Dynamics of Magnetization Switching in Models of Magnetic Nanoparticles and Ultrathin Films

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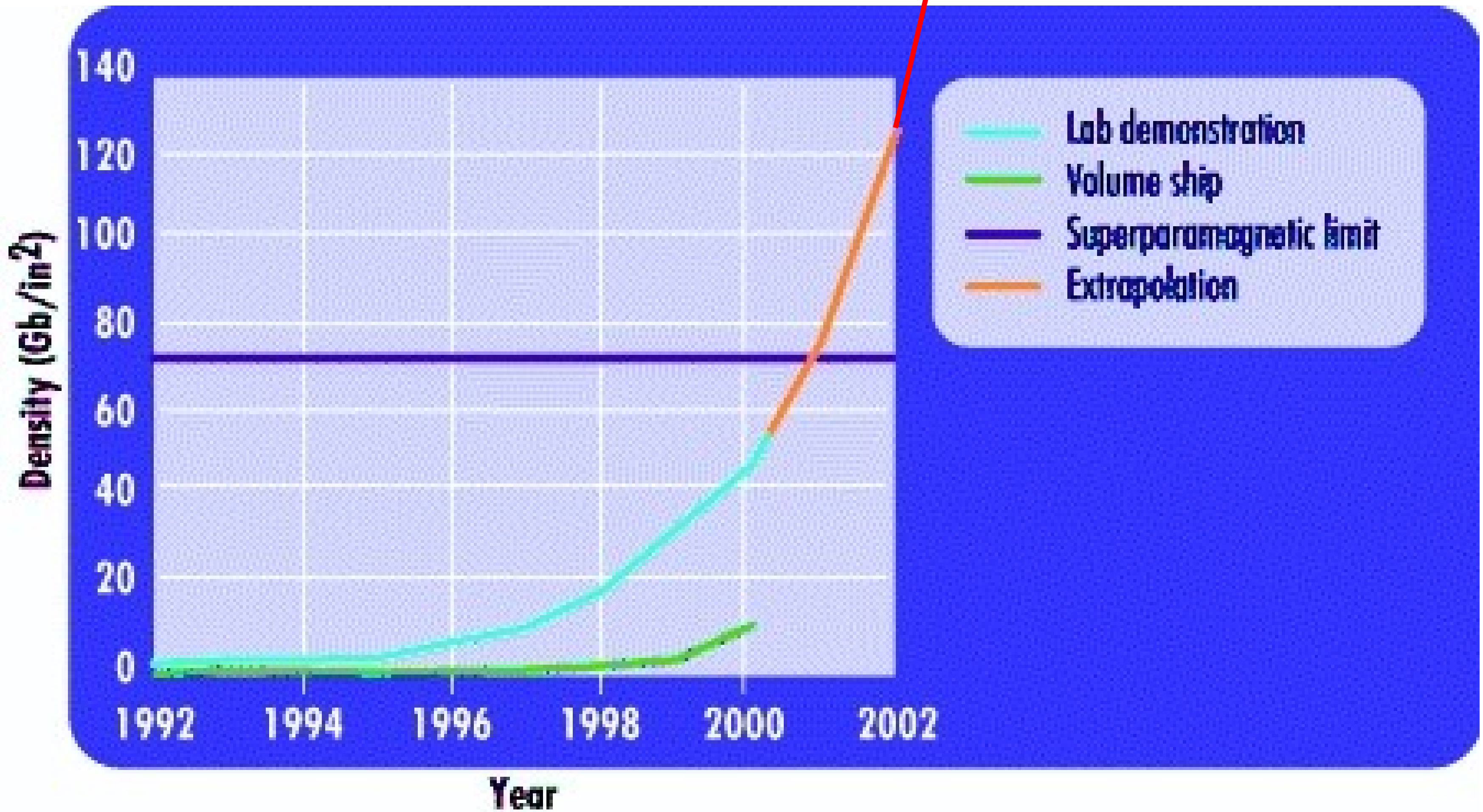
Why are anisotropic magnetic nanoparticles interesting?

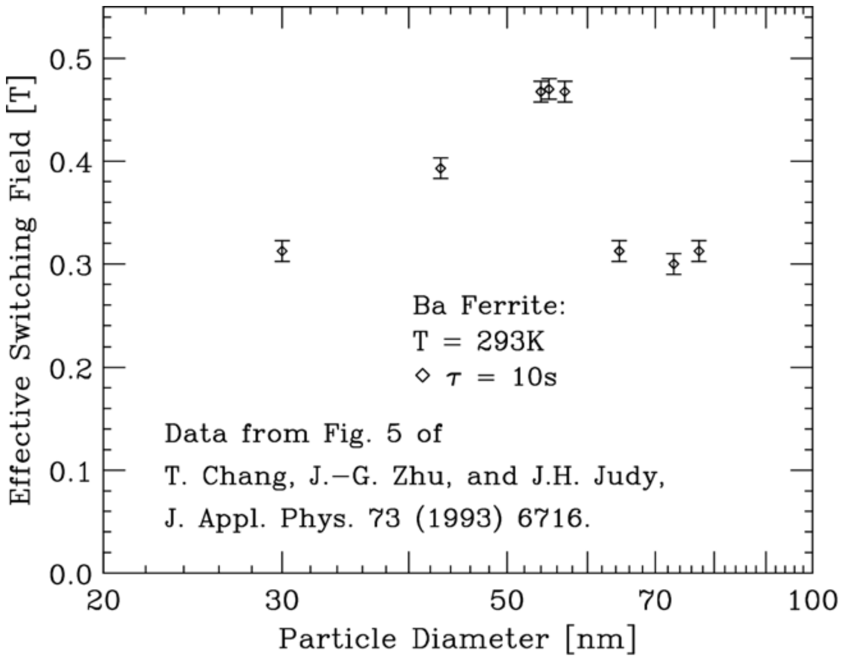
- Hot candidate materials for ultra-high density magnetic recording media
- Only recently observable by methods such as Magnetic Force Microscopy (MFM) and Atomic Force Microscopy (AFM)
- Switching behavior a technologically important problem in nonequilibrium statistical mechanics

