The magnetization reversal of the finite-size Co and Fe chains on Pt(664) surface: a comparation of the analytical and the computational results

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The Hamiltonian of the system

$$H = H_{ex} + H_{MAE} + H_{dip} + H_{int},$$

where

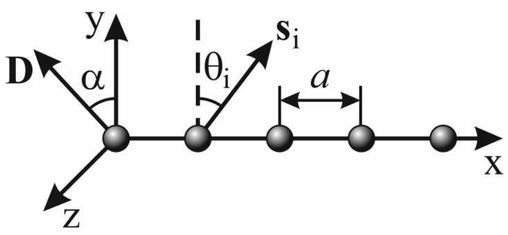
$$H_{ex} = -J\sum_i (\mathbf{s}_i \cdot \mathbf{s}_{i+1}) - \mathbf{D}\sum_i [\mathbf{s}_i \times \mathbf{s}_{i+1}],$$

$$H_{MAE} = \sum_i \left[-K\left(s_i^y\right)^2 + E\left((s_i^z)^2 - (s_i^x)^2\right)\right],$$

$$H_{dip} = \frac{\mu_0\mu^2}{4\pi}\sum_{i>j}\frac{(\mathbf{s}_i\cdot\mathbf{s}_j)r_{ij}^2 - 3(\mathbf{s}_i\cdot\mathbf{r}_{ij})(\mathbf{s}_j\cdot\mathbf{r}_{ij})}{r_{ij}^5},$$

$$H_{int} = -\mu\sum_i (\mathbf{s}_i\cdot\mathbf{B}),$$

where $\mathbf{B} = B\mathbf{e}_y$ is external magnetic field, $J > 0$ is the exchange energy, $\mathbf{D}$ is the Dzyaloshinskii vector (it lies in the plane perpendicular to the atomic chain), K and E are the magnetic anisotropy energy (MAE) coefficients, $K > |E|$, y is the easy axis of magnetization, μ is the magnetic moment, $\mu_0/4\pi = 10^{-7}$ H/m, $\mathbf{r}_{ij} = \mathbf{r}_i - \mathbf{r}_j$ is the radius vector between the i-th and j-th atoms. The schematic view of the atomic chain is presented below:



Parameters of the Hamiltonian for Co/Pt(664) and Fe/Pt(664) chains [1]:

TM	J, meV	K, meV	E, meV	D, meV	α, deg.	μ, μ_B	a, Å
Co	61.8	1.31	0.34	1.92	131°	2.39	2.82
Fe	45.9	1.73	-0.89	1.98	74°	3.41	2.82

Co chains on Pt(664)

In the continuous XY-model the magnetic energy is the following functional:

$$E[\theta] = \frac{1}{a}\int\left[\frac{Ja^2}{2}\left(\frac{\mathrm{d}\theta}{\mathrm{d}x}\right)^2 + D_z a\frac{\mathrm{d}\theta}{\mathrm{d}x} + \widetilde{K}\sin^2\theta + \mu B_y(1-\cos\theta)\right]\mathrm{d}x,$$

where $\widetilde{K} = K - E$ and $D_z = D\sin\alpha$. Varying the functional we get the equation

$$\frac{\mathrm{d}^2\theta}{\mathrm{d}x^2} = A\sin\theta\cos\theta + C_y\sin\theta, \qquad (1)$$

where $A = 2\widetilde{K}/Ja^2$ and $C_y = \mu B_y/Ja^2$.

The case $B_y = 0$

Eq. (1) has well-known solutions:

$$f_1(x) = \arccos\left(\tanh\left(x\sqrt{\frac{2\widetilde{K}}{J}}\right)\right)$$

is anticlockwise domain wall (ACDW) and

$$f_2(x) = \arccos\left(-\tanh\left(x\sqrt{\frac{2\widetilde{K}}{J}}\right)\right)$$

is clockwise domain wall (CWD).

