# A multiscale approach to Artificial Spin Ice thermal simulations

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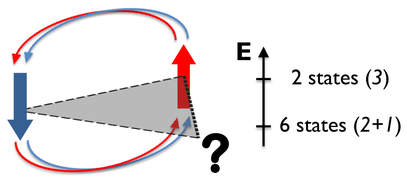
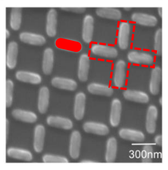
## *Introduction*: Artificial Spin Ice

Introduced in 2006, Artificial Spin Ice (ASI) systems are metamaterials consisting of arrays of dipolar-coupled nanomagnets arranged in ***frustrated geometries*** [1].




***Frustration***: the inability of a physical system to satisfy all the interactions simultaneously, leading to a large *degeneracy* of low-energy states.

***Square lattice ASI*** [2]

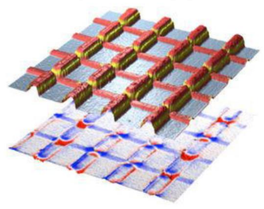



***Shakti lattice ASI*** [3]

***Interesting features***

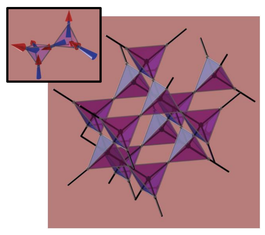
- 2D model systems in which the lowest-energy state can be obtained at *room temperature* and imaged through lab-scale imaging techniques (e.g., MFM, MOKE, LTEM);
- Advanced fabrication techniques (EBL) allow for the *systematic variation of the key parameters* governing the system (size, distance, arrangement, height offset, …).

***Double-height square ASI*** [4]



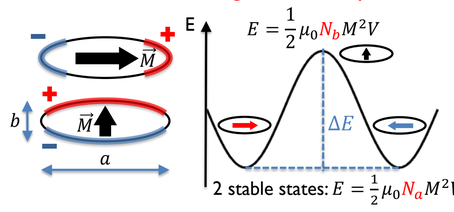
same degeneracy as

***Spin-ice compounds*** [5]



***Key structures***

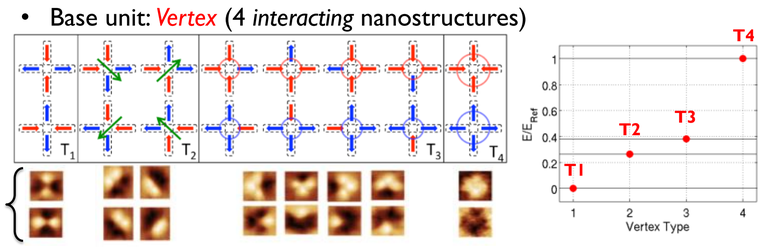
- Base element: *Ising-like macrospin nanostructure*




Assuming a magnetization reversal by *coherent rotation*, the energy barrier is given by

$$\Delta E = \frac{1}{2}\mu_0 (N_b - N_a) M^2 V$$

- Base unit: *Vertex* (4 *interacting* nanostructures)



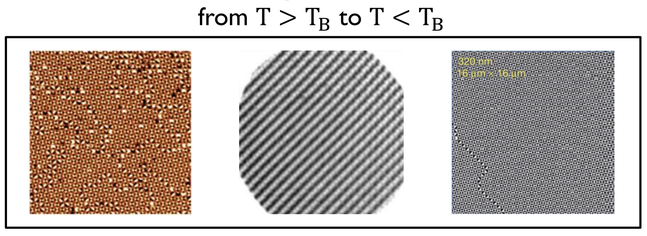

## *μm-scale*: thermal protocol and kMC

The ***key process*** in ASI systems consist in the formation of *low-energy states* (*rarely observed*): (1) the system is *melted* and (2) the frozen state (*equilibrium*) is recorded.