Increasing magnetic data recording density

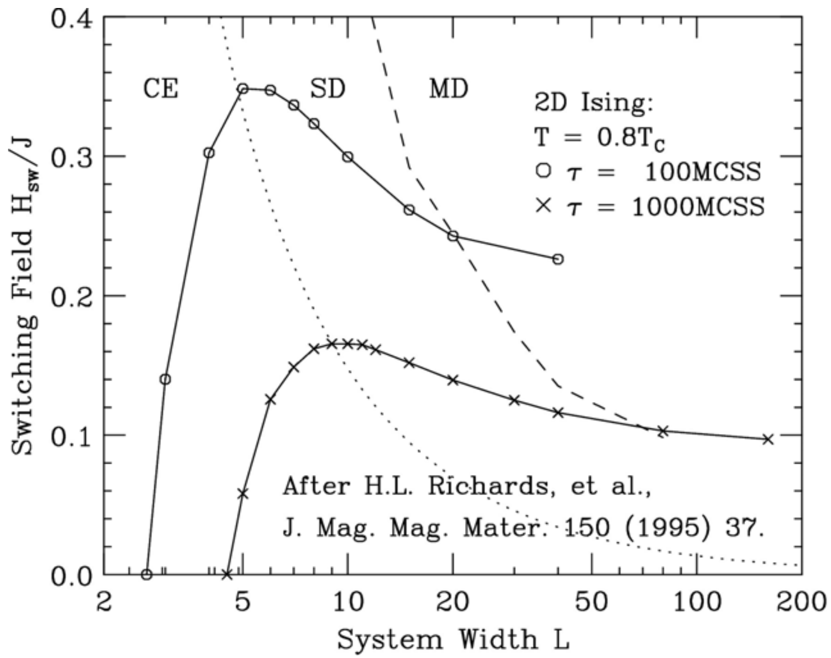


From *Data Storage*, July 2000

Superparamagnetic limit



MFM experiments

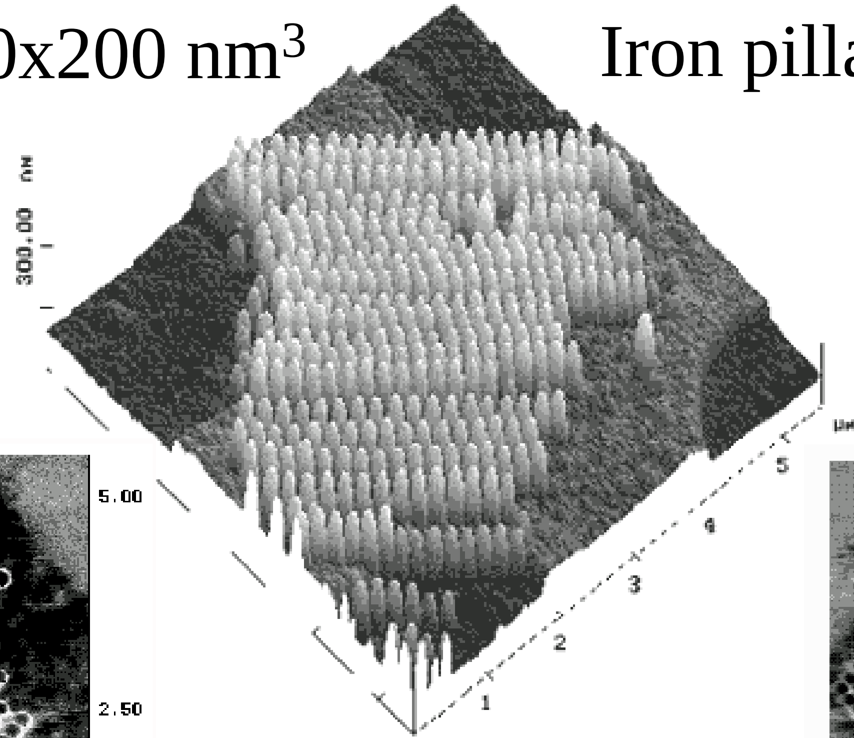


Kinetic Ising model

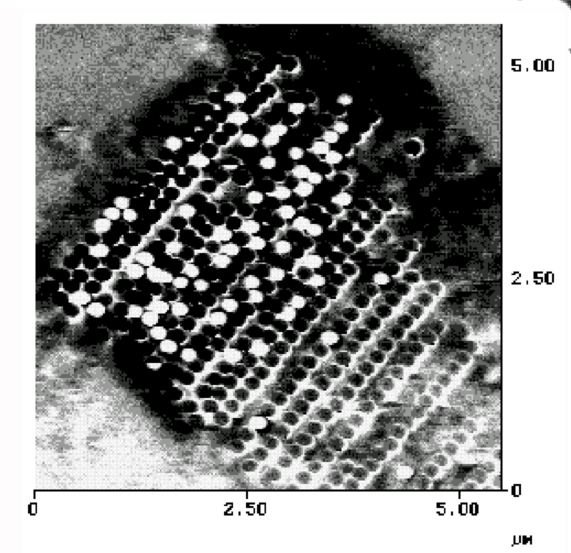
Example of potential recording medium

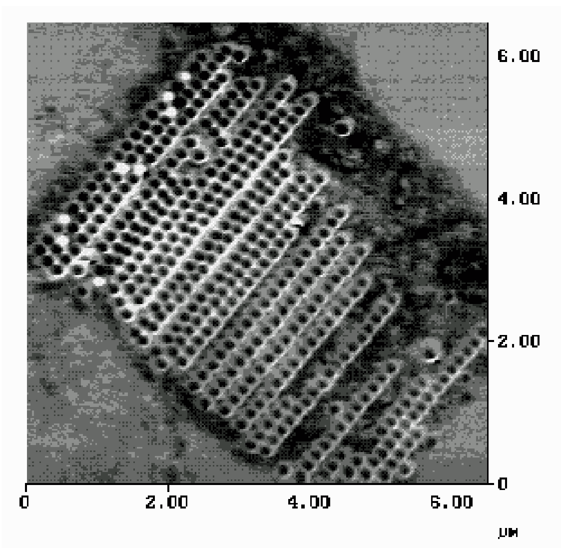
40x40x200 nm^3

Iron pillars



AFM image



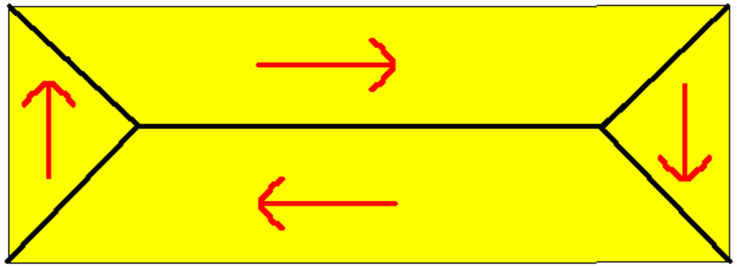


MFM, random magnetization

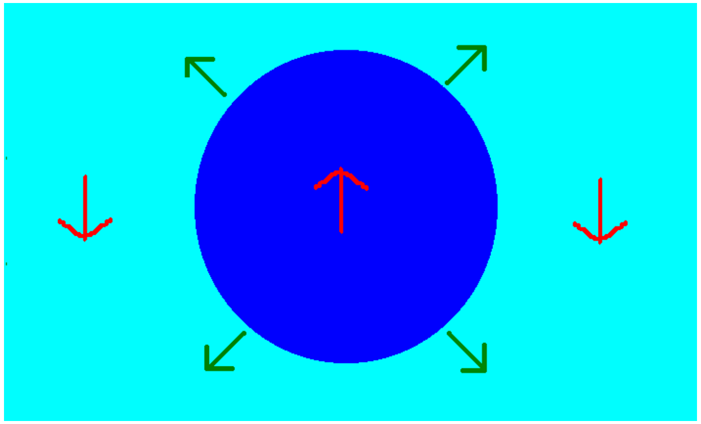
Oriented in 200 G field

D.D. Awschalom, J. Shi, S. von Molnár, http://www.qi.ucsb.edu/awsch

Droplets versus domains



Domains are equilibrium structures that minimize the magnetic energy. Nanometer sized particles can be single-domain.



Droplets are nonequilibrium structures that only exist during the process of magnetization switching.

Models and methods

1. Dynamic Monte Carlo simulations of kinetic Ising models
2. Nucleation theory of metastable decay
3. Finite-temperature micromagnetics simulations

Kinetic Ising Model

Simple model Hamiltonian:

$$\mathcal{H} = -J \sum_{\langle i,j \rangle} s_i s_j - H \sum_i s_i$$

Order parameter is magnetization:

$$m = N^{-1} \sum_i s_i$$

For temperature T below critical value T_c, m for $H{=}0$ takes one of two equilibrium values:

$$m(T < T_c,\ H{=}0) \ = \ \pm m_{\mathrm{s}}(T)$$

For $H \neq 0$, m at equilibrium has same sign as H. The phase with m antiparallel to H is metastable.

Stochastic Dynamics

Ising models don't have intrinsic kinetics.

Construct one to mimic the coupling to the environment.

