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# Magnetic anisotropy and anisotropic ballistic conductance of thin magnetic wires

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# Magnetic anisotropy and anisotropic ballistic conductance of thin magnetic wires

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**Abstract:** The magnetocrystalline anisotropy of thin magnetic wires of iron and cobalt is quite different from the bulk phases. The spin moment of monatomic Fe wire may be as high as 3.4 $\mu_B$, while the orbital moment as high as 0.5 $\mu_B$. The magnetocrystalline anisotropy energy (MAE) was calculated for wires up to 0.6 nm in diameter starting from monatomic wire and adding consecutive shells for thicker wires. I observe that Fe wires exhibit the change sign with the stress applied along the wire. It means that easy axis may change from the direction along the wire to perpendicular to the wire. We find that ballistic conductance of the wire depends on the direction of the applied magnetic field, i.e. shows *anisotropic* ballistic magnetoresistance. This effect occurs due to the symmetry dependence of the splitting of degenerate bands in the applied field which changes the number of bands crossing the Fermi level. We find that the ballistic conductance changes with applied stress. Even for thicker wires the ballistic conductance changes by factor 2 on moderate tensile stain in our 5×4 model wire. Thus, the ballistic conductance of magnetic wires changes in the applied field due to the magnetostriction. This effect can be observed as large *anisotropic* BMR in the experiment.

**Keywords:** Magnetic anisotropy; Magnetic properties of nanostructures

## 1. Introduction

Anisotropy of nanomagnets is an active area of research pushed forward by needs of magnetic storage industry and possible spintronic applications. Properties of magnetic materials at nanoscale cannot be frequently explained just by combining knowledge of surface properties and bulk. For example, anisotropy of freestanding nanoparticles and clusters is determined in large degree by the symmetry of the cluster. Small nanoparticles of Co exhibit complicated dependence of energy on the orientation of the magnetization [1] and can be described in terms of biaxial anisotropy model. Complicated magnetization reversal behavior was reported for nanowires [2]. The reversal may not show classic astroid of magnetization reversal as function of the angle between wire and the applied field. Moreover, the switching field may not be symmetric for positive and negative direction of the applied field.

Experimental studies show that anisotropy oscillates with the wire thickness [3] in agreement with the theoretical predictions [4], [5] and [6]. Gambardella et al. have shown that wires grown on the surface steps may exhibit unusual direction of magnetization at 20° to the direction of the atomic chain on the step of Pt surface. Besides the magnetocrystalline anisotropy one need to take into account the shape anisotropy originating from the dipole–dipole interactions. This contribution can be readily estimated for high-symmetry shapes such as cylinder, ellipsoid or parallelogram. For nanowires this contribution is of the order of 0.1 meV/atom, i.e. smaller than the magnetocrystalline anisotropy energy (MAE). The effects of the substrate on the anisotropy energy

are extremely important. Substrate having interaction with nanowire changes its electronic states, symmetry and spin–orbit coupling. As a result it changes anisotropy and orbital moment of nanowire drastically. We will leave this effect for future consideration.

We present in this work the first-principle calculations of MAE of Fe and Co nanowires. We show that anisotropy easy axis may change direction with the stress applied to the wire as well as change in the symmetry of the wire to the previously established dependence on the wire diameter or width.

The ballistic transport in ferromagnetic metal constrictions has recently received a great deal of attention due to unexpectedly large MR values obtained in experiments on Ni break junctions [7]. These results were attributed to a creation and annihilation of a constrained DW during a magnetic field sweep. Although the results of these experiments are currently under debate, they stimulated a number of theoretical studies of spin-dependent transport in constrained geometries using free-electron models. Imamura et al. [8], Tagirov et al. [9] and Dugaev et al. [10] demonstrated that the interplay between quantized conductance and an atomic scale domain wall results in MR that oscillates with the cross section of the constriction and leads to enhanced MR values. The conductance and magnetoresistance fluctuations were also found by Tagirov et al. [11], who used a quasi-classical approach to calculate the MR due to a constrained DW that was approximated by a step-like potential. Dugaev et al. [10] found an analytical solution for the MR of a narrow DW limiting their consideration of electronic transport by one quantum channel.

We show that conductance of nanowires strongly depends on the applied strain. Moreover, the magnetization direction may change conductance as well leading to anisotropic ballistic magnetoresistance. Separating these two effects in experiment, however, may be difficult because magnetostriction could create conditions for strain-induced change in the conductance.