Now the ground state, the metastable state and the saddle points can be constructed from CDWs and ACDWs [2]:

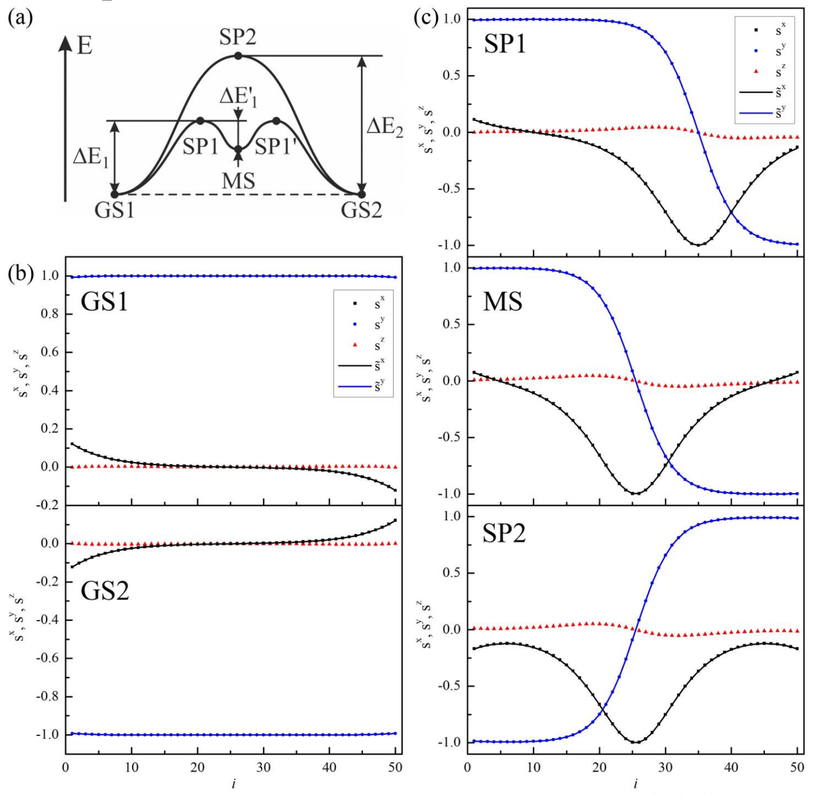
$$\theta_i^{GS} = f_1(i - i_0 - i_{10}) + f_1(i - i_0 + i_{10}) - \pi,$$
$$\theta_i^{MS} = f_1(i - i_0 - i_{11}) + f_1(i - i_0 + i_{11}) + f_1(i - i_0),$$
$$\theta_i^{SP1} = f_1(i - i_{12}) + f_1(i + i_{22}) + \pi,$$
$$\theta_i^{SP2} = f_2(i - i_0) + f_1(i - i_0 - i_{13}) + f_1(i - i_0 + i_{13}),$$

where $i_0 = (N+1)/2$ is the middle of the atomic chain and i_{10}, i_{11}, i_{12}, i_{13}, i_{22} are positive real numbers. The energies of the states are the functions of these numbers: $E_{GS}(i_{10})$, $E_{MS}(i_{11})$, $E_{SP1}(i_{12}, i_{22})$ and $E_{SP2}(i_{13})$. For example, the energy of the ground state can found via minimization of the function $E_{GS}(i_{10})$.

In the framework of the XY-model

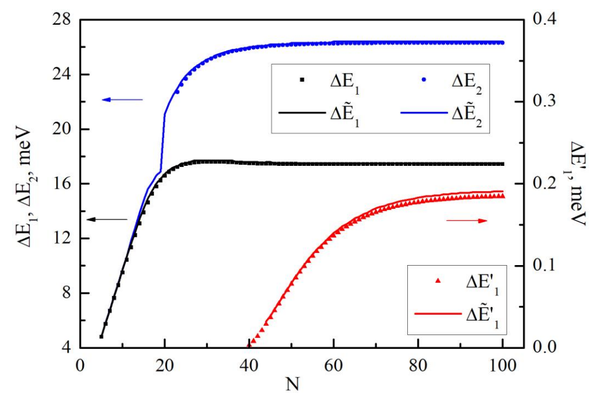
$$s_i^x = \sin\theta_i, \quad s_i^y = \cos\theta_i \quad \text{and} \quad s_i^z = 0.$$

Comparation with GNEB results



Here the points are GNEB results and the solid lines are analytical results.