***Demagnetizing protocol*** [2]

*VS*

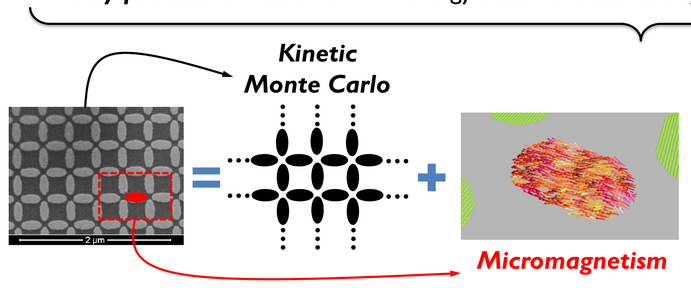
***Thermal protocol*** [2,7]: from $T > T_B$ to $T < T_B$




*Bigger ground-state domains with respect to the demagnetizing protocol*

The equlibrium configurations are usually simulated by Monte Carlo techniques [8], considering that

- ***Key structures***: Ising-like nanostructures (≤ 500 nm).
- ***Key process***: formation of low-energy states in extended systems (≈ 20 – 50 μm, so up to $10^4$ nanostructures).

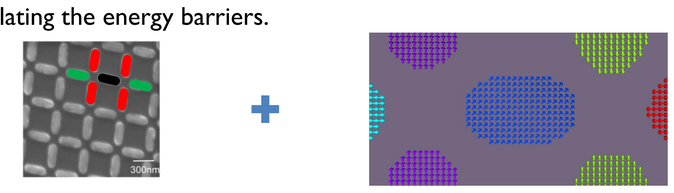



Our idea was to move a step further (beyond the macrospin approximation) and consider a ***multiscale approach*** (*μm-* and *nm-scale*):

- *Kinetic Monte Carlo* (kMC) combined with a more detailed analysis of the switching process;
- *Micromagnetic analysis* of the thermally-induced magnetization reversal ($T \neq 0$ K).

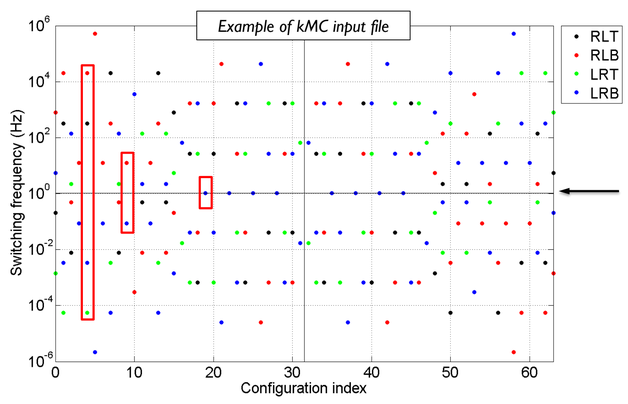
***Kinetic Monte Carlo*** [9] **+ *precomputed* switching frequencies**

- The considered event is the magnetization reversal of a single nanostructure (*single flip*);
- The base unit is composed by 7 nanostructures (**center**, **first n.n.** and **second n.n.**);
- The 7 nanostructures are uniformly magnetized and the magnetization reversal in the central one occurs by *coherent rotation*, but the *actual shape* of the nanostructure is taken into account for calculating the energy barriers.




The *input* for the kMC consists in **64 x 4** switching frequencies $\nu_{Sw}^i = \nu_0 \exp\left(-\frac{\Delta E_{CR}^i}{k_B T}\right)$:

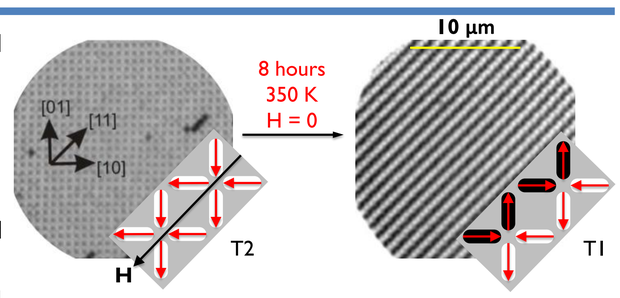
Right to Left via Top **RLT** | Left to Right via Top **LRT** | Right to Left via Bottom **RLB** | Left to Right via Bottom **LRB**



