Estimation of the magnetization reversal time of ferromagnetic and antiferromagnetic monoatomic and biatomic chains in the Heisenberg model in the framework of the single domain-wall approximation.

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COMPUTATIONAL METHODS

Classical Heisenberg Hamiltonian with uniaxial anisotropy:

$$H = -\sum_{i<j} J_{ij}(s_i \cdot s_j) - K\sum_i (\boldsymbol{s_i}\cdot \boldsymbol{e})^2 - \mu \sum_i (\boldsymbol{s_i}\cdot \boldsymbol{B})$$

where s_i and e are the unit vectors of the magnetic moments of atoms and the easy axis of magnetization, K is MAE, $J_{ij} = J(\delta_{i,j+1} + \delta_{i,j-1})$ is the exchange energy.
For ferromagnetic chains $J>0$ and for antiferromagnetic chains $J<0$.

Simple kinetic Monte Carlo (kMC) model of Li and Liu [1]:

- **Only one magnetic moment rotates at the each kMC step.**
- **Other magnetic moments are directed "up" or "down" .**
- **If $2K > |h_i|$, then** $v_i = v_0\, exp\left(-\frac{(2K+h_i)^2}{4Kk_BT}\right)$
- **If $2K \le |h_i|$, then** $v_i = v_0 \frac{exp(-2h_i/k_BT)}{1+exp(-2h_i/k_BT)}$

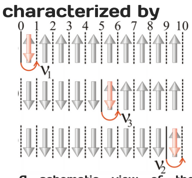
where $h_i = \sum_j J_{ij}(s_i \cdot s_j)$

The random walk of the domain wall for ferromagnetic chains is characterized by three frequencies:

$$v_1 = \begin{cases} v_0 \exp\left(-\frac{(2K+|J|)^2}{4Kk_BT}\right), if\ 2K > |J|; \\ v_0 \frac{exp(-2|J|/k_BT)}{1+exp(-2|J|/k_BT)}, if\ 2K \le |J|; \end{cases}$$

$$v_2 = \begin{cases} v_0 \exp\left(-\frac{(2K-|J|)^2}{4Kk_BT}\right), if\ 2K > |J|; \\ v_0 \frac{exp(2|J|/k_BT)}{1+exp(2|J|/k_BT)}, if\ 2K \le |J|; \end{cases}$$

$$v_3 = v_0 exp\left(-\frac{K}{k_BT}\right)$$



A schematic view of the atomic chain consisting of N=10 magnetic moments.

Time of spontaneous remagnetization of a monatomic chain:

$$\tau_{sp} = \frac{1}{2a}\left\{\frac{a}{v_3}\left(\frac{N-1}{2}\right)\left[N - \frac{2(1-2a)}{1-a}\right] + \frac{1}{v_1}[N(1-a) - 2(1-2a)]\right\}$$

where $a = v_3/(v_2+v_3)$

Time of remagnetization of a monatomic antiferromagnetic chain using an STM tip:

$$\tau = \frac{1}{v_3}\left(\frac{N-1}{2}\right)\left[N - \frac{2(1-2a)}{1-a}\right]$$

$v_1,\ v_2 \longrightarrow v_{1\pm},\ v_{2\pm}$ **, if** $J \longrightarrow J \pm \mu B$

Time of remagnetization of a monoatomic ferromagnetic chain in an external magnetic field[2]:

$$\tau = \frac{1}{2(1-a_-)}\left\{\frac{a_-}{v_{3-}} + \frac{(N-2)(1-a_-) + (a_- - \beta)S_{N-2}}{v_{3+}(1-\beta)} + \frac{S_{N-2} - (a_- - \beta a_+)S_{N-3} + \beta a_+ a_- S_{N-3}}{v_{1+}a_+}\right\},$$

where $S_N = (1-\beta^N)/(1-\beta).$

$a_+ = v_{3+}/(v_{2-}+v_{3+}),\ a_- = v_{3-}/(v_{2+}+v_{3-}),\ b = v_{3+}/(v_{3-}+v_{3+}),\ \beta = \frac{1-b}{b},$