## 2. Method of calculations

We consider free standing nanowires of ferromagnetic FCC cobalt and iron. We consider two nanowire configurations having different atomic arrangements: (i) monatomic and (ii) 5×4. The nanowires are built along the [0 0 1] direction ($z$-axis) by periodic repetition of a supercell made up of 1 atom (monatomic wire) or two FCC (0 0 1) planes (for a square 5×4 wire as shown in Figure 1). To use the advantage of the k-space representation within a first-principles calculation, we considered a periodic array of these wires separated by empty space.

Magnetocrystalline anisotropy in lowest order of perturbation theory is

$$\mathrm{MAE} = K_1\sin^2(\theta)+K_2\sin^2(\theta)\sin^2(\phi).$$

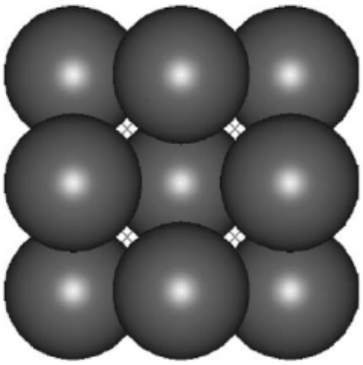

**Figure 1.** 5×4 wire representing a periodically repeated super cell of two FCC (0 0 1) layers with 5 and 4 Co atoms in each layer.

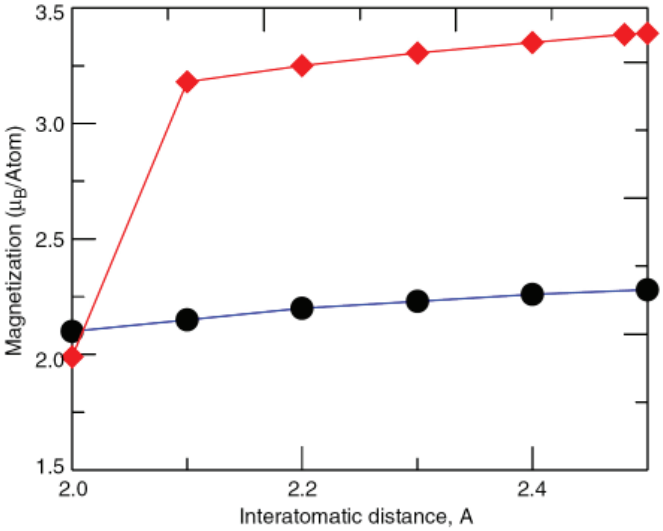


**Figure 2.** Spin moments of Fe (diamonds) and Co (circles) for monatomic wires as function of temperature.

Technically, the difference of total energies were found using force theorem to find $K_1$

$$\mathrm{MAE} = E(\|) - E(\perp).$$

We performed our calculations using VASP (version 4.6.23). Distance between atomic chains is chosen to 10 times the interlayer distance. Integration over Brillouin zone is performed by tetrahedron method with 80 k-points along $z$-direction for monatomic wires, while 2×2×26 k-points were used for 5×4 wires. Cut-off energy is 400 eV.

## 3. Electronic and magnetic structure

Magnetic properties of Fe and Co are quite different in the bulk. While Co exists in HCP phase and has a moment of about 1.7 $\mu_B$, Fe crystallizes in BCC phase and moment of 2.21 $\mu_B$. These moments do not show strong dependence on the applied stress. Both elemental metals can be stabilized in FCC phase in thin film geometry or by doping with other metal (in case of Co only few percent of Cu is needed). In FCC phase iron shows strong magnetovolume effect, i.e. dependence of magnetization on the lattice spacing. Iron mag-

netization decreases sharply in ferromagnetic state if the lattice compressed.