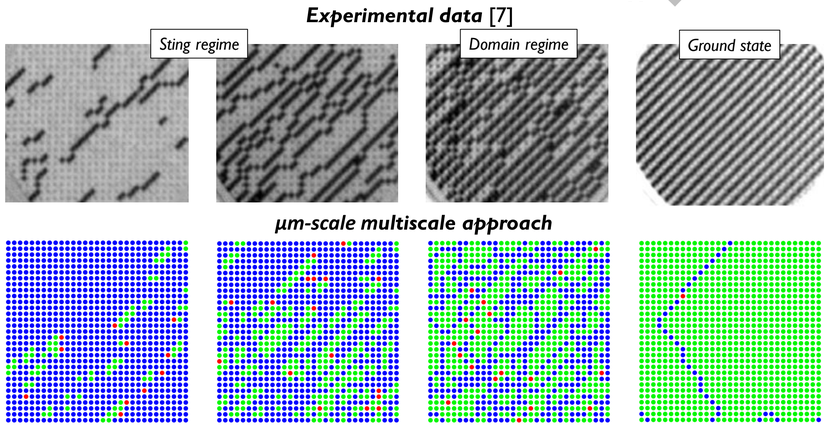

Switching frequency corresponding to $\Delta E_0$ (energy barrier for the coherent reversal of an *isolated* nanostructure)

This approach allowed us to analyze experimental data available in literature [7]:

- $Ni_{83}Fe_{17}$
- 470 nm x 170 nm x 3 nm
- 130 nm edge-to-edge distance
- M = 350 kA/m
- Sample saturated in a magnetic field applied along [11] and measured by XMCD




***Experimental data*** [7]

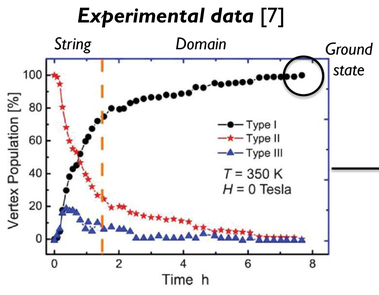



***μm-scale multiscale approach***

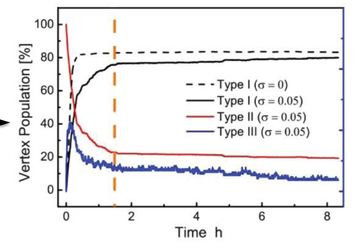


*T1 Vertices* | *T2 Vertices* | *T3 Vertices*

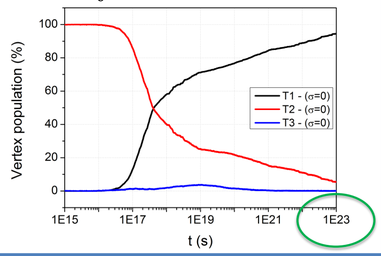
***Experimental data*** [7]




***KMC*** from [7], where $\Delta E_0$ and $\tau_0$ have been *set* to **1.05 eV** and $2 \cdot 10^{-12}$ s to get the right time scale




***μm-scale multiscale approach:*** $\Delta E_0$ turns out to be **2.15 eV**



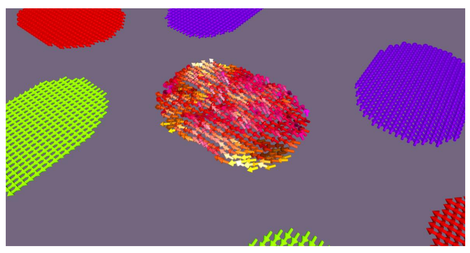

## *nm-scale*: micromagnetism

The difference in the kMC time scale (given by the energy barrier's difference) led us to consider a better approach for the magnetization reversal modelling at $T \neq 0$ K.

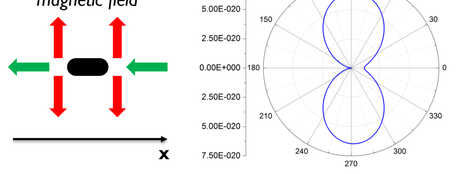
***Micromagnetism***

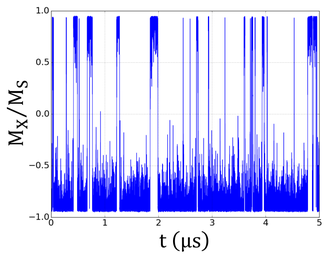
**mumax**[3] GPU-accelerated micromagnetism

- Stadium-like Permalloy nanostructures (150 nm x 100 nm x 3 nm) with 5 x 5 x 3 $nm^3$ cell volume;
- Analysis of the central nanostructure time evolution with *fixed* magnetization in the 6 n.n.;
- 5th order Runge-Kutta scheme with 4th order error correction [10] and *adaptive timestep*;
- At each temperature, 10 μs have been simulated and $M_S$ has been accordingly *adjusted*.

