An improved kinetic Monte Carlo model for computational and analytical investigations of the magnetic properties of finite-size atomic chains

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Computational methods

Classical Heisenberg Hamiltonian with uniaxial anisotropy:

$$H = -\sum_{i>j} J_{ij}(\mathbf{s}_i \cdot \mathbf{s}_j) - K\sum_i (\mathbf{s}_i \cdot \mathbf{e})^2$$

where $\mathbf{s}_i$ and $\mathbf{e}$ 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 $\nu(h_i) = \nu_0 \exp\left[-\frac{(2K+h_i)^2}{4Kk_BT}\right]$
- If $2K \le |h_i|$, then $\nu(h_i) = \nu_0 \frac{\exp(-2h_i/k_BT)}{1+\exp(-2h_i/k_BT)}$

where $h_i = \sum_j J_{ij}(\mathbf{s}_i \cdot \mathbf{s}_j)$

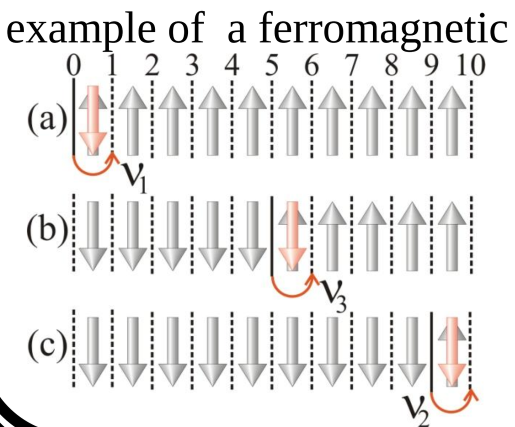
Improved kMC models take the relaxation of the magnetic moments into account. There are two cases:

Model 1 ($J << K$):
- The same states as in the simple kMC model [1].
- Diffusion barriers are calculated with GNEB method [2].

Model 2 ($J \sim K$):
- Searching of stable states by mapping with domain walls.
- Existence of clockwise and anti-clockwise domain walls.

Analytical calculations of the reversal time of magnetization in the framework of a single domain-wall approximation [3–6]:

The main idea of the method can be demonstrated on the example of a ferromagnetic chain consisting of 10 atoms:



(a) the rate of formation of the domain wall ν_1, (b) the rate of motion of the domain wall along the chain ν_3, and (c) the rate of the domain wall disappearance ν_2.

We assume that the reversal time of magnetization can be calculated as the average time of the random walk of the domain wall.
According to the mean rate method [7] we should to:
- find the transition probability matrix $T_{ij} = \tau_j^1 \nu_{j\to i}$
- solve the system of linear equations $\sum_{j=0}^{N-1}(\delta_{ij} - T_{ij})P_j = P_i^{\text{init}}$
- obtain the average time of the random walk $\tau_{\text{tot}} = \sum_{i=0}^{N-1} \tau_i^1 P_i$

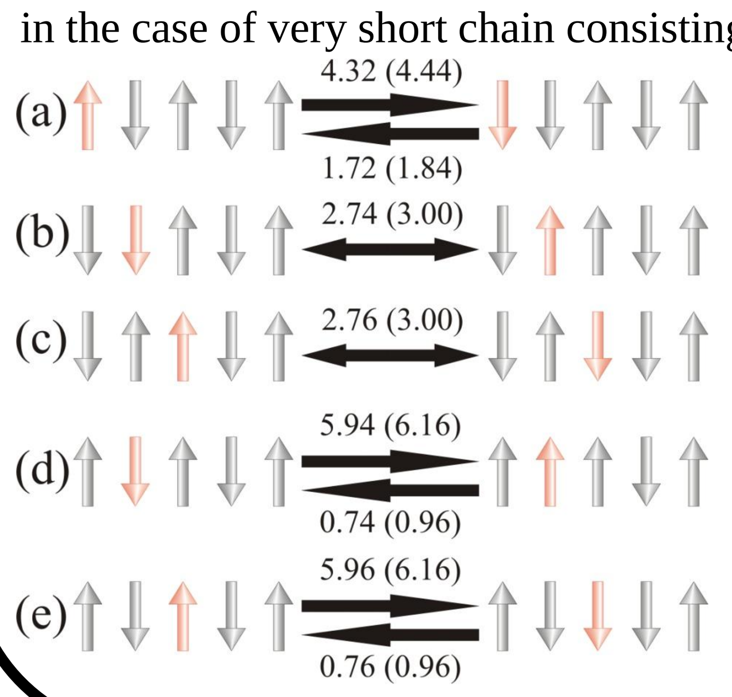
The reversal time of magnetization of a single-atomic chain consisting of N atoms:

$$\tau = \frac{1}{2a}\left\{\frac{a}{\nu_3}\left(\frac{N-1}{2}\right)\left[N - \frac{2(1-2a)}{1-a}\right] + \frac{1}{\nu_1}[N(1-a) - 2(1-2a)]\right\}$$

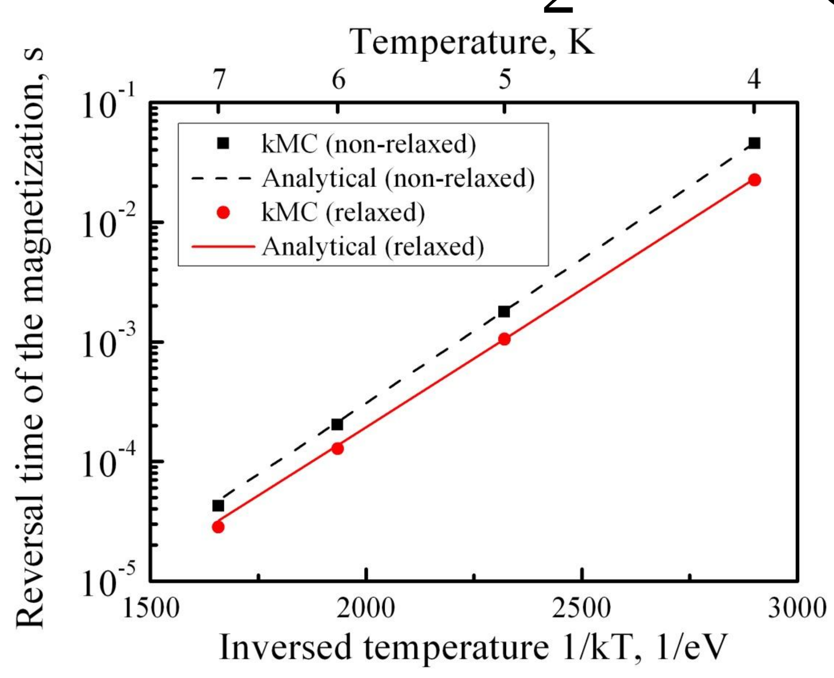
where $a = \nu_3/(\nu_2 + \nu_3)$

Antiferromagnetic Fe chains on Cu_2N/Cu(001) surface

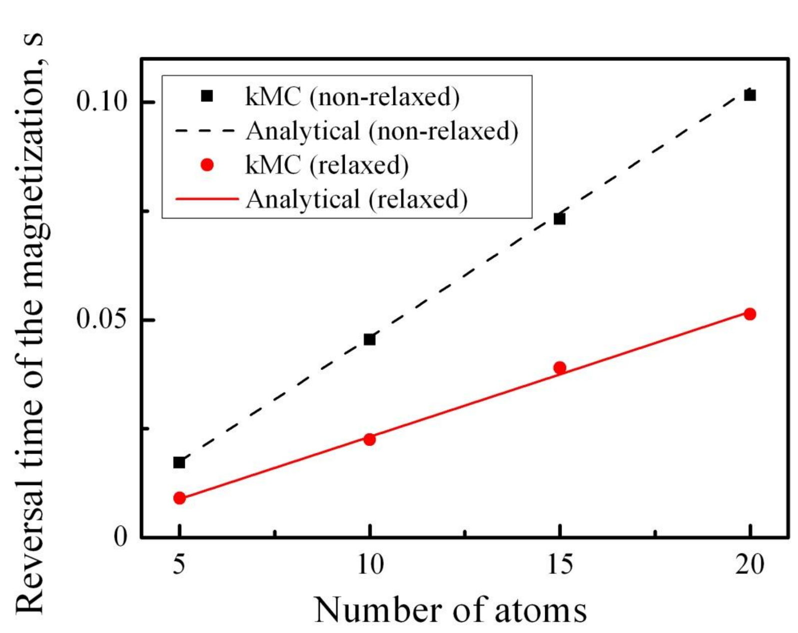
We use the following parameters of the Heisenberg Hamiltonian: J = 1.3 meV, K = 3.0 meV [8,9]. The kMC **model 1** is applicable. For example, let us consider the effect of relaxation of the magnetic moments in the case of very short chain consisting of 5 atoms:



(a) formation of the domain wall at the edge,
(b,c) motion of the domain wall along the chain,
(d,e) formation of the pair of domain walls.
All values are given in meV. The non-relaxed values are given in brackets.



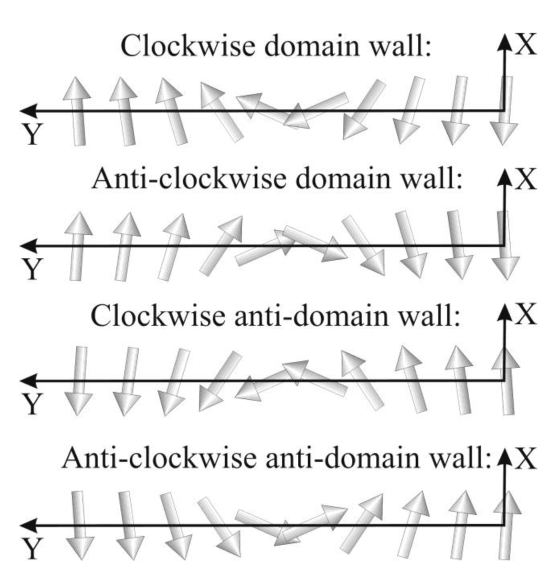
The temperature dependence of the reversal time of the magnetization of the Fe chain consisting of 10 atoms in the framework the simple kMC model [1] and the improved kMC **model 1**.



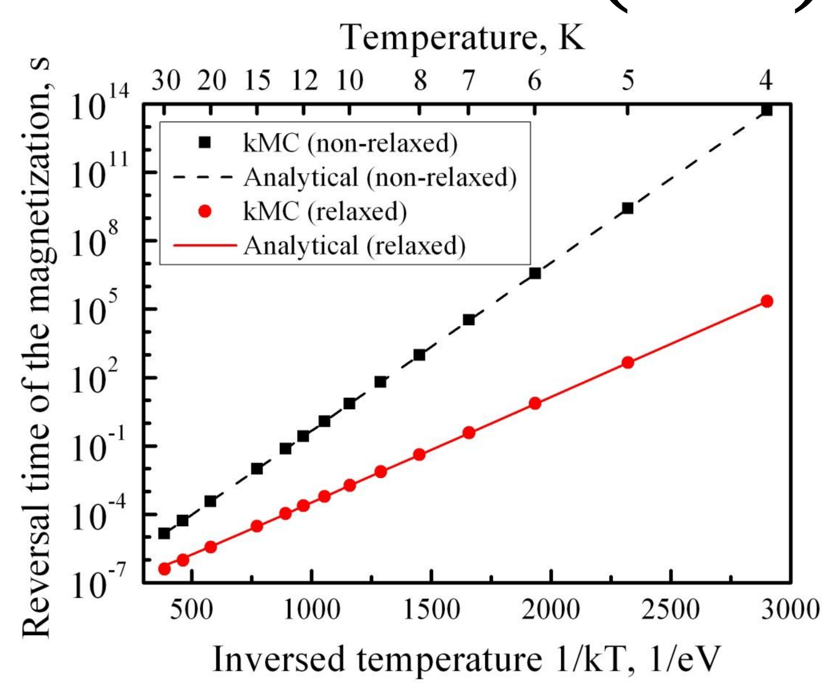
Dependence of the reversal time of the magnetization on the length of the Fe chain at T = 4K in the framework the simple kMC model [1] and the improved kMC **model 1**.

