Nucleation Theory of Magnetization Switching in Nanoscale Uniaxial Ferromagnets

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Why interesting?

Nanometer-sized particles of highly anisotropic ferromagnets

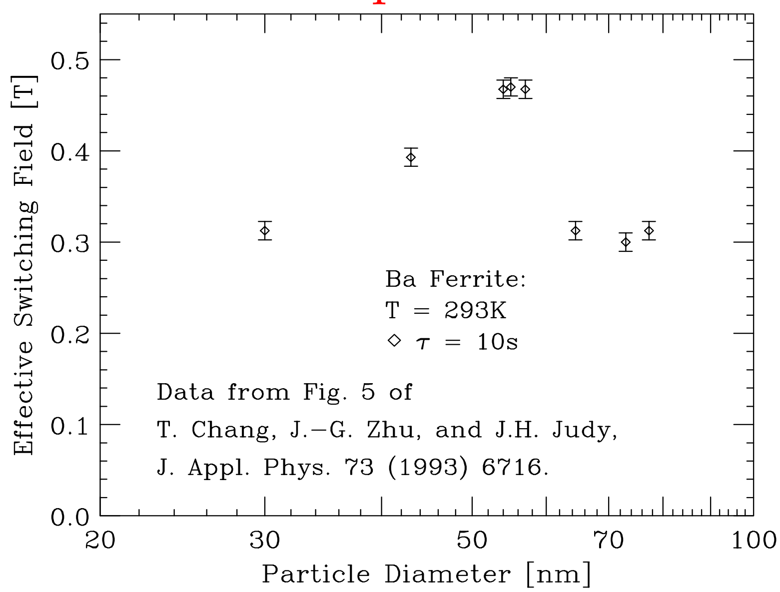
- are hot candidate materials for magnetic recording media.
- have only recently become individually observable by methods such as Magnetic Force Microscopy (MFM).
- should be single domain in equilibrium.

Why nucleation theory?

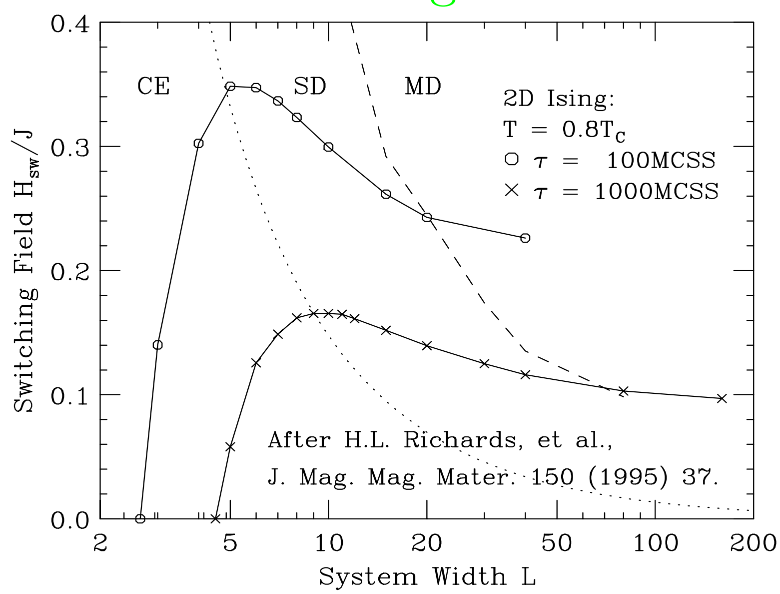
- Provides nonuniform switching mechanism for single-domain particles.

Switching Fields

MFM experiments



Kinetic Ising model



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 "their own" kinetics. Construct one to mimic the coupling to the environment.

Choose spin and ask: *"Would you like to flip?"*

Answer: *"Yes"* with *probability* $W(s_i \to -s_i)$

Answer: *"No"* with *probability* $1 - W(s_i \to -s_i)$

Different W that lead to equilibrium:
Metropolis:

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

Glauber:

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

Nucleation theory of metastable decay

Relevant fluctuations are compact droplets of radius R and volume $\Omega_d R^d$ with free energy

$$F(R) \approx d\Omega_d \sigma_0(T) R^{d-1} - |H| 2 m_{\rm s}(T) \Omega_d R^d$$

$\sigma_0(T)$: Droplet surface tension.

