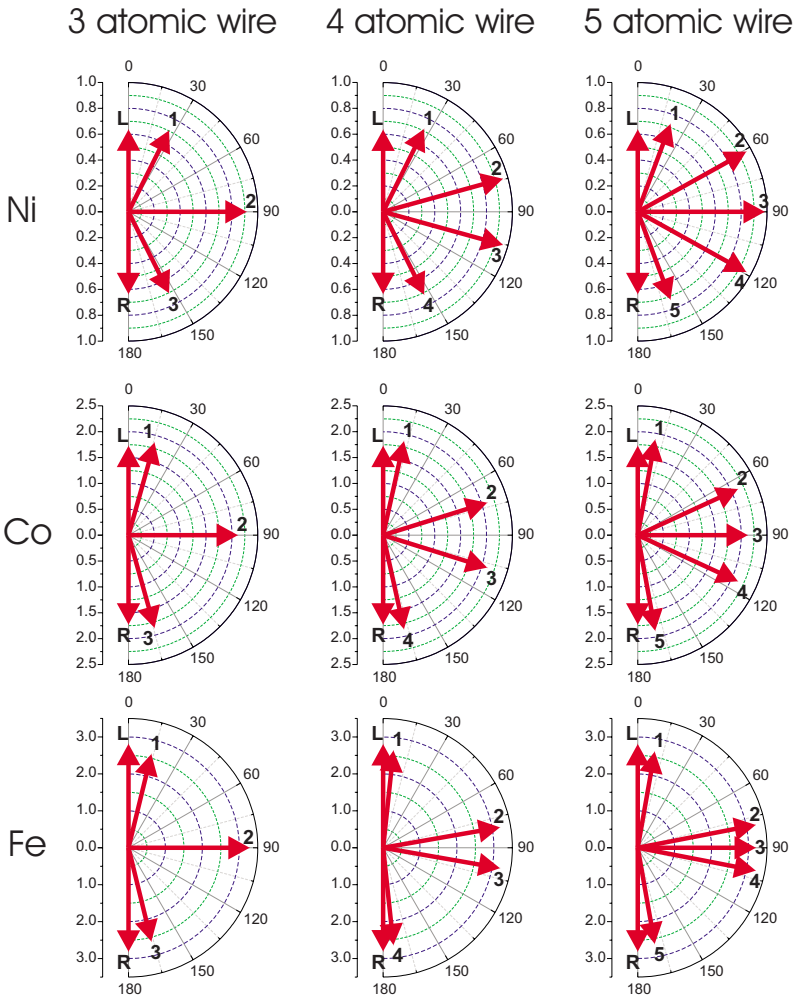

FIG. 2. (Color online) Direction and size of the moments along the wire for antiparallel aligned lead magnetization in the fully relaxed magnetic structure. From left to right, the length of the wire is increased from three to five atoms. In all cases, the lead and the wire are made of the same material, which changes from top to bottom from Ni to Co to Fe.

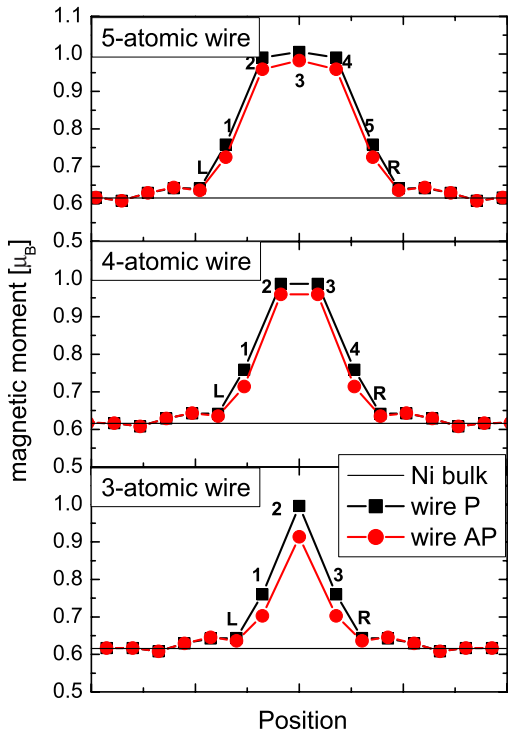

FIG. 3. (Color online) Size of the magnetic moments along the Ni wire in the parallel (P) and antiparallel (AP) configuration for different lengths. L denotes the surface atom in the left lead (R in the right lead), and the numbers indicate the positions of the atoms in the wire, counted from left to right. For comparison, the bulk magnetic moment is given as a straight line.

