First principles study of domain walls through a Co nanocontact

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Motivation

Magnetic properties of low dimensional systems often differ considerably from their bulk counterparts. We studied the effect of the enhanced magnetic anisotropy on the formation of a domain wall through a point contact.

Computational details

Model of the point contact: two identical pyramids facing each other between (001) interfaces of fcc Co.

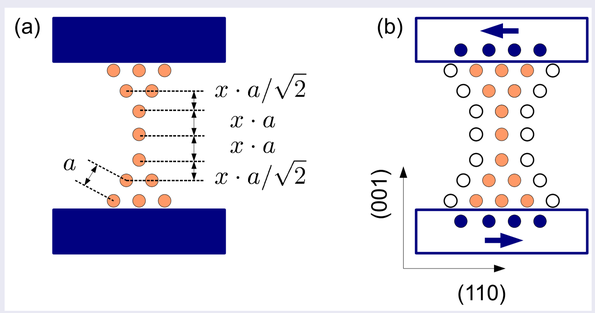


Figure: **(a) The geometry of the contact** viewed from the $(1\bar{1}0)$ direction. The length of the contact is tuned via $x = 0.85$, 0.90, 0.95, 1.00, 1.05, 1.10, and 1.15. (Note: only the marked distances were scaled; a denotes the nearest neighbor distance in the fcc structure.) **(b) Sketch of the embedded cluster.** Blue circles: selected atoms of the cobalt leads, orange circles: cobalt atoms in the nanocontact, and empty circles: empty spheres around the contact. The directions of magnetization in the leads are marked by blue arrows.

Electronic structure calculation:

- Fully relativistic screened KKR embedded cluster Green's function method. [1]
- The magnetic ground state configurations were determined by a Newton-Raphson algorithm using analytical derivatives of the band energy. [2, 3]

Domain wall configuration

From symmetry reasons, two different orientations are possible for the central atom. In a *cycloidal* wall the magnetization of the central atom points to the $(1\bar{1}0)$ direction; in a *helical* wall it is parallel to the axis of the point-contact.

The cycloidal and the helical spin configurations can be transformed into each other in term of a spin rotation around the axis parallel to the magnetization of the leads. **According to a non-relativistic description, the energy of the system remains constant in such a spin rotation.**

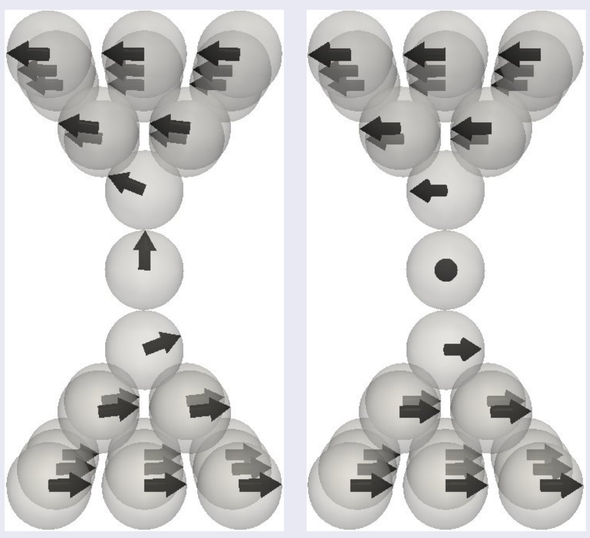


Figure: **Sketch of the cycloidal (left) and the helical (right) domain wall.** In the cycloidal case, all the spin moments are confined to the plane of the sheet. In the helical case, the magnetic moments at all sites remain perpendicular to the axis of the point contact.