$m_{\rm s}(T)$: Spontaneous magnetization.

$F(R)$ is maximum for the critical radius

$$R_{\rm c} \approx \frac{(d-1)\sigma_0(T)}{2 m_{\rm s}(T)|H|}$$

Nucleation rate:

$$\Gamma(T,H) \propto |H|^K \exp\left[-\frac{\beta \Xi(T)}{|H|^{d-1}}\right]$$

No sharp spinodal for short-range-force system!

Nucleation and growth

KJMA (Avrami) theory.

Large supercritical droplets grow at constant velocity (Lifshitz-Allen-Cahn approximation):

$$
\begin{aligned}
v_\perp &= (d-1)\nu\left(R_c^{-1} - R^{-1}\right) \\
&\xrightarrow{R\to\infty} (d-1)\nu R_c^{-1} \equiv v_0 \propto |H|
\end{aligned}
$$

Volume fraction of stable phase
(randomly placed, freely overlapping droplets):

$$
\begin{aligned}
\phi_s(t) &\approx 1 - \exp\left[-\Gamma \int_0^t \Omega_d (v_0 s)^d \mathrm{d}s\right] \\
&= 1 - \exp\left[-\frac{\Omega_d}{d+1}\left(\frac{t}{t_0}\right)^{d+1}\right]
\end{aligned}
$$

where $t_0 = (v_0^d \Gamma)^{-1/(d+1)}$ is the average time of free growth.

With t_0 is associated the

characteristic distance of free growth:

$$R_0 = v_0 t_0$$

Recall nucleation rate:

$$\Gamma \propto |H|^K \exp\left[-\frac{\beta\Xi(T)}{|H|^{d-1}}\right]$$

Using this, we have:

$$t_0(T,H) \propto \exp\left[\frac{1}{d+1}\,\frac{\beta\Xi(T)}{|H|^{d-1}}\right]$$

and

$$R_0(T,H) \propto \exp\left[\frac{1}{d+1}\,\frac{\beta\Xi(T)}{|H|^{d-1}}\right]$$

Finite-size effects

Multi-droplet regime, $L \gg R_0 \gg R_c$

$$\tau \propto \exp\left[\frac{1}{d+1}\frac{\beta\Xi}{|H|^{d-1}}\right]$$

Single-droplet regime, $R_0 \gg L \gg R_c$

$$\tau \approx \left[L^d \Gamma\right]^{-1} \propto L^{-d} \exp\left[\frac{\Xi}{k_{\mathrm{B}}T|H|^{d-1}}\right]$$

Coexistence regime, $R_c > L$

$$\tau \approx \exp\left[const \cdot L^{d-1}\right]$$

Scott's SD/MD slide here.

Crossover fields

$R_0 \approx L$: Dynamic Spinodal (DSP)

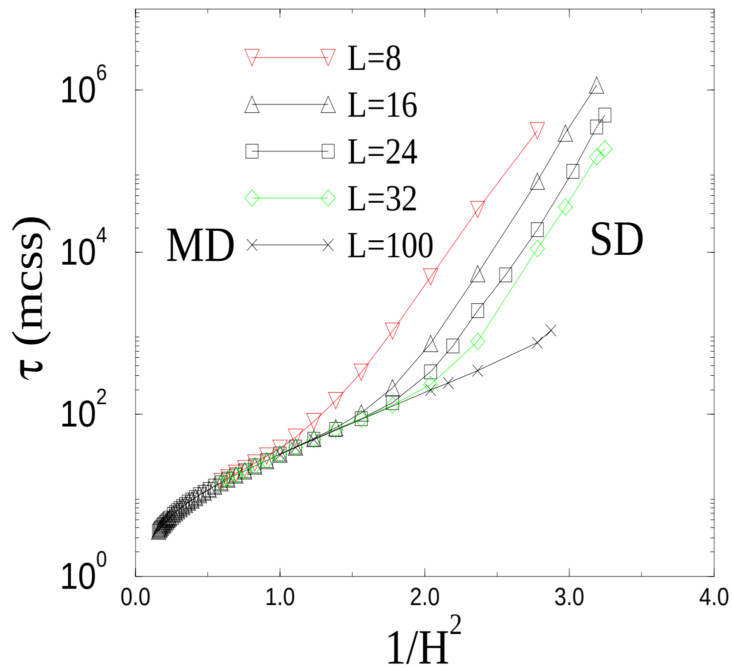
$$H_{\mathrm{DSP}} \approx \left(\frac{1}{d+1} \; \frac{\beta \Xi(T)}{\ln L} \right)^{\frac{1}{d-1}}$$