Choose random spin s_i and

propose update $s_i \rightarrow -s_i$

Accept with probability $W(s_i \rightarrow -s_i)$

Reject with probability $1 - W(s_i \rightarrow -s_i)$

Some different W that lead to equilibrium:

Metropolis:

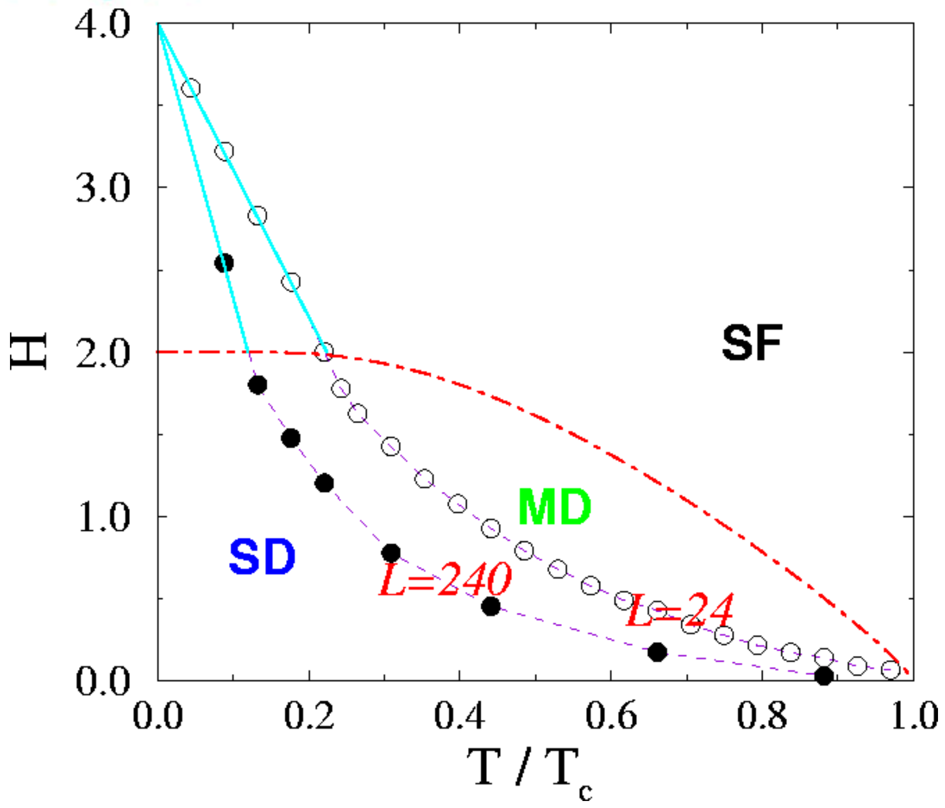
$$W(s_i \rightarrow -s_i) = \min[1, \exp(-\beta \Delta E_i)]$$

Glauber:

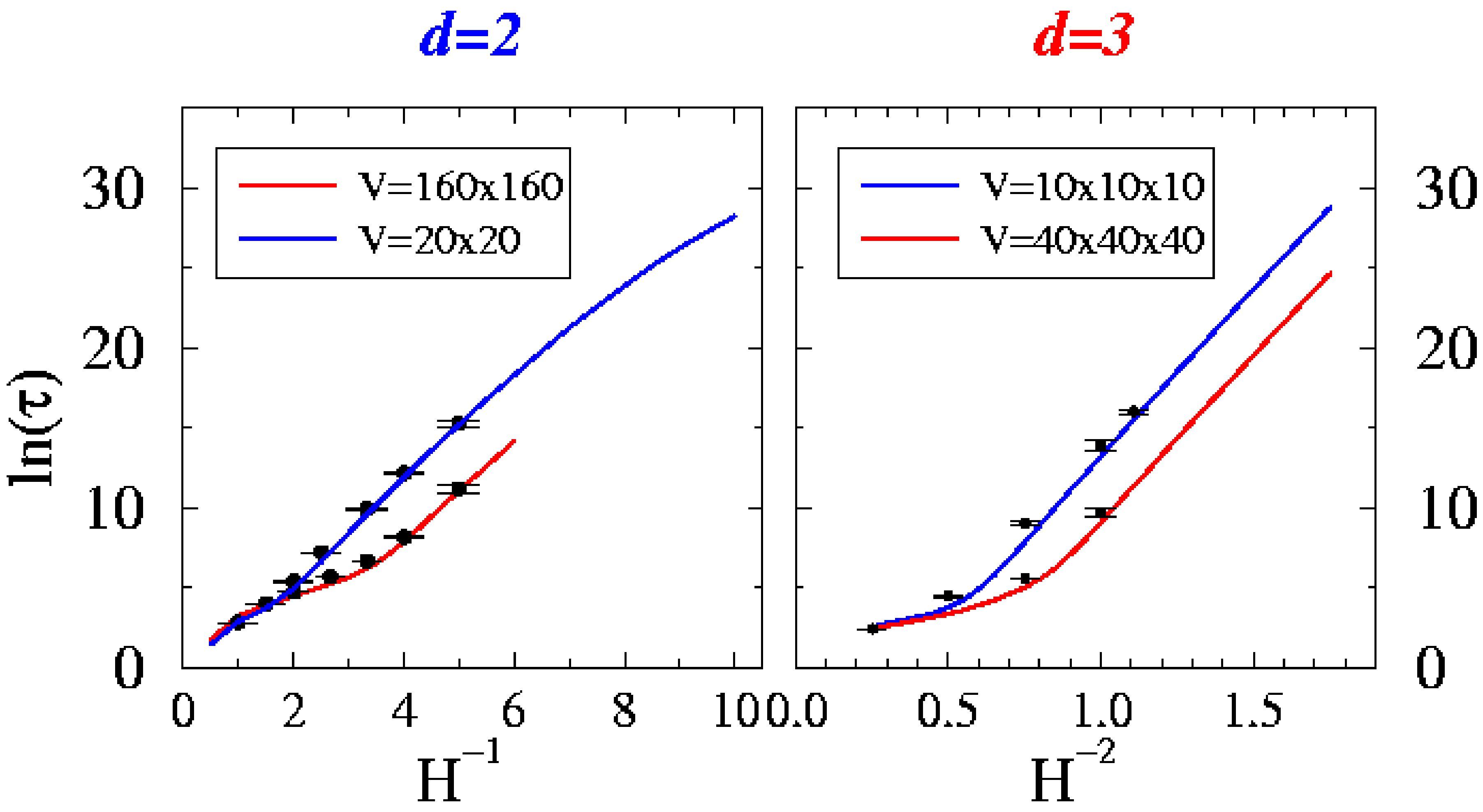
$$W(s_i \rightarrow -s_i) = \frac{\exp(-\beta \Delta E_i)}{1 + \exp(-\beta \Delta E_i)}$$

"Metastable Phase Diagram"

- 4 length scales, different decay regimes
  - SD (Single Droplet) $a{<<}R_c{<<}L{<<}R_o$
  - H_{DSP} between SD and MD
  - MD (Multi-Droplet) $a{<<}R_c{<<}R_o{<<}L$
  - SF (Strong Field) $a{\approx}R_c{\approx}R_o$
  - H_{DSP} about where $r{=}\frac{1}{2}$