Now the energy barriers can be calculated and compared:



Simple analytical expressions can be found in the case of long chains

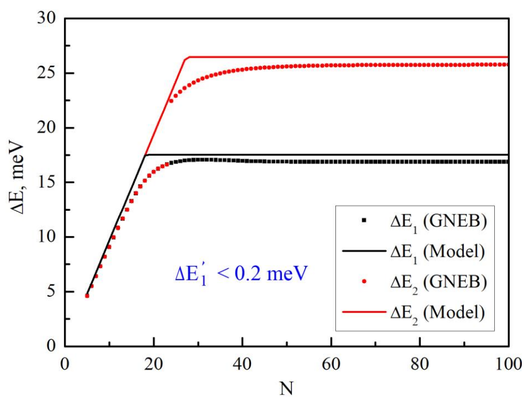
$$\Delta E_1 = \sqrt{8J\widetilde{K}} - \pi D_z + \frac{D_z^2}{\sqrt{2J\widetilde{K}}},$$

$$\Delta E_2 = \sqrt{8J\widetilde{K}} + \pi D_z \quad \text{and} \quad \Delta E'_1 = D_z^2/\sqrt{2J\widetilde{K}},$$

and in the case of short chains

$$\Delta E_1 = \Delta E_2 = N\widetilde{K}.$$

These energy barriers are in a qualitative agreement with the GNEB results



The case $B_y > 0$

Eq. (1) has the following solution

$$\cos\theta(x) = \frac{\alpha\left(\cosh\left(\sqrt{\frac{8\widetilde{K}}{J}(1-\alpha)}\frac{x}{a}\right) + 3\right) - 2}{\alpha\left(\cosh\left(\sqrt{\frac{8\widetilde{K}}{J}(1-\alpha)}\frac{x}{a}\right) - 1\right) + 2}, \qquad (2)$$

where $\alpha = C_y/A = \mu B_y/Ja^2$.

This solution is the coupled state of CDW and ACDW. It can be presented in the form

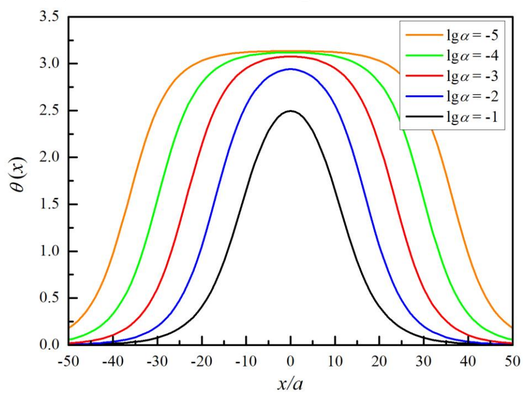
$$\cos\theta(x) = \frac{\beta^2 - 2\beta(2-3\alpha)\varphi(x) + \alpha^2\varphi(x)^2}{\beta^2 + 2\beta(2-\alpha)\varphi(x) + \alpha^2\varphi(x)^2}, \qquad (3)$$

where

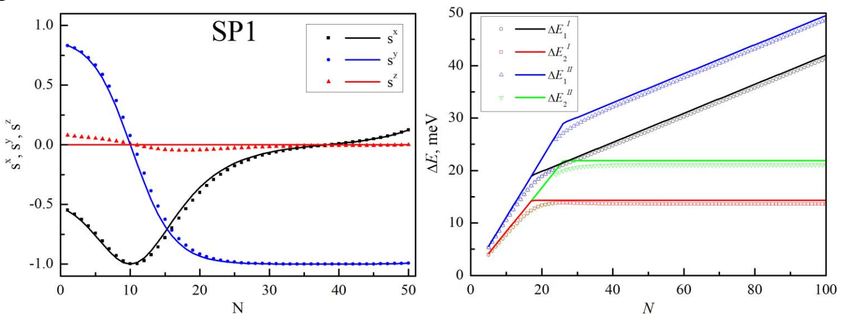
$$\varphi(x) = \exp\left(\sqrt{\frac{8\widetilde{K}}{J}(1-\alpha)}\frac{x - x_0}{a}\right)$$

and $\beta = 2 - 3\alpha + 2\sqrt{(1-\alpha)(1-2\alpha)}$.