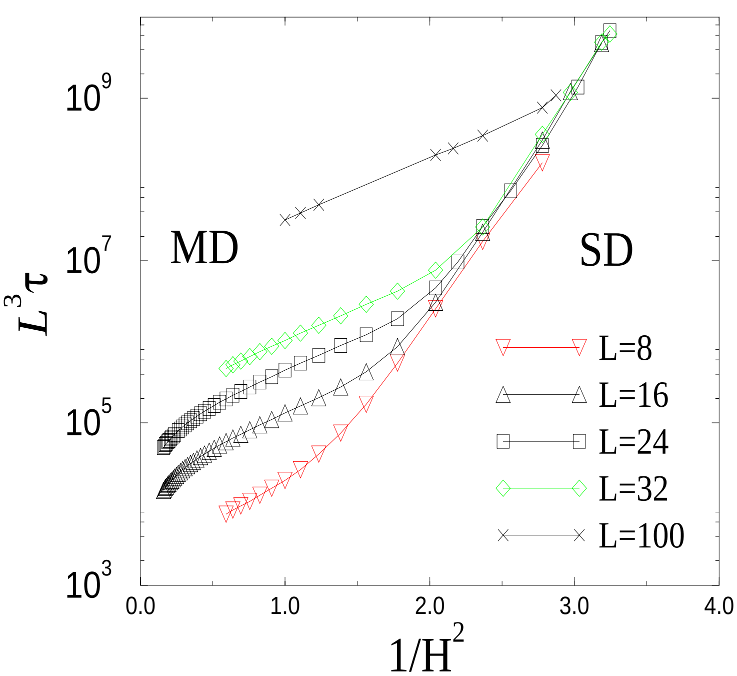
EXCEEDINGLY SLOW CONVERGENCE WITH L !!!

$R_c \approx L$: Thermodynamic Spinodal (THSP)

$$H_{\mathrm{THSP}} \propto \frac{1}{L} \; \frac{(d-1)\sigma_0(T)}{m_{\mathrm{s}}(T)} \; .$$

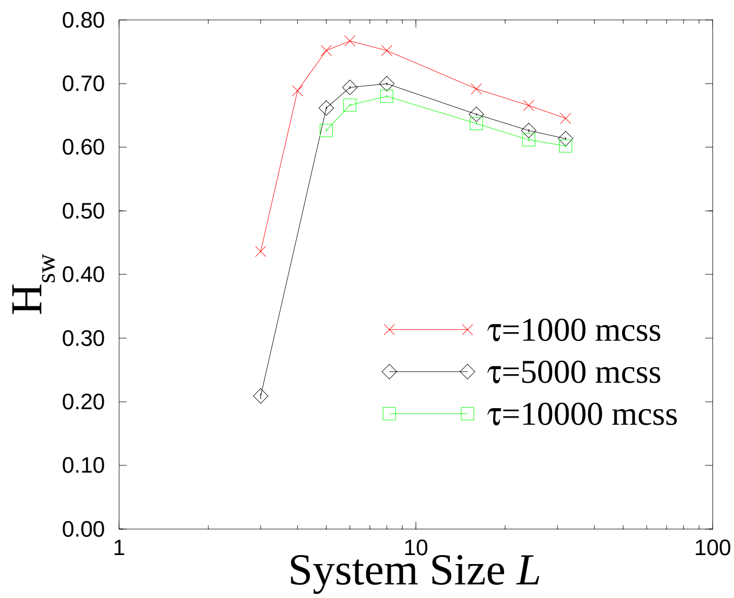
Lifetime data [$d = 3$, $T = 0.6T_c$]



