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.

- **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, STEM).

- **Advanced fabrication techniques** (EBL) allow for the systematic variation of the key parameters governing the system (size, distance, arrangement).

Interesting features

- **Double-height square ASI**\(\[4\]**
- **Spin-ice compounds**\(\[5\]**

The key process in ASI systems consist in the formation of low-energy states (towards observed):

1. The system is melted and (2) the frozen state (equilibrium) is recorded.

Demagnetizing protocol [7]

- **Thermal protocol [2,4,7]**: From \(T > T_e\) to \(T < T_e\).

**Kinetic Monte Carlo** [7] + precomputed switching frequencies

- The considered event is the magnetization reversal of a single nanostructure (single flip).
- The base unit is composed of 7 nanostuctures (center, first n.n. and second n.n.).
- The 7 nanostuctures 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.

This approach allows us to analyze experimental data available in literature [7].

- \(N_{kMC}, P_{kMC} = 470 \text{ nm } \times 170 \text{ nm } \times 3 \text{ nm}\)
- \(130 \text{ nm} \text{-edge to edge distance}\)
- \(M = 330 \text{ kA/m}\)
- Sample saturated in a magnetic field applied along [111] and measured by XMCD.

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

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

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

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

**KMC** [7] where \(E_{kMC}\) and \(E_{kMC}(\Delta E)\) have been used:

1. 1.65 eV and 2-10\(^-15\) to get the right time scale

**nm-scale: micromagnetics**

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 \(T > 0 \text{ K}\).

- **Micromagnetic** • Stadium-like Permalloy nanostructures (150 nm x 100 nm x 3 nm) with 5  \times 5  \times 3 \text{ nm}^3\) cell volume;
• Analysis of the central nanostructure time evolution with fixed magnetization in the 6 n.n.:
• 5\(^{th}\) order Runge-Kutta scheme with 4\(^{th}\) order error correction [10] and adaptive time step;
• At each temperature, 10\(^{4}\) have been simulated and \(M_e\) has been accordingly adjusted.

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Conclusions

- We showed that, at high temperature (T close to \(T_e\)), the energy barrier can be about 63 % of the coherent reversal energy barrier and \(E_k\) 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


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