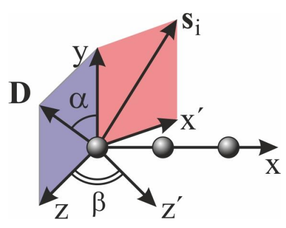
The solution (2) is shown in the Figure below



The function (3) can be used in order to construction of the ground state, the metastable state and the saddle points of the atomic chain instead of functions $f_1(x)$ and $f_2(x)$. The parameters of the approximation can found via minimization of the energy. The example of such approximation and the energy barriers at $B_y = 1$ T are showing below



Fe chains on Pt(664)

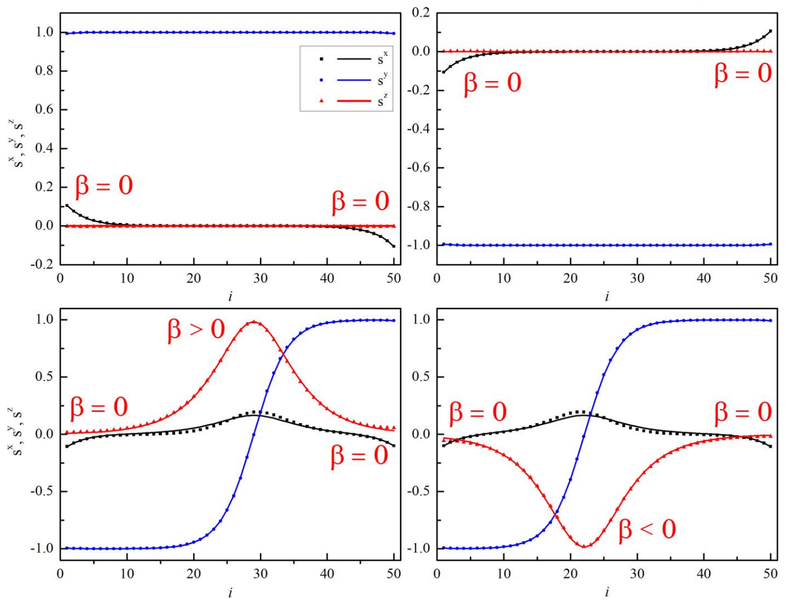


In general, Fe chains are analogous to Co ones. However, the negative value of the parameter E and DMI lead to the rotation of the plane of the domain walls. The rotation angle can be found in the framework of the continuous approximation:

$$\cos\beta = \sqrt{\frac{K - |E|}{2|E|\left(\frac{16J|E|}{\pi^2 D_z^2} - 1\right)}}.$$

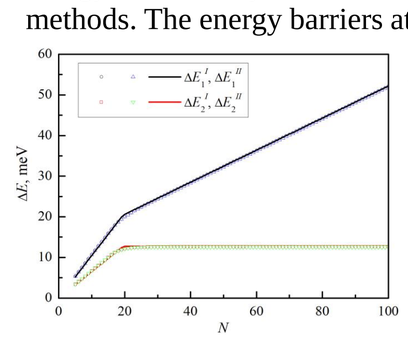
The case $B_y = 0$

The functions $f_1(x)$ and $f_2(x)$ can be used for the approximation of the states of chain as shown in the Figure:



The case $B_y > 0$

Analogously to the system Co/Pt(664) we can calculate the energy barriers by the means of the analytical and GNEB methods. The energy barriers at $B_y = 1$ T are showing below



References

[1] PRB **94**, 024403 (2016)

[2] JMMM 579, 170869 (2023)