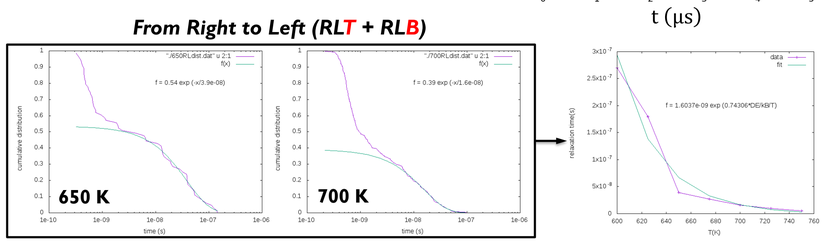


*no applied magnetic field*

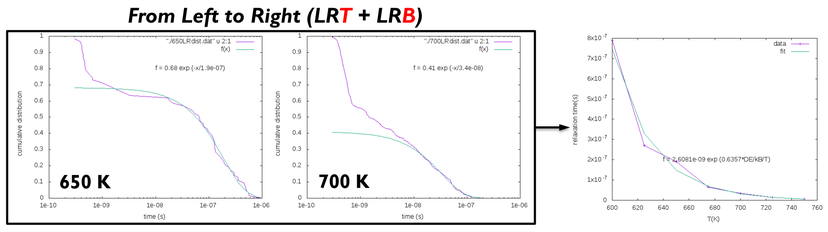


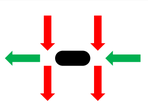
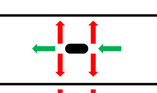
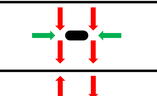
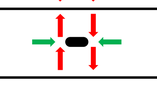

***From Right to Left (RLT + RLB)***




***From Left to Right (LRT + LRB)***




$\tau^i = \tau_0^i \exp\left(\frac{c^i \Delta E_{CR}^i}{k_B T}\right)$, where $\Delta E_{CR}^i$ is the coherent reversal energy barrier for configuration $i$

| Configuration ($i$) | Transition | $\tau_0^i$ (ns) | $c^i$ |
|---|---|---|---|
| (0)  | LRB | $3.5 \pm 0.6$ | $0.61 \pm 0.03$ |
| | LRT | $2 \pm 1$ | $0.63 \pm 0.12$ |
| | RLB | $2.6 \pm 0.7$ | $0.62 \pm 0.07$ |
| | RLT | - | - |
| (9)  | LR | $2.6 \pm 0.8$ | $0.63 \pm 0.04$ |
| | RL | $1.6 \pm 0.7$ | $0.74 \pm 0.08$ |
| (16)  | B | $2.0 \pm 0.3$ | $0.71 \pm 0.03$ |
| | T | $2.2 \pm 0.6$ | $0.51 \pm 0.04$ |
| (19)  | - | $3.0 \pm 0.7$ | $0.59 \pm 0.03$ |
| | | $\mathbf{2.320 \pm 0.003}$ | $\mathbf{0.6322 \pm 0.0002}$ |

***Conclusions***

- We showed that, at high temperature (T close to $T_B$), the energy barrier can be about 63 % of the coherent reversal energy barrier and $\tau_0$ lies in a range consistent with literature data. Anyway, a general analysis including room T is still missing (*future outlook*).
- The whole work points out the necessity of considering both the actual nanostructure's shape and the effect of temperature in order to calculate the proper energy barrier.

## References

[1] R. F. Wang et al., *Nature* **439,** 303 (2006).
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[7] A. Farhan et al., *Phys. Rev. Lett*. **111,** 057204 (2013).
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[9] A. B. Bortz et al., *J. Comp. Phys.* **17,** 10 (1975).
[10] A. Vansteenkiste et al., *AIP Advances* **4,** 107133 (2014).

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