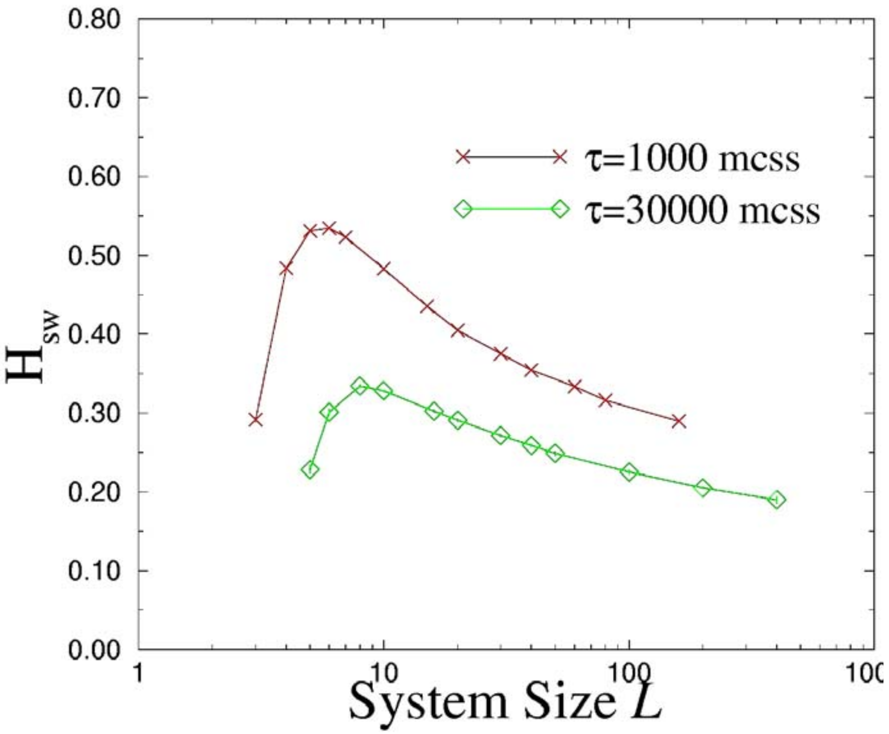


Lifetime vs $H^{-(dimension-1)}$

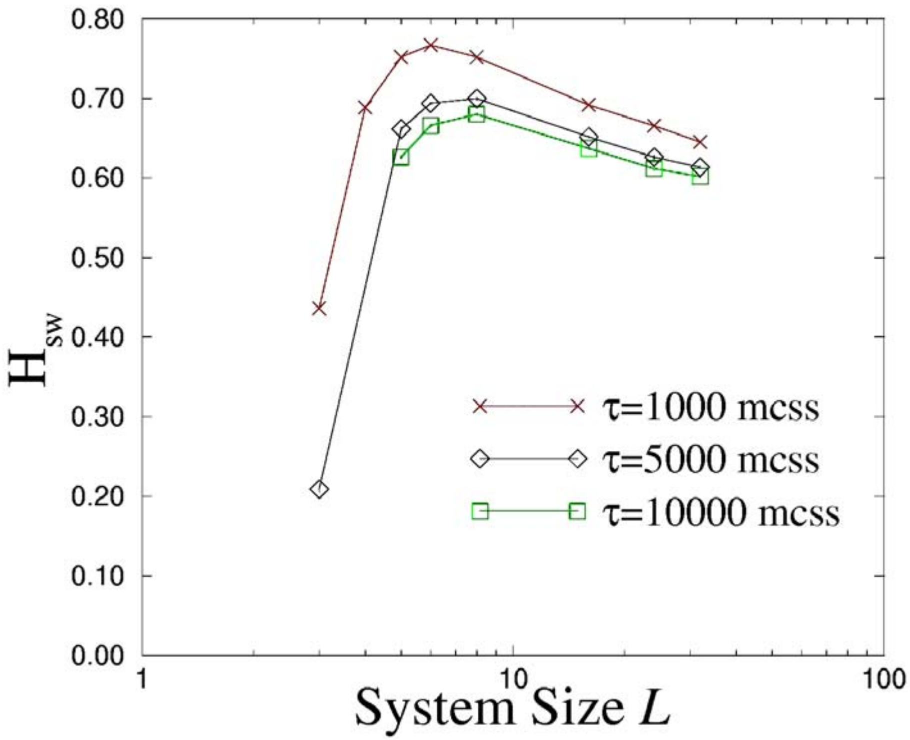


Switching Field

2D square, $T = 0.57T_c$



3D cubic, $T = 0.60T_c$



Bells and Whistles

The hypercubic Ising model with periodic boundary conditions is obviously far too simple to describe real systems.

We have considered several generalizations.

- Modified boundary conditions (free, or with modified fields or interactions at the surface).
- Different forms of disorder.
- Demagnetizing field
- Coercivity of magnetic sesquilayers.

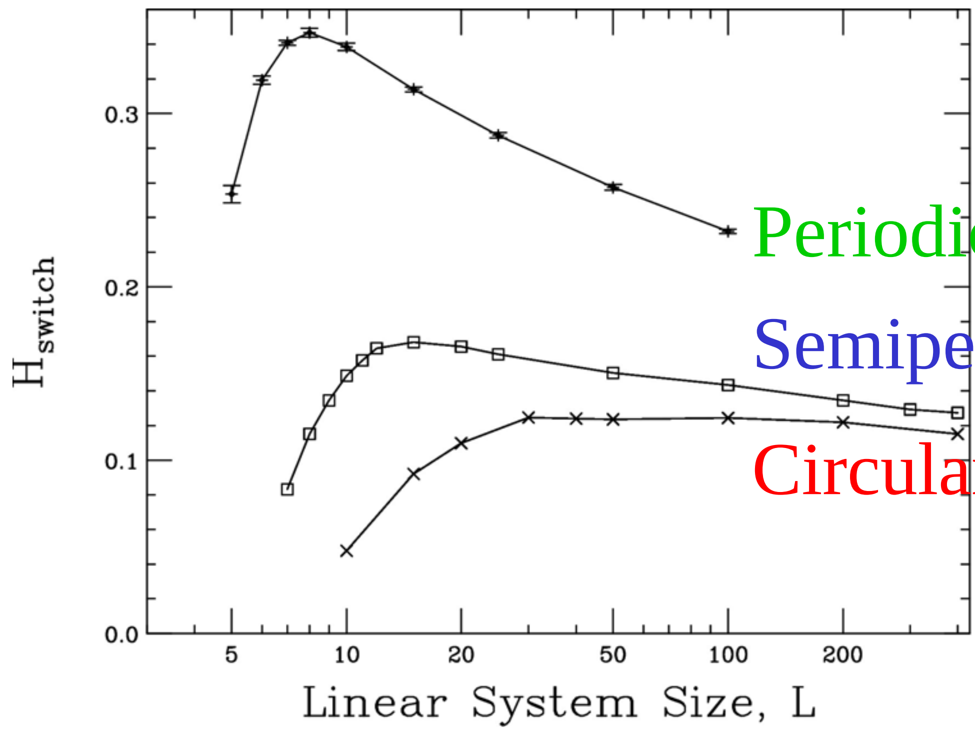
These lead to *quantitative*, but in general little *qualitative*, change. In the next few slides I will show some examples.

Different Boundary Conditions

Modified Hamiltonian with boundary interactions and fields:

$$\mathcal{H} = -J\sum_{\langle i,j \rangle} s_i s_j - H\sum_i s_i - J_\Sigma \sum_{\langle i,j \rangle_\Sigma} s_i s_j - H_\Sigma \sum_{i_\Sigma} s_i$$

d=2, T=1.3J≈0.57T_c, τ=30000 MCSS



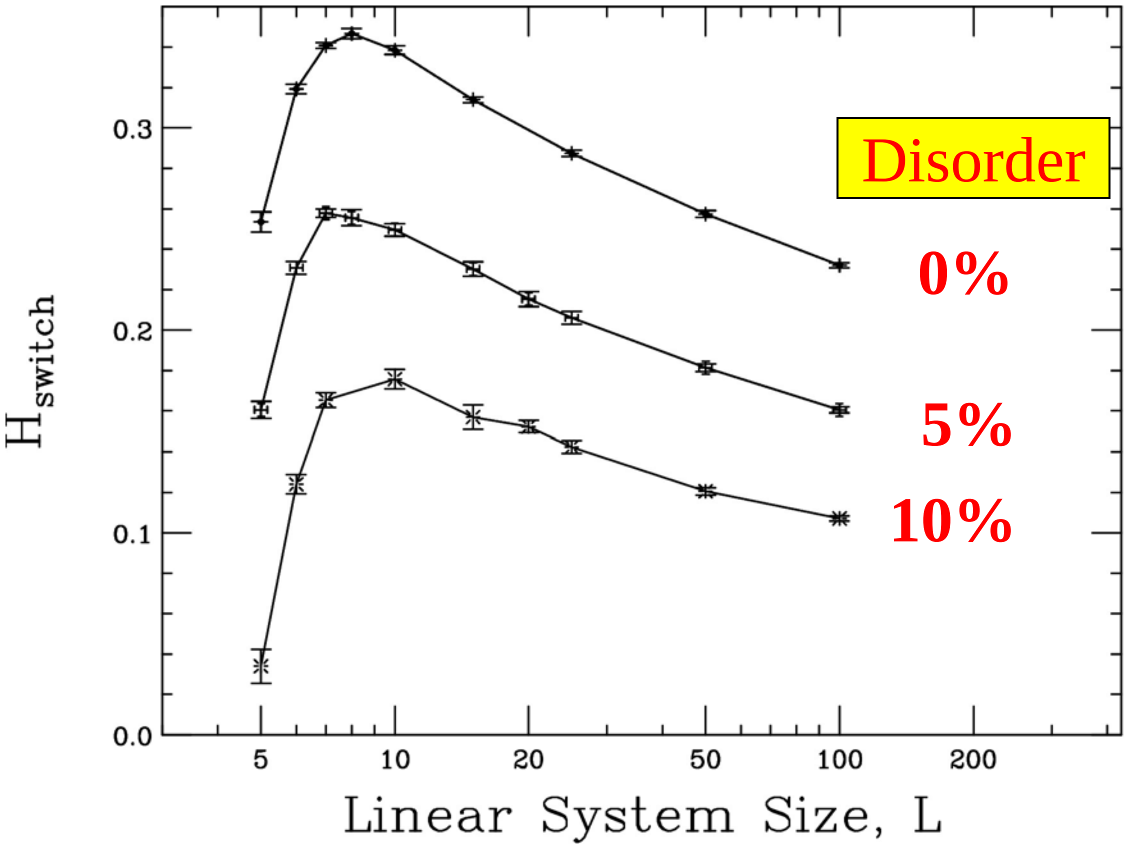
Periodic b.c.