To construct magnetic hysteresis loops, we use the Cauchy problem:

$$\begin{cases} \frac{dM(t)}{dt} = \mathfrak{A}(t)M(t) + \mathfrak{B}(t) \\ M(0) = M_0 \end{cases}$$

where $\mathfrak{A} = -\nu_{\uparrow\to\downarrow} - \nu_{\downarrow\to\uparrow}$ **and** $\mathfrak{B} = \nu_{\downarrow\to\uparrow} - \nu_{\uparrow\to\downarrow}$

M - magnetization

$M \in [-1,1]$ $\qquad M = P_\uparrow - P_\downarrow$ $\qquad P_\uparrow + P_\downarrow = 1$

P - probability

Time of spontaneous remagnetization of a biatomic chain[3]:

$$\tau^{\text{strong}} = \frac{1}{2\tilde{a}}\left\{\frac{\tilde{a}}{2\tilde{\nu}_3}\left(N - 3 + 2\frac{\tilde{\nu}_3}{\tilde{\nu}'_3}\right)\left[N - \frac{2(1-2\tilde{a})}{1-\tilde{a}}\right] + \frac{1}{\tilde{\nu}_1}[N(1-\tilde{a}) - 2(1-2\tilde{a})]\right\},$$

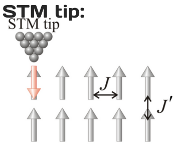
where $\tilde{a} = \tilde{\nu}'_3/(\tilde{\nu}_2 + \tilde{\nu}'_3)$

Time of remagnetization of a biatomic antiferromagnetic chain using an STM tip:

$$\tau^{\text{strong}}_{\text{STM}} = \left(\frac{N-3}{2\tilde{\nu}_3} + \frac{1}{\tilde{\nu}'^{\text{STM}}_3}\right)\left[N - \frac{2(1-2a)}{1-a}\right] + \frac{a}{1-a}\left(\frac{1}{\tilde{\nu}'^{\text{STM}}_3} - \frac{1}{\tilde{\nu}'_3}\right) + \frac{1}{a^{\text{STM}}\tilde{\nu}^{\text{STM}}_1} \times \left[N(1-a^{\text{STM}}) - 2(1-2a^{\text{STM}}) + \frac{a - a^{\text{STM}}}{1-a}\right]$$

where $a = \tilde{\nu}'_3/(\tilde{\nu}_2 + \tilde{\nu}'_3)$

$a^{\text{STM}} = \tilde{\nu}'^{\text{STM}}_3/(\tilde{\nu}^{\text{STM}}_2 + \tilde{\nu}'^{\text{STM}}_3)$



A schematic view of the interaction between the STM tip and biatomic chains.

Time of remagnetization of a bioatomic ferromagnetic chain in an external magnetic field[3]:

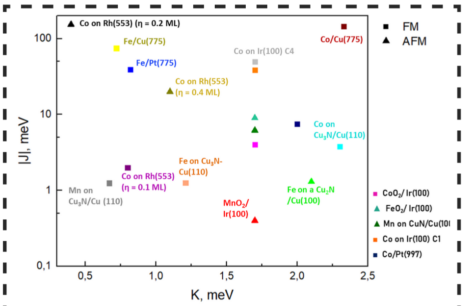
$$\tau^{\text{strong}}_B(B) = \frac{1}{2(1-a'_-)}\left\{\frac{a'_-}{\tilde{\nu}'_{3-}} + \frac{(N-2)(1-a'_-) + (a'_- - \alpha)S_{N-2}}{\tilde{\nu}_{3+}(1-\alpha)} + \frac{S_{N-2} - (a'_- + \alpha a'_+)S_{N-3} + \alpha a'_+ a'_- S_{N-4}}{\tilde{\nu}_{1+}a'_+} + \left(\frac{1}{\tilde{\nu}'_{3+}} - \frac{1}{\tilde{\nu}_{3+}}\right)(1-\alpha)[1-(a'_- - \alpha)S_{N-3}]\right\},$$