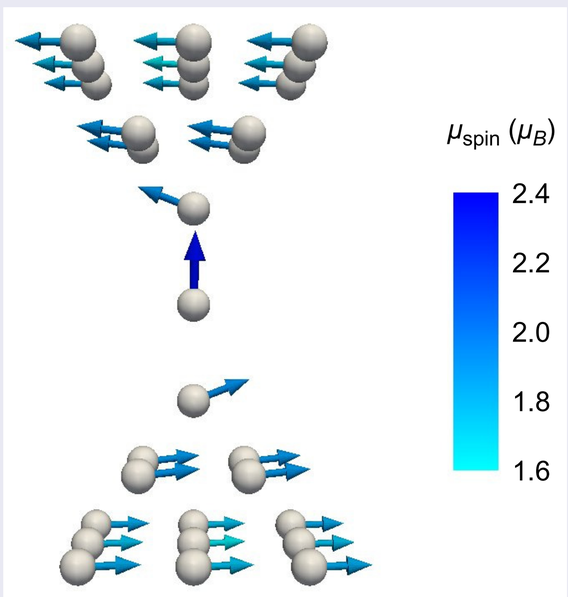
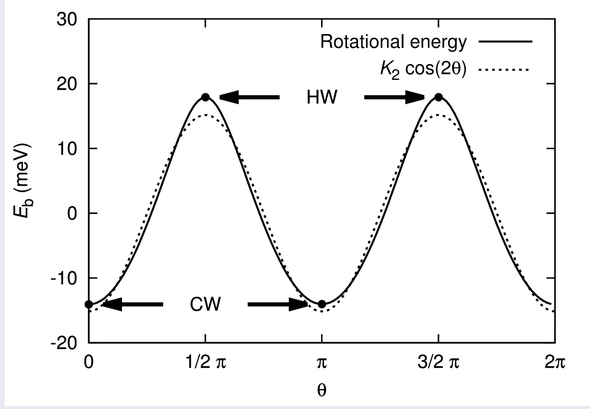


Figure: **The ground state configuration: cycloidal domin wall.** The lengths of the arrows, indicated also with color coding, are proportional to the size of the spin magnetic moments.

Ground state: the *cycloidal domain wall* turned out to be the ground state in the whole stretching range.

Why the cycloidal domain wall has lower energy?

Rotational energy of the domain walls



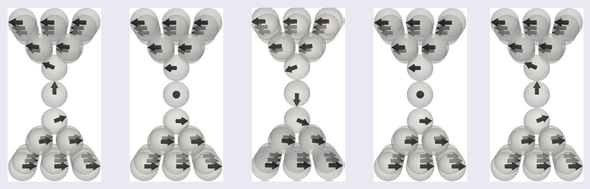


Figure: The band energy of the nanocontact while rotating the exchange field at each atomic sites simultaneously around the (110) axis. By rotating all the spins by 90° the system goes over from the cycloidal wall (CW) into the helical wall (HW). The dashed line denotes the leading Fourier component of the band energy, -15.2 [meV] $\cos(2\theta)$.

Symmetry

The band energy along the simultaneous rotation of the spin directions around the axis parallel to the magnetization of the leads is analyzed. Due to time reversal symmetry, the cycloidal and the helical domain wall configurations are two fold degenerate.

Fourier expansion

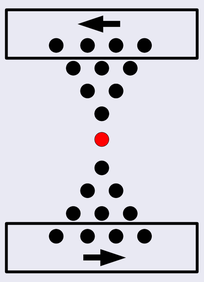
The rotational energy can be expanded in term of the $\cos(2k\theta)$ functions. We found that in each case the $K_2 \cos(2\theta)$ adds the largest weight.

Energy barrier

The energy barrier between the two different domain wall configurations is plotted in the previous section. For the unstretched nanocontact it is $E_{HW} - E_{CW} = 32.0$ meV.

Magnetic anisotropy of the central atom

Spherical harmonics expansion



We analyzed the band energy of the point-contact, $E_b(\boldsymbol{\sigma})$, with $\boldsymbol{\sigma}$ denoting the spin-orientation at the central atom, whereas the spin-orientations of all the other sites in the contact were kept fixed. The following expansion was carried out:

$$E_b(\boldsymbol{\sigma}) = \sum_{\ell,m} K_\ell^m R_\ell^m(\boldsymbol{\sigma}) \qquad (1)$$

Table: Expansion coefficients K_ℓ^m (in units of meV) of the band energy of the contact, see Eq. (1), according to real spherical harmonics R_ℓ^m up to $\ell = 4$. The first row corresponds to the Weiss field and the second row to the uniaxial anisotropy.

ℓ	m	R_ℓ^m	$x = 0.85$	$x = 0.90$	$x = 0.95$	$x = 1.00$	$x = 1.05$	$x = 1.10$	$x = 1.15$
1	0	$\frac{1}{2}\sqrt{\frac{3}{\pi}}z$	−240	−247	−235	−212	−192	−176	−159
2	0	$\frac{1}{4}\sqrt{\frac{5}{\pi}}(3z^2-1)$	−25.3	−30.0	−33.2	−32.4	−30.9	−28.4	−25.6
2	2	$\frac{1}{4}\sqrt{\frac{15}{\pi}}(x^2-y^2)$	4.30	2.54	1.39	0.51	−0.29	−0.92	−1.36
3	0	$\frac{1}{4}\sqrt{\frac{7}{\pi}}(5z^3-3z)$	4.12	3.06	1.63	0.71	−0.28	−1.43	−2.67
3	2	$\frac{1}{4}\sqrt{\frac{105}{\pi}}(x^2-y^2)z$	−0.199	−0.093	0.004	0.108	0.196	0.267	0.293
4	0	$\frac{3}{16}\sqrt{\frac{1}{\pi}}(35z^4-30z^2+3)$	−0.63	1.72	4.60	4.94	5.05	4.85	4.32
4	2	$\frac{3}{8}\sqrt{\frac{5}{\pi}}(x^2-y^2)(7z^2-1)$	0.033	0.125	0.184	0.108	0.051	0.001	−0.052
4	4	$\frac{3}{16}\sqrt{\frac{35}{\pi}}(x^4-6x^2y^2+y^4)$	−0.007	−0.005	−0.018	−0.041	−0.088	−0.187	−0.345