Semiperiodic, $J_\Sigma = H_\Sigma = 0$

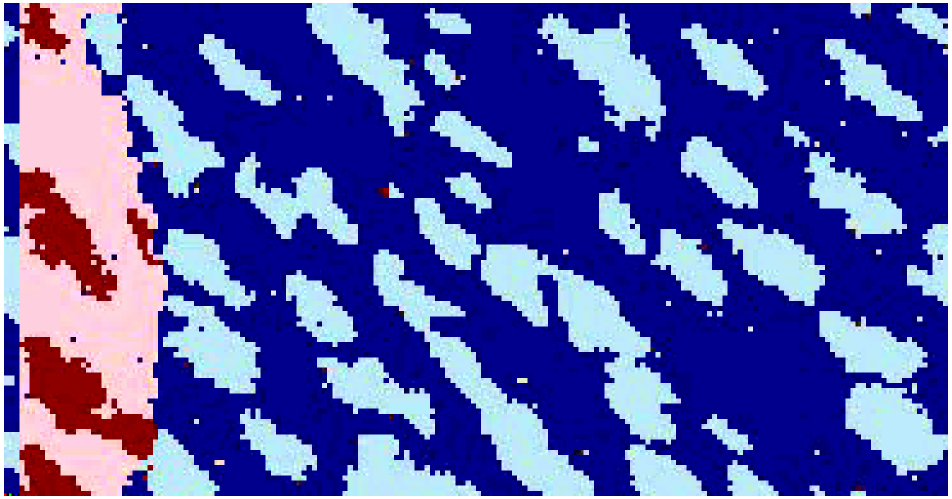
Circular, $J_\Sigma = H_\Sigma = 0$

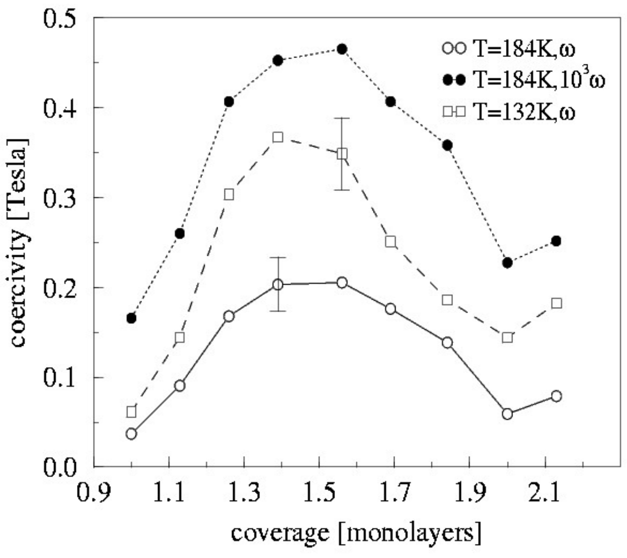
Different Amounts of Bond Disorder

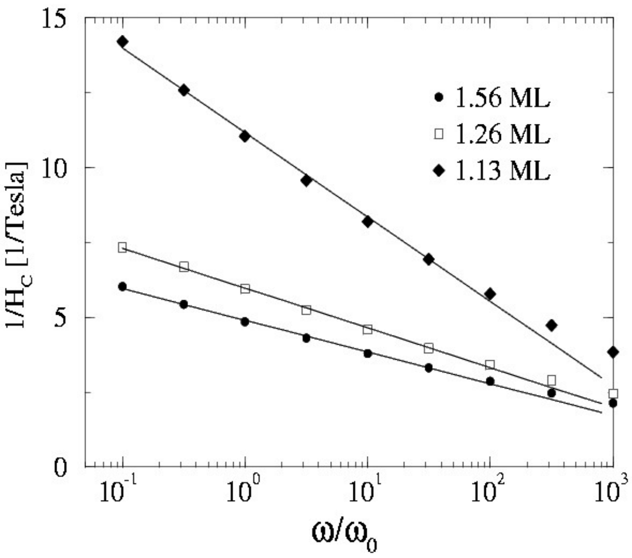
d = 2, T = 1.3J, τ = 30,000 MCSS



Coercivity of Fe Sesquilayers on W(100)







Continuum Spins:

Finite-temperature Micromagnetics

Landau-Lifshitz-Gilbert equation:

$$\frac{d\tilde{\mathbf{M}}(\tilde{\mathbf{r}}_i)}{d\tilde{t}} = \frac{\gamma_0}{1+\alpha^2}\tilde{\mathbf{M}}(\tilde{\mathbf{r}}_i) \times \left(\tilde{\mathbf{H}}(\tilde{\mathbf{r}}_i) - \frac{\alpha}{M_s}\tilde{\mathbf{M}}(\tilde{\mathbf{r}}_i) \times \tilde{\mathbf{H}}(\tilde{\mathbf{r}}_i) \right)$$

$\tilde{\mathbf{M}}(\tilde{\mathbf{r}}_i)$: magnetization vector at $\tilde{\mathbf{r}}_i$

γ_0 : electron gyromagnetic ratio

$\alpha = 0.1$: phenomenological damping parameter

$\tilde{\mathbf{H}}(\tilde{\mathbf{r}}_i)$: local magnetic field, contains exchange, anisotropy, dipole-dipole, thermal noise, and applied field

Fluctuation-dissipation relation for noise field:

$$\langle \tilde{H}_{\mathrm{n}\mu}(\tilde{\mathbf{r}}_i, \tilde{t}) \tilde{H}_{\mathrm{n}\mu'}(\tilde{\mathbf{r}}_i', \tilde{t}') \rangle = \frac{2\alpha k_{\mathrm{B}} T}{\gamma_0 M_s V} \delta\left(\tilde{t} - \tilde{t}'\right) \delta_{\mu,\mu'} \delta_{i,i'}$$

Fast Multipole Method

- The dipole-dipole interactions are computed with the Fast Multipole Method (FMM) [Greengard, J. Comp. Phys. **73**, 325 (1987)]
- Fast (order *N*)
- Easily handles empty space, as in arrays of magnets
- Can be generalized to irregular grids

Fast Multipole Method

Multipole Expansion

$$\phi_{\mathrm{M}}(r,\theta,\varphi) = \sum_{i=0}^{\infty} \sum_{j=-i}^{i} \left(L_i^j r^i + \frac{M_i^j}{r^{i+1}} \right) Y_i^j(\theta,\varphi)$$