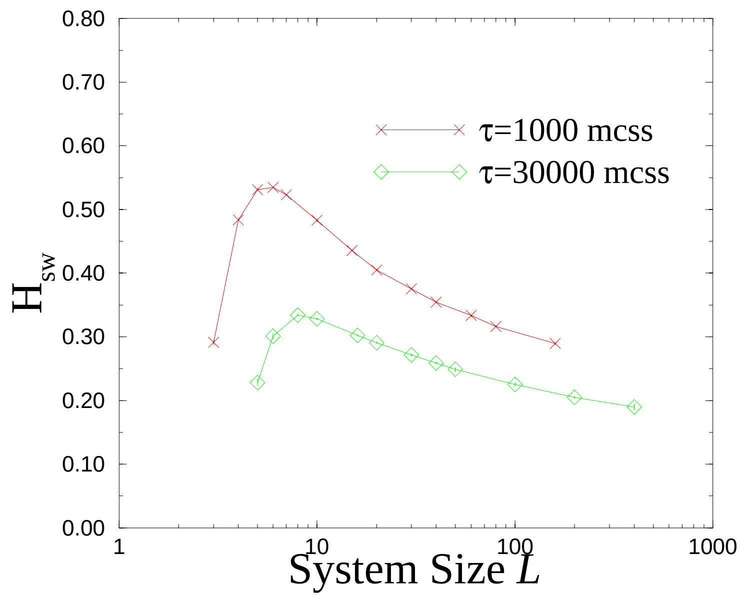


Switching Field

3D Cubic, $T = 0.6T_c$



2D Square, $T = 0.57T_c$



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.

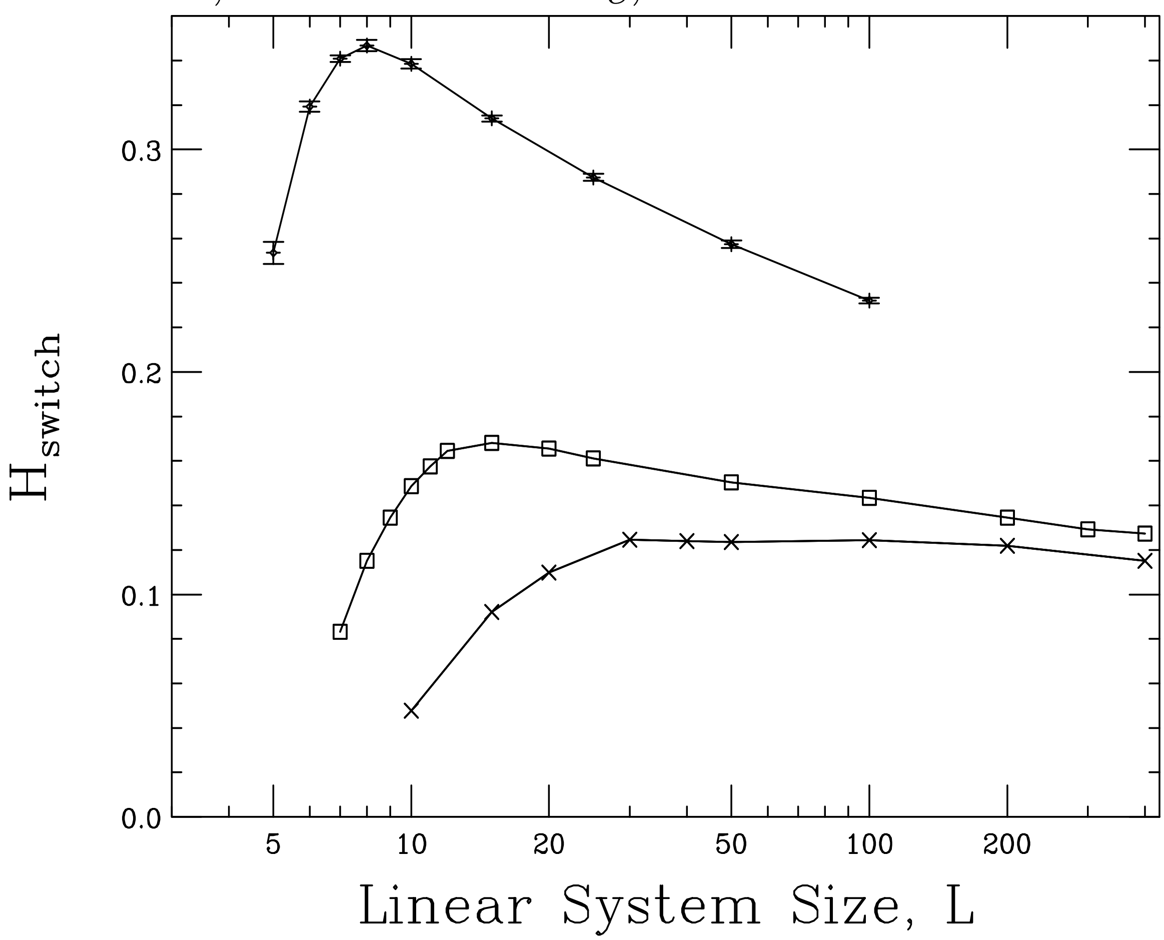
These lead to *quantitative*, but in general little *qualitative*, change. In the next few slides I will show some examples.