We find that spin moment of atomic scale wires is much larger than the bulk values as shown in Figure 2. There is smooth variation of moment for Co with strain, while Fe wires have sharp reduction of spin moment at very small interatomic spacing. Interesting to notice that the orbital moment of wires is very large as shown in Figure 3. This is a result of symmetry reduction in the wires comparing to the bulk systems, where the second-order contribution to MAE and the orbital moment are quenched. The MAE of Co wire is negative at lower lattice parameters and is negative, i.e. easy axis is perpendicular to the wire. At larger lattice parameters it is changing the sign, i.e. having spin-reorientation transition on the applied strain. Fe has negative MAE only in low spin state, while in high spin state its MAE is positive meaning that easy axis is along the wire. Spin reorientation happens when exchange splitting causes the band shift its crossing with respect to the Fermi energy in the center of 1D Brilloine zone as can be seen in Figure 4. It changes the relative contribution from each *k*-point in such a way that the right part of oscillation lowers its energy (see bottom panel of Figure 4)

The number of bands crossing Fermi energy is not very sensitive to the orientation direction. We did not find anisotropic ballistic magnetoresistance in monatomic wires of either Co or Fe. The 5×4 wire of Co shows strong dependence on applied strain. MAE is changing its sign similarly to the monatomic wire situation as can be seen from Figure 5. Magnetic moment is sensitive to the strain as well. Table 1 shows spin and orbital magnetic moments on inequivalent sites of Co 5×4 wire. They are much closer to the bulk Co result.

Band structure of this wire is more complicated. It shows although strong change in conductance. For example, at lattice spacing 2.5 Å it shows 8 quantum of conductance, while at 2.2 Å it is 16 quantum of conductance. This means that magnetoresistance of such straining would be 100% to the conductance of expanded wire. Moreover, there is a dependence of the ballistic conductance on the orientation of the applied magnetic field. When spin moment is along the Co wire at lattice spacing of 2.5 Å, for example, the conductance is