$Y_i^j(\theta,\varphi)$ is spherical harmonic

Truncate sum in i

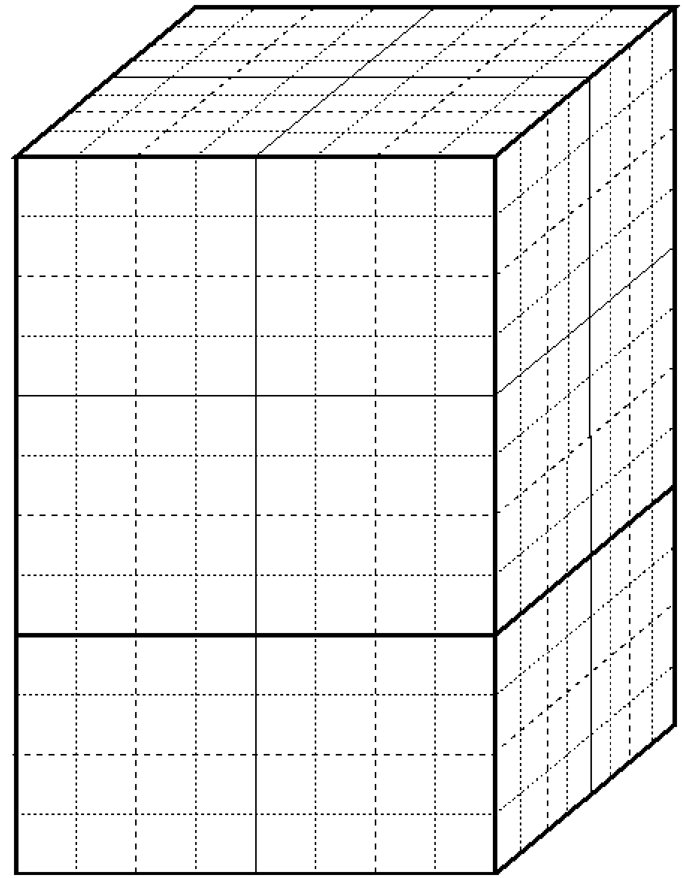
$$M_i^j = \int_V d\mathbf{r} \left[\rho_{\mathrm{M}}(r,\theta,\varphi) + \sigma_{\mathrm{M}}(r,\theta,\varphi) \right] r^i Y_i^j(\theta,\varphi)$$

Rules for transforming information

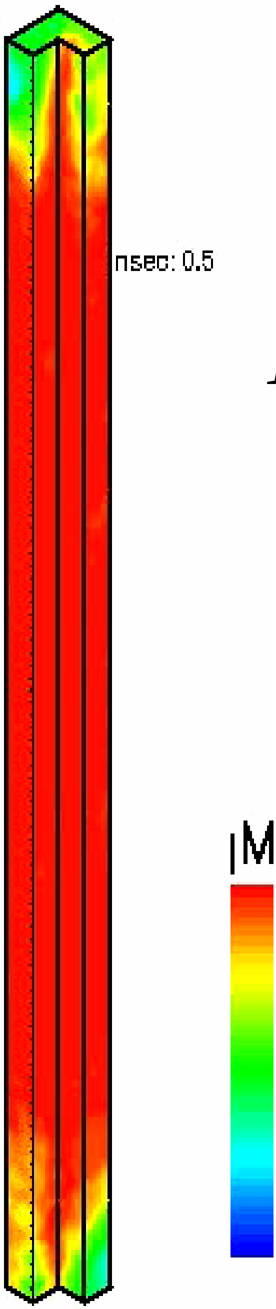
- Multipole at $\mathbf{r}'$ to multipole at $\mathbf{r}$
- Local at $\mathbf{r}'$ to local at $\mathbf{r}$
- Multipole source at $\mathbf{r}'$ to local field at $\mathbf{r}$

$$L_i^j = \sum_{k=0}^{p} \sum_{l=-k}^{k} M_k^l \frac{J_k^{j,l} A_k^l A_i^j}{A_{i+k}^{l-j}} \frac{Y_{i+k}^{l-j}(\theta,\varphi)}{\varrho^{i+k+1}}$$