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



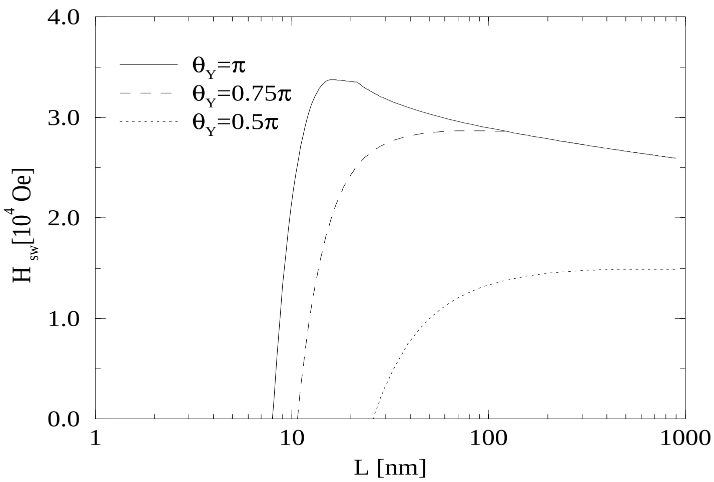
Example with "physical" numbers

Lattice constant: 3 nm.

$J = 1.42 \times 10^{-2}$ eV $\Rightarrow$ 300 K $\approx 0.8 T_c$.

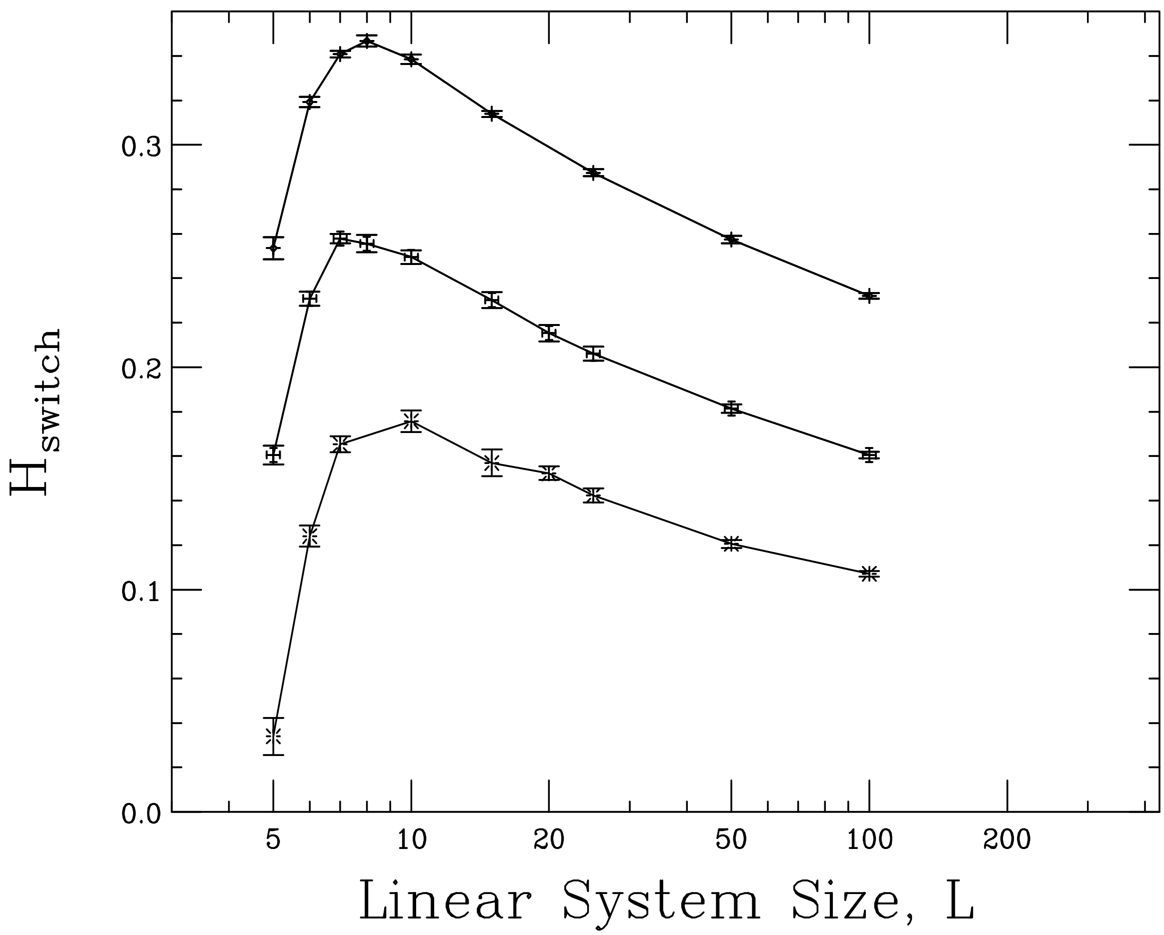
Spin magnetic moment: $\mu_\mathrm{B} = 5.788 \times 10^{-5}$ eV/T.

