Nucleation Theory of Switching in Magnetic Nanoparticles and Ultrathin Films

P.A. Rikvold and M.A. Novotny
Florida State University, Tallahassee, FL, USA

with

G. Brown, M. Kolesik, G. Korniss,
P.-A. Lindgård, H.L. Richards, S.W. Sides,
D.M. Townsley, C.J. White

Supported by US NSF, US DOE, and
Florida State University

http://www.scri.fsu.edu/materials/matsci-mag.html

Why interesting?

Nanometer-sized particles of highly anisotropic ferromagnets