where $a'_+ = \tilde{\nu}'_{3+}/(\tilde{\nu}_{2-} + \tilde{\nu}'_{3+}),\ a'_- = \tilde{\nu}'_{3-}/(\tilde{\nu}_{2+} + \tilde{\nu}'_{3-})\ b = \tilde{\nu}_{3+}/(\tilde{\nu}_{3-} + \tilde{\nu}_{3+})$

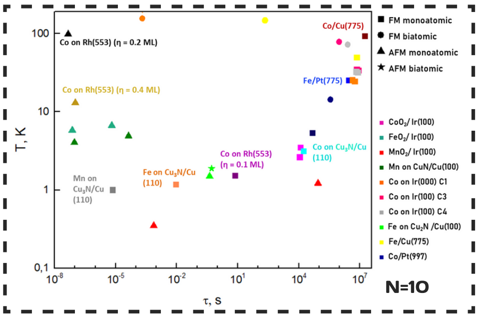
$\alpha = (1-b)/b, S_N = (1-\alpha^N)/(1-\alpha)$

RESULTS

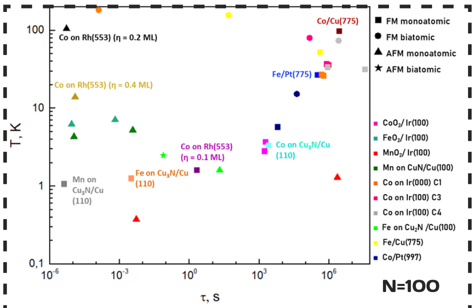
We calculated the temperatures at which the spontaneous magnetization reversal time is 1 year, as well as the magnetization reversal time in an external magnetic field of 5 T at the obtained temperatures. The parameters J and K are taken from the literature[4]-[13]. The calculation results are presented in the diagrams.



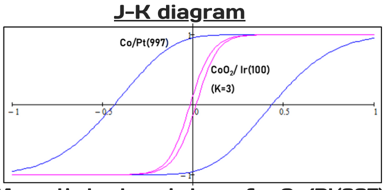
J-K diagram



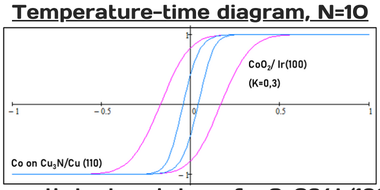
Temperature-time diagram, N=10



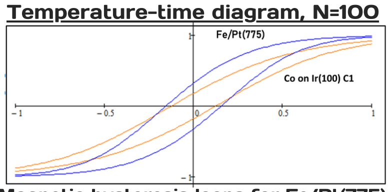
Temperature-time diagram, N=100



Magnetic hysteresis loops for Co/Pt(997) and CoO2/ Ir(100) (K=3), T=15 K



Magnetic hysteresis loops for CoO2/ Ir(100) (K=0,3) and Co on Cu3N/Cu (110), T=10 K



Magnetic hysteresis loops for Fe/Pt(775) and Co on Ir(100) C1, T=85 K

CONCLUSION

1. Magnetic properties of a wide range of ferromagnetic and antiferromagnetic atomic and biatomic chains are investigated by means of the the analytical method [4]-[13].
2. The biatomic chains can be used as a bit of information at higher temperatures T bit then the same single-atomic chains. The ratio α = τ/τ' between the spontaneous and induced remagnetization times is also higher in the case of biatomic chains.
3. Nitriding the substrate or oxidation the atomic chain usually leads to decreasing the temperature T bit and the increasing of the ratio α.
4. According our results the Co chains on Rh(553) surface seems the most prospective to the creation of stable bits of information.

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