Waiting time: 10^{13} MCSS $\Leftrightarrow$ order of seconds.



Different Amounts of Bond Disorder

d=2, T=1.3J, τ=30000 MCSS



Effect of demagnetizing field

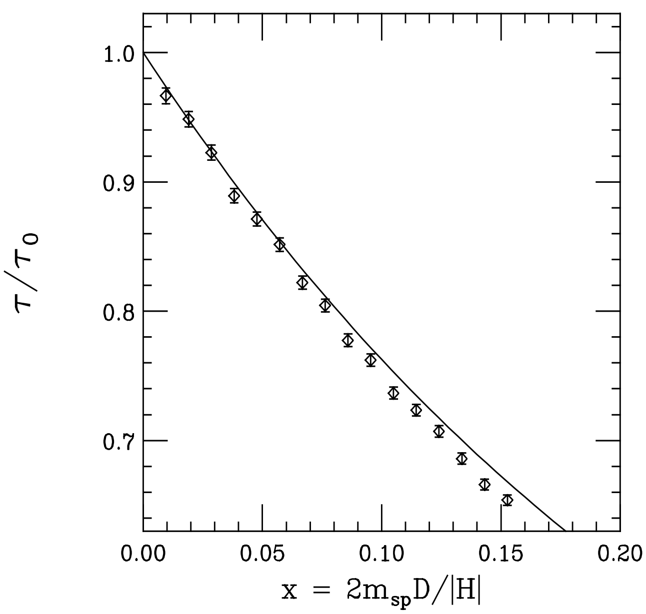
Modified Hamiltonian:

$$\mathcal{H} = -J \sum_{\langle i,j \rangle} s_i s_j - H \sum_i s_i + NDm^2$$

d=2, T=0.8T_c

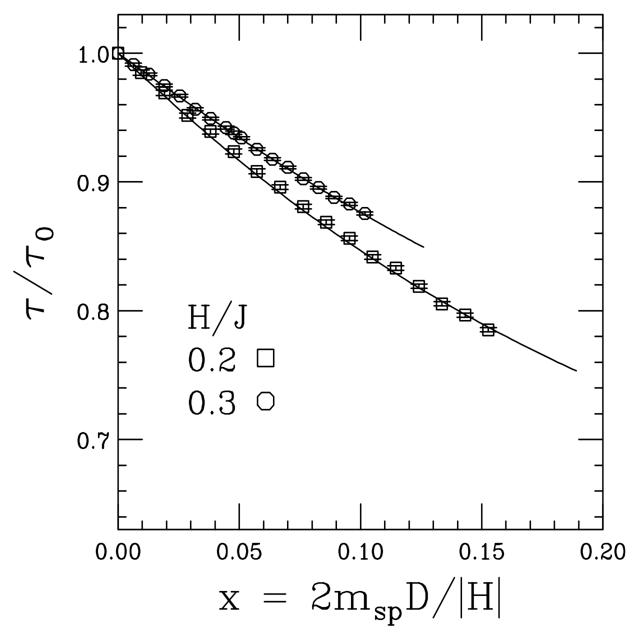
Single-droplet:

$H = 0.2J$, $L = 10$

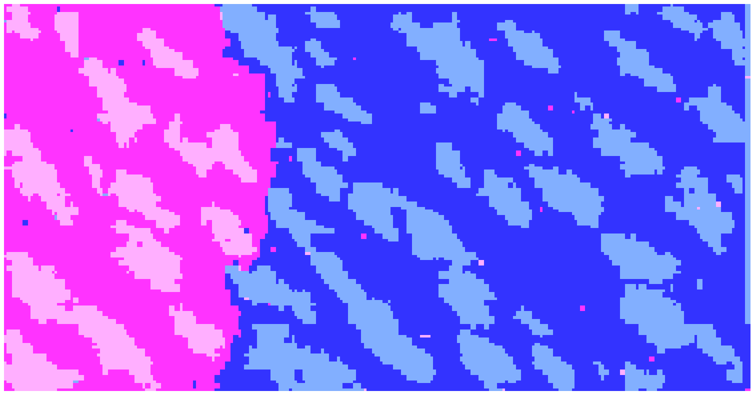


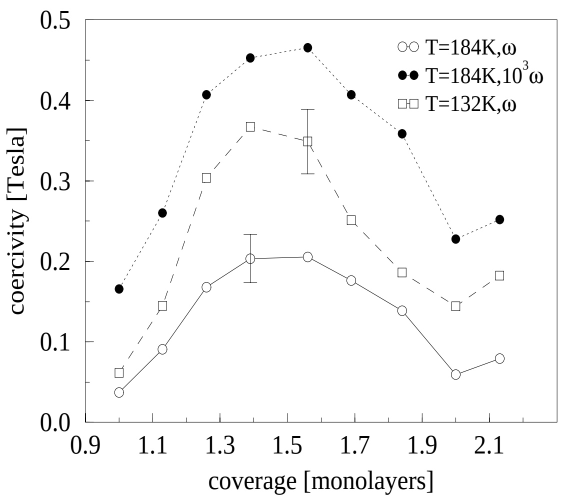
Multi-droplet:

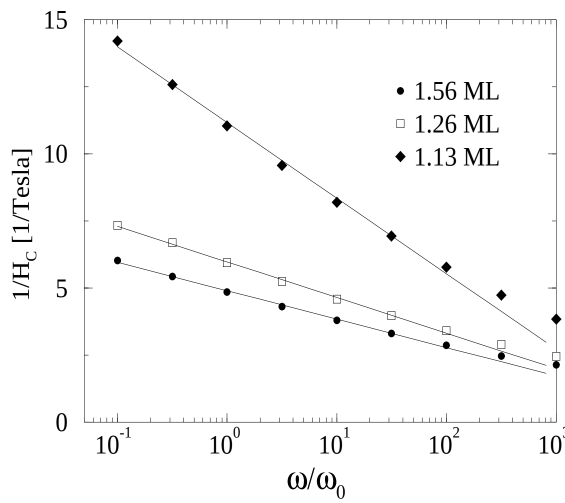
$L = 100$



Coercivity of Fe Sesquilayers on W(110)







CONCLUSIONS

- Simulations of kinetic Ising model predict behavior of single-domain uniaxial particles.
- Switching behavior is analyzed with droplet theory
  - Coexistence Region: $L < R_{\mathrm{c}}$
  - Single-Droplet Region: $R_{\mathrm{c}} \ll L \ll R_0$
  - Multi-Droplet Region: $R_0 \ll L$
- Single-domain particles can have a maximum in H_{switch} vs. L, corresponding to $R_c \approx L$
- Modifications to increase realism mostly do not change the qualitative behavior