Hierarchical lattice decomposition



Simulated Nanomagnets



M_z

9 nm x 9 nm x 150 nm

Fe particle

H_0=800 Oe, T=20 K

Landau-Lifshitz-Gilbert

Langevin simulation

4949 lattice points

Time: 1.2 ns

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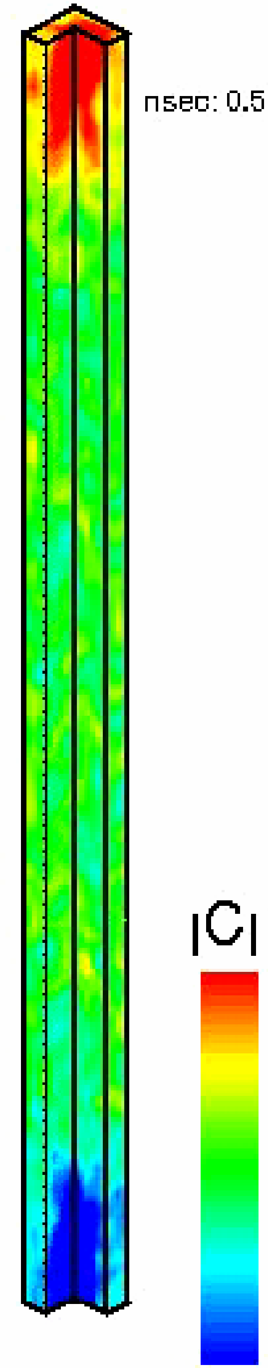
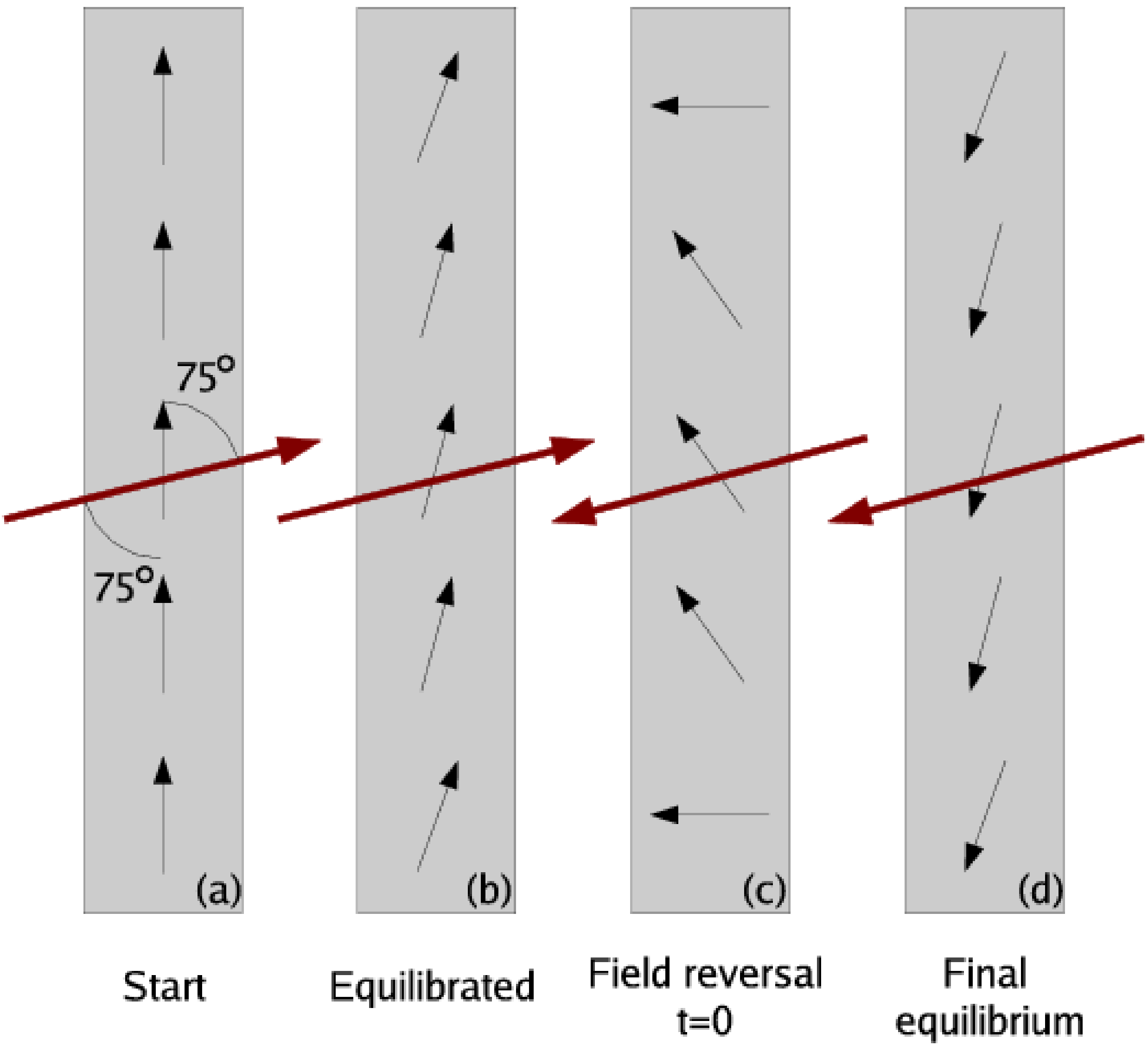
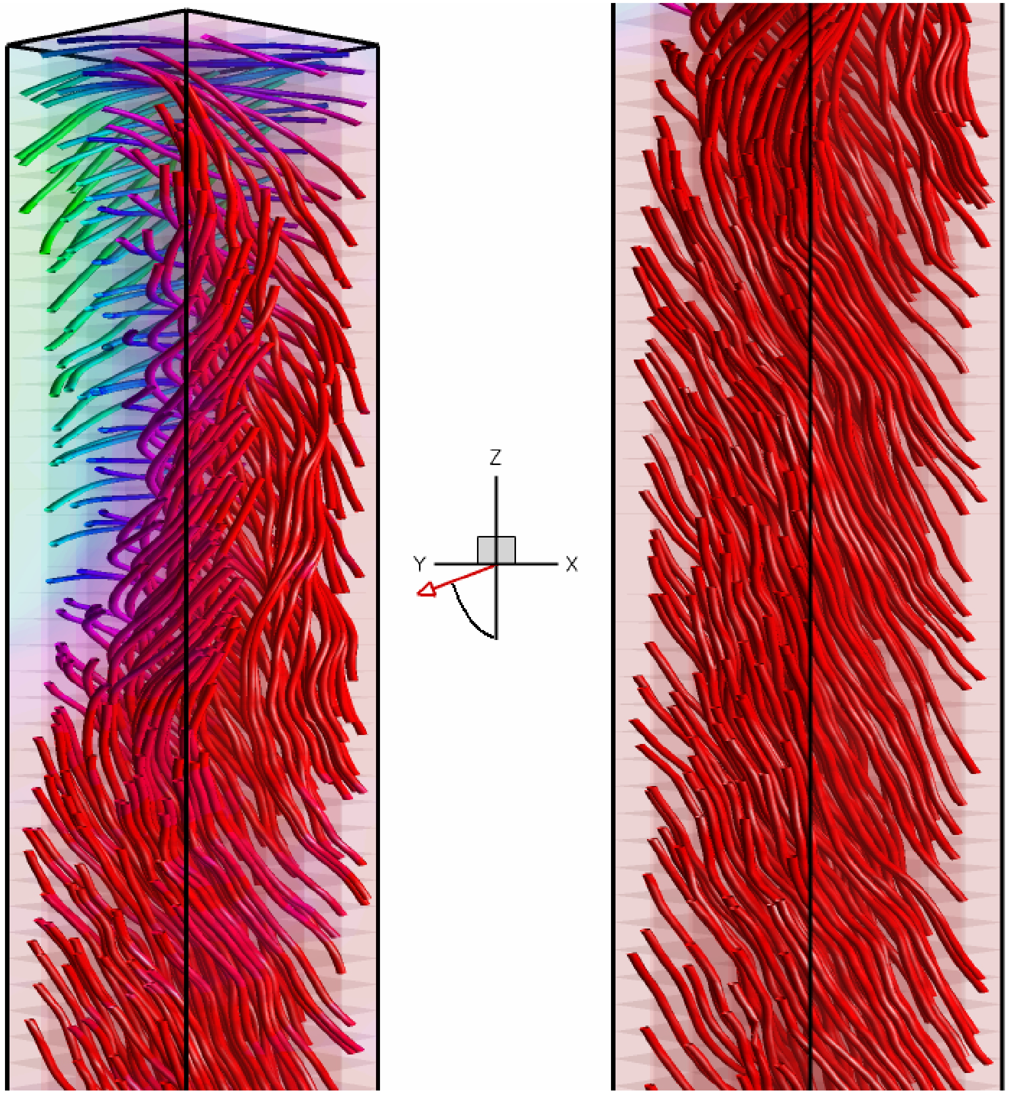