Relation with the Heisenberg model

According to a Heisenberg model extended by relativistic corrections [2, 4] the energy in Eq. (1) can be expressed as

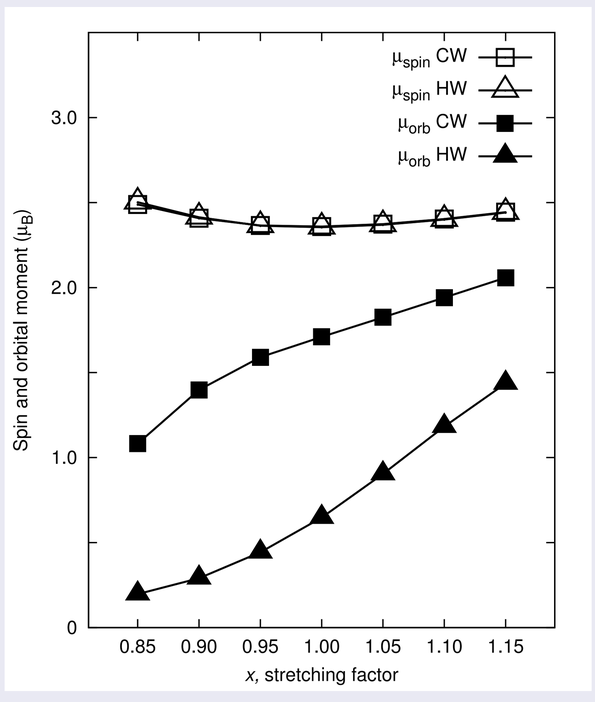
$$E_{Heis}(\boldsymbol{\sigma}) = \boldsymbol{\sigma} \sum_j \mathbf{J}_{cj} \boldsymbol{\sigma}_j + E_{anis}(\boldsymbol{\sigma}). \qquad (2)$$

The second term can be further expanded (up to $\ell = 4$) in agreement with the tetragonal, D_{4h}, point-group symmetry:

$$E_{anis}(\boldsymbol{\sigma}) = K_2^0 R_2^0(\boldsymbol{\sigma}) + K_4^0 R_4^0(\boldsymbol{\sigma}) + K_4^4 R_4^4(\boldsymbol{\sigma}). \qquad (3)$$

The other terms ($(\ell, m) = (2,2)$, $(3,0)$, $(3,2)$ and $(4,2)$) which are not consistent with the D_{4h} symmetry are related to *higher order spin interactions*.

Magnetic moments



Energetics

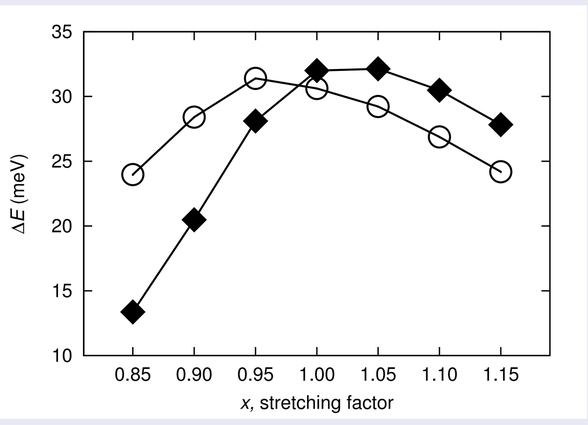


Figure: **Enhancement, as well as anisotropy of the orbital moment at the central site of the contact.**
Left: The spin- and orbital moments of the central atom.
Above: Diamonds: Calculated energy differences between the helical and cycloidal domain walls, $E_{HW} - E_{CW}$, circles: on-site uniaxial magnetic anisotropy energy of the central atom (see below).

References

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Acknowledgments

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