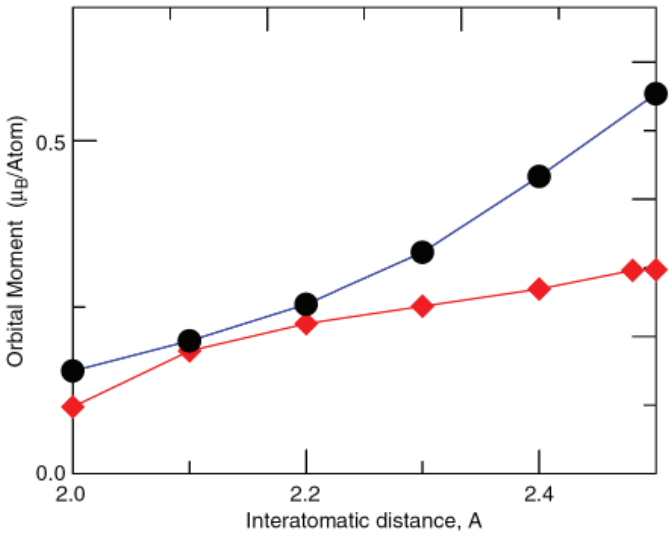


**Figure 3.** Orbital magnetic moments of Fe (diamonds) and Co (circles) for monatomic wires as function of temperature.

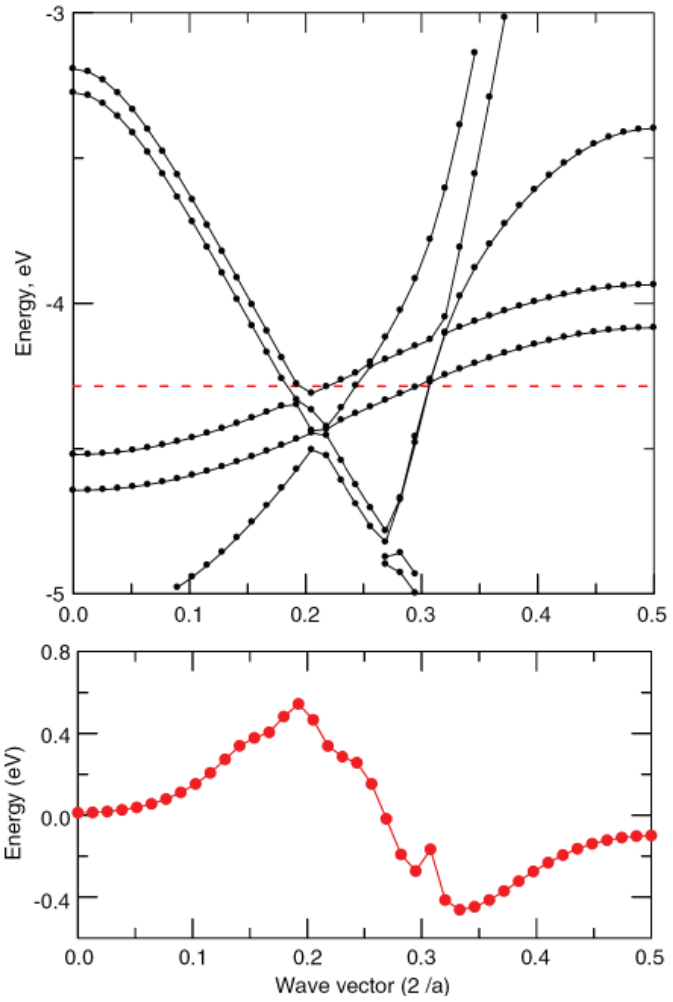


**Figure 4.** 1D band structure for monatomic Co (upper panel) and the *k*-resolved contribution to MAE (bottom panel).

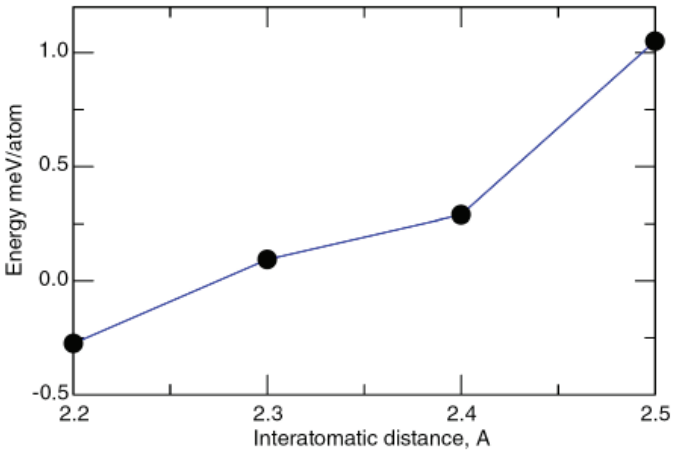


**Figure 5.** MAE of 5×4 cobalt wires.

**Table 1.** Spin ($M$) and orbital ($L$) moments on three inequivalent sites in 5×4 wires as function of interatomic distance ($d$)

| $d$ | $M1$ | $M2$ | $M3$ | $M_{av}$ | $L1$ | $L2$ | $L3$ | $L_{av}$ |
|---|---|---|---|---|---|---|---|---|
| 2.2 | 0.96 | 1.34 | 1.22 | 1.25 | 0.01 | 0.08 | 0.06 | 0.07 |
| 2.3 | 1.34 | 1.67 | 1.68 | 1.64 | 0.02 | 0.12 | 0.09 | 0.10 |
| 2.4 | 1.55 | 1.80 | 1.78 | 1.79 | 0.04 | 0.16 | 0.11 | 0.13 |
| 2.5 | 1.70 | 1.90 | 1.86 | 1.86 | 0.05 | 0.25 | 0.11 | 0.17 |

8$G$, while when magnetization is directed perpendicular to the wire the conductance is 10$G$, giving 20% of ballistic magnetoresistance, where $G=Ne^2/h$ is quantum of conductance, here $N$ is the number of open conducting channels, i.e. the number of transverse modes at the Fermi energy. The reason for such effect lays in the different way spin–orbit coupling affects the splitting and shifting of bands. SO coupling does not affect split bands when polarization is perpendicular to the wire, while provide such splitting when polarization is along the wire. This value of anisotropic ballistic magnetoresistance is much larger than values of AMR in bulk materials being of the order of a few percent at room temperature. At the same time they are comparable to the magnetoresistance values observed in the experiments [12]. The theory of this effect is described in detail in Ref. [13].

In conclusion, we show that Fe and Co wires change sign of MAE with the stress applied along the wire. It means that easy axis may change from the direction along the wire to perpendicular to the wire. The ballistic conductance of the wire depends on the direction of the applied magnetic field. This effect occurs due to the symmetry dependence of the splitting of degenerate bands in the applied field which changes the number of bands crossing the Fermi level. We find that the ballistic conductance changes with applied stress. The ballistic conductance changes by factor 2 on stain in 5×4 Co wire. The ballistic conductance of magnetic wires changes in the applied field due to the magnetostriction and symmetry effects. These effects can manifest itself as large *anisotropic* BMR in the experiment.

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