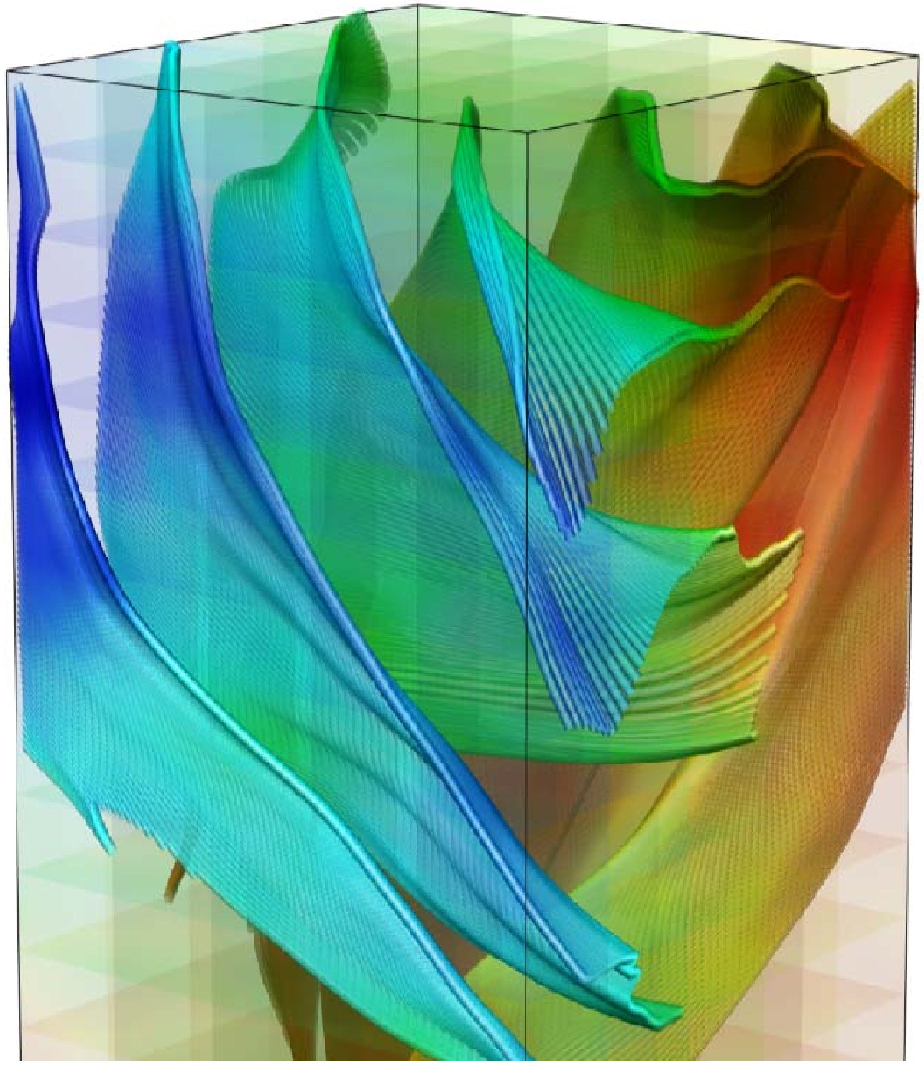
Switching in 75° oblique field



Flux line visualization

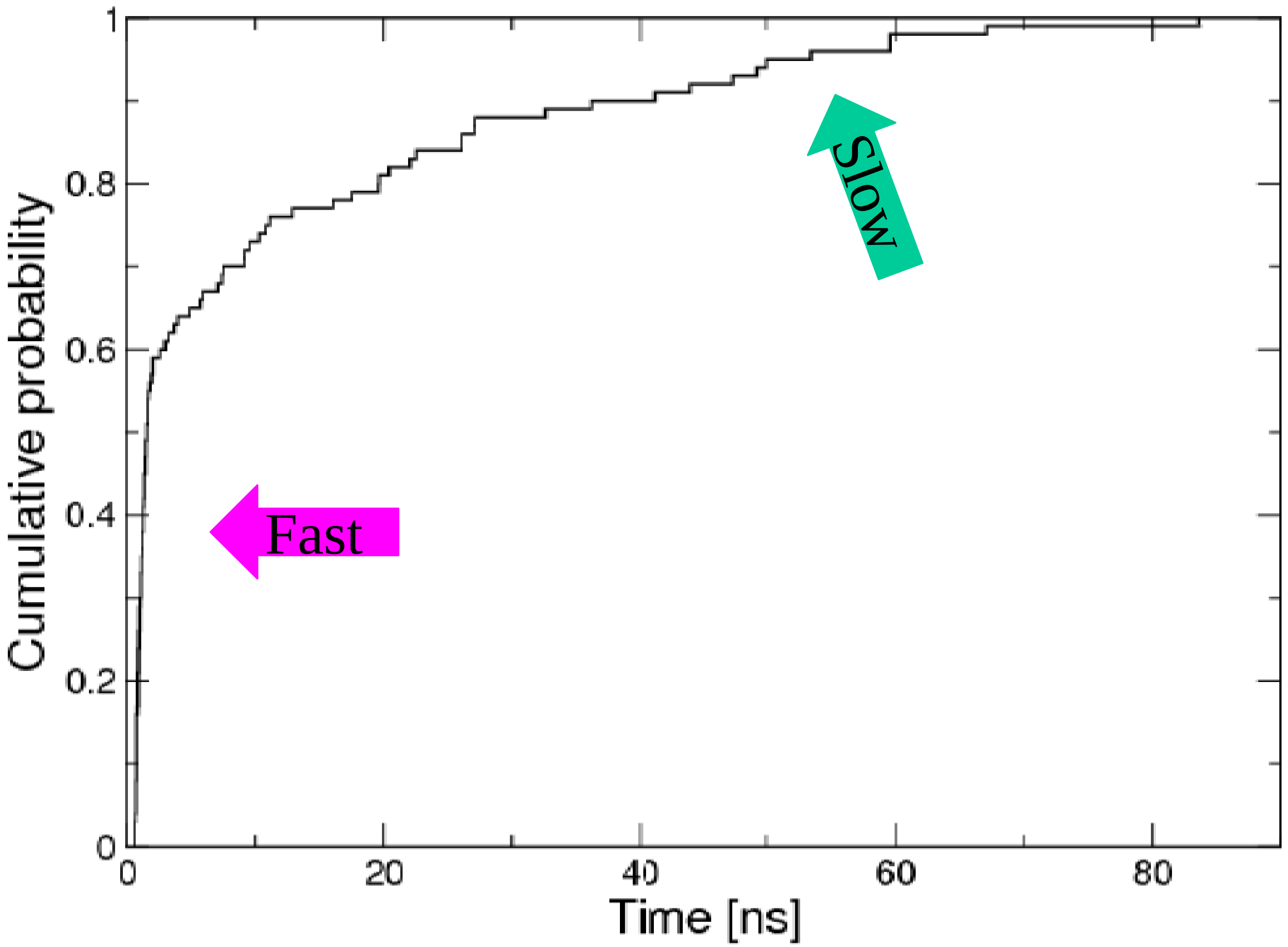


Flux lines at field angle 75°. Metastable state.

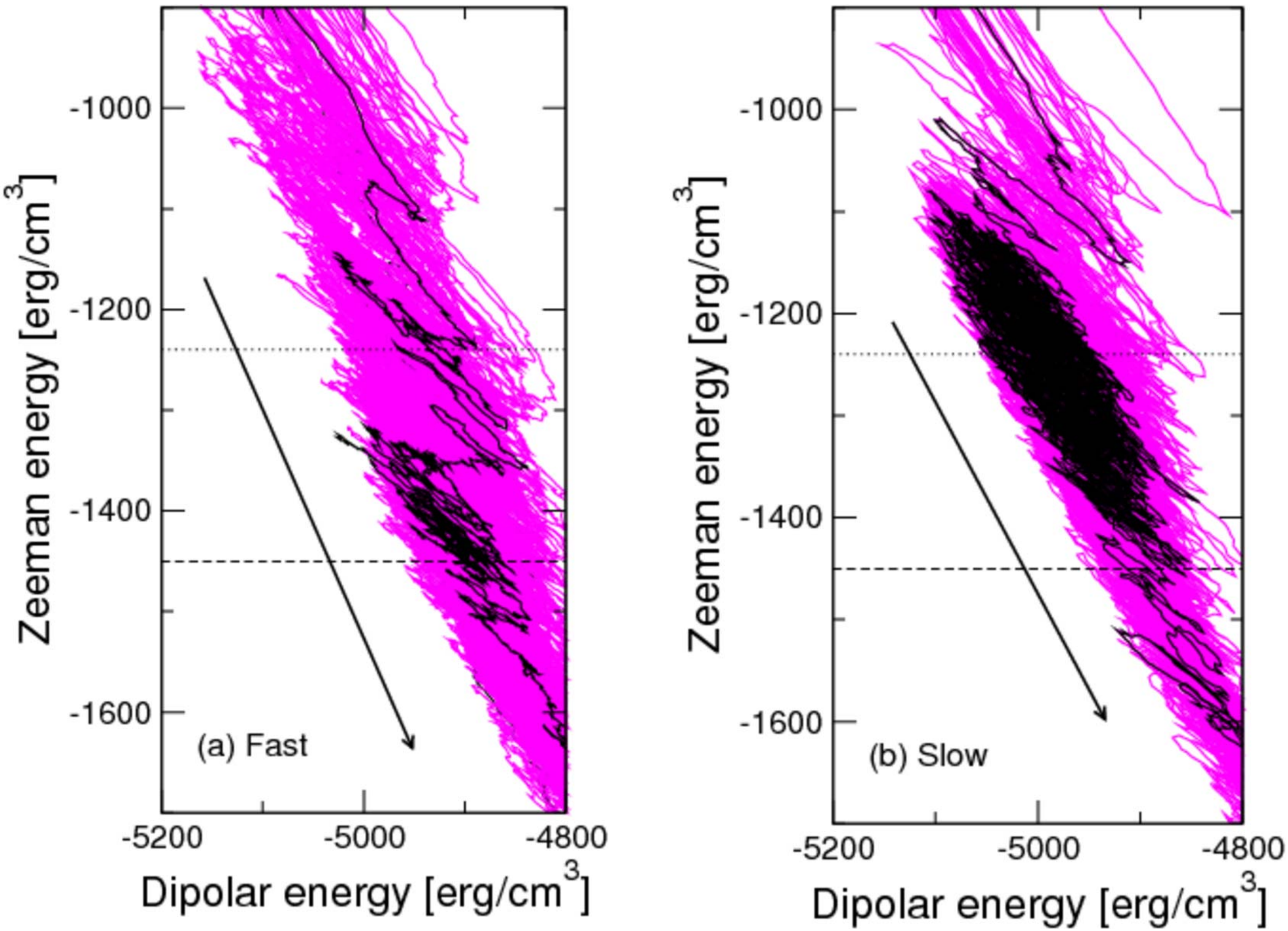


End cap detail

“Fast” and “slow” switching



Different paths in phase space



Conclusions

- Single-domain, uniaxial magnetic nanoparticles important for magnetic recording
- Monte Carlo and Micromagnetic simulations at nonzero *T* predict switching behavior
- Switching behavior analyzed with nucleation theory
- Single-domain particles can have characteristic maximum in coercivity vs size, entirely determined by dynamics
- Modifications to enhance realism mostly only change quantitative behavior
- Hysteresis shows interesting behavior