nearest neighbors in the surface of the electrode, which leads to a stronger coupling to the electrodes than to the atoms in the wire. On the other hand, the reduced coordination number for the inner atoms of the wire causes an enhancement of the magnetic moments, which gives rise to a stronger coupling between these moments than to the outermost ones and results in the formation of a bunch of magnetic moments oriented, with a small misalignment, along the bisectrix of the angle between the lead magnetizations. The alignment of the moments of the outermost atoms close to the magnetization of the electrodes in combination with the bunching of the inner moments of the wire leads to a formation of the "separation angle" between magnetizations of the first and next (from the surface) atoms of the wire. Our analysis of the magnetic structure of the DW in the nanocontacts supports the suggestion of Bruno,[9] based on the simple continuum model, that in the constriction between two wider regions a magnetic wall of a new kind, besides Bloch and Néel walls, is formed. In addition, our self-consistent calculations show that the special features of this DW, i.e., the separation angle and the bunching, become more pronounced along with the increasing size of the magnetic moment from Ni via Co to Fe.

The size of the moments in the wire and the surface region of the electrodes, for both parallel and antiparallel alignments of the lead magnetizations for the three-, four-, and five-atom long nanowires of Ni is shown in Fig. 3. In addition to the already mentioned enhancement of the moments in the inner part of the DW, i.e., for the antiparallel alignment, we found this effect to be even more pronounced for the parallel alignment. The increase of the moments in the center of the wire is a geometrical effect originating from the coexistence of bulk-like (three dimensions) behavior far in the leads, and reduced dimensionality at the lead surfaces (two dimensions), and in the nanowire (one dimension) between the leads. For this reason, the effect was not observed by Burton *et al.*,[18] who considered a DW in a freestanding wire. At the same time, a small reduction of the moments inside the DW for the antiparallel alignment relative to the parallel one is certainly similar to the "magnetic moment softening" discussed by these authors.

It should be noted that structural relaxation was not included in our calculations to study the magnetic relaxation separately. However, we showed in previous publications[24,25] that the effect of geometrical relaxation leads mainly to a larger bond length between the outermost atom and the next atom in the wire in comparison to the bond length in the center of the wire. Based on these results, we expect a further increase of the separation angle. Furthermore, it should be noted that spin-orbit coupling (SOC) was neglected as mentioned in Ref. 26. SOC may change the magnetic profile of the DW considering the magnetic anisotropy.

Ballistic conductance of the nanocontacts was calculated within the Landauer-Büttiker approach combined with the SKKR method modified to noncollinear magnetic systems.[21] While for every self-consistent calculation the twist angle α between the magnetizations of the leads was fixed at one of the values from 0° (parallel) to 180° (antiparallel) going up in steps of 30°, the magnetic moments in the DW were allowed to relax. Figure 4 shows the dependence of the conductance on the twist angle for the three-, four-, and five-atom long nanowire of Co. For all three lengths, the conductance is a smoothly decreasing function of α, i.e., the system acts as a spin valve.

In order to demonstrate the effect of the fully relaxed magnetic structure on the transport in the nanocontacts, we calculated ballistic conductance for two systems with predetermined magnetization directions. In both cases, the twist angle α was fixed to be 180° (antiparallel alignment). The first system is the collinear one with an abrupt DW. In the second system, local magnetization along the wire rotates between the lead magnetizations in constant steps of $180°/(N+1)$, where N is the number of atoms in the wire. This spiral-like configuration is a typical one for a Bloch or Néel wall.[26] Corresponding conductance values for the Co nanocontacts with $N=3$, 4, and 5 are also mapped in Fig. 4 (open symbols).

For all lengths of the wire, the systems with a fully relaxed magnetic structure provide values which are approximately 1.5 times larger than the conductances for the abrupt DW and about 10% smaller values than the systems with a spiral-like DW. The decrease of the conductance along the spiral-like DW via the fully relaxed DW to the abrupt DW is obviously related to the magnetic disorder in the system. The abrupt DW causes stronger spin scattering than both noncollinear structures and has consequently the smallest conductance. The separation angle between the near-surface and following magnetic moments causes additional spin

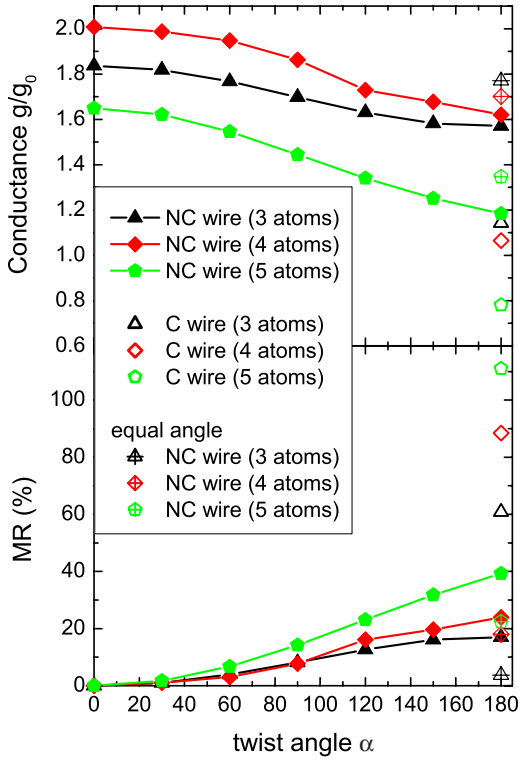

FIG. 4. (Color online) Calculated conductance and MR ratios for Co wires with different lengths. The magnetic configurations are fully relaxed (closed symbols), spiral-like structures with equal angles (open symbols with cross), and collinear magnetic order (open symbols).

mistracking with respect to the spiral-like DW, and in this way, reduces electron transmission through the wall.

The lower panel of Fig. 4 shows the MR ratio for the Co nanocontacts in the presence of DW. We used the following definition:

$$\mathrm{MR} = \frac{g_P - g_{DW}}{g_{DW}},$$

where $g_P = g(0)$ is the conductance in the parallel case and $g_{DW} = g(\alpha)$ the conductance of the system with a (fully relaxed) DW at a fixed value α of the twist angle between the lead magnetizations. For comparison, corresponding values for the systems with abrupt and the spiral-like DWs at $\alpha = 180°$ are also shown. While the MR ratios of the fully relaxed magnetic structure in the antiparallel case are about 20% for the three- and four-atom wire and about 40% for the five-atom wire, in the systems with an abrupt DW, they increase strongly with the length from 60% at $N=3$ to 110% at $N=5$. The spiral-like DW provides very small MR ratios, especially the three-atom wire with 3.7%. These major differences are caused by the change of the conductance values in the antiparallel case for the different descriptions.

It should be mentioned again that SOC was neglected in our calculation. Inclusion of SOC leads to a dependence of the conductance on the orientation of the magnetic moments with respect to the lattice, i.e., anisotropic magnetoresistance.[27,28]

IV. CONCLUSIONS

In conclusion, we have investigated the fully relaxed magnetic structure of the Ni, Co, and Fe nanowires suspended between two macroscopic electrodes of the same material. We show that a DW pinned in a short monatomic wire has a magnetization profile which is significantly different from that of a Bloch or Néel wall. In particular, a separation angle between the moments of the two outermost atoms of the wire is formed, while the magnetizations of the inner atoms form a bunch mainly oriented near the bisectrix of the angle between the magnetizations of the leads. The effect of the fully relaxed magnetic structure on ballistic transport was also studied. We found significant changes in the magnetotransport properties if one assumes collinear or spiral-like magnetic order instead of the fully relaxed one.

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