Ferromagnetic Co chains on Pt(997) surface

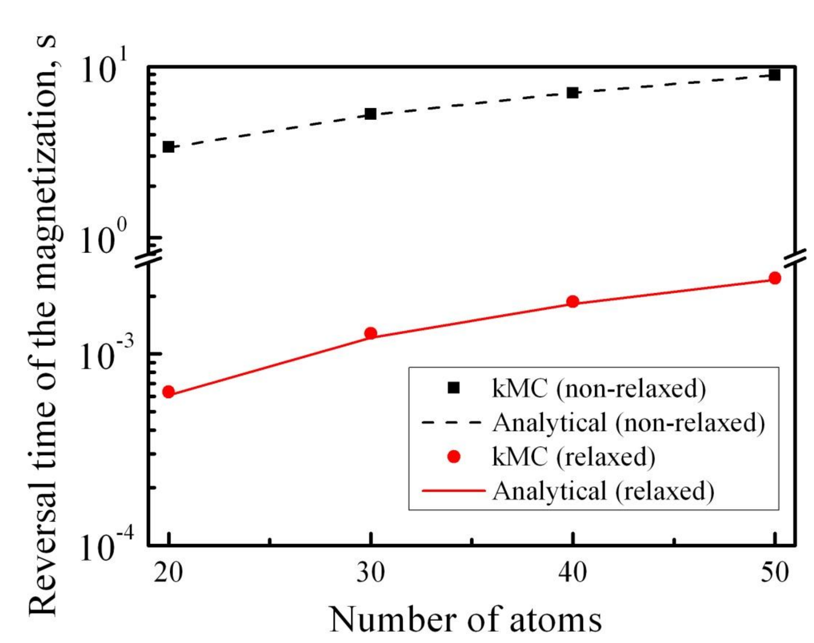
We use the following parameters of the Heisenberg Hamiltonian: J = 7.5 meV, K = 2.0 meV [10,11]. The kMC **model 2** is applicable. In this case we need to search the metastable states of the chain. The searching algorithm consist of the mapping the chain with following 4 types of domain walls and the relaxation of the chain.



Existence of wide domain walls leads to the following effects:
- The domain walls can appear at the edge only with rotating of 6 atoms. Thus, the effective length of the chain decreases to (N –10) .
- The number of states increases twice (clockwise and anti-clockwise states). Thus, the additional factor ½ arises in the analytical equation.



The temperature dependence of the reversal time of the magnetization of the Co chain consisting of 40 atoms in the framework the simple kMC model [1] and the improved kMC **model 2**.



Dependence of the reversal time of the magnetization on the length of the Co chain at T = 10K in the framework the simple kMC model [1] and the improved kMC **model 2**.

Conclusion

The main results are the following:
- At all parameters of the Heisenberg Hamiltonian the effect of relaxation of the magnetic moments leads to the decrease of diffusion barriers and to the decrease of the reversal time of the magnetization.
- If $J << K$, then the effect of relaxation does not influence on the possible number of metastable states of the chain. The example of such system is the antiferromagnetic Fe chain on Cu_2N/Cu(001) surface. The reversal time of the magnetization of this chain decreases by factor 2-3 at T = 4-7K.
- If $J \sim K$, then the effect of relaxation leads to the decrease of the effective length of the chain and to the appearance of clockwise and anti-clockwise states. The example of such system is the ferromagnetic Co chain on Pt(997) surface. The reversal time of the magnetization of this chain decreases dramatically by several orders of magnitude at T = 4-30K.
- In both cases the analytical approach [3-6] can be successfully used to estimates of the reversal time of the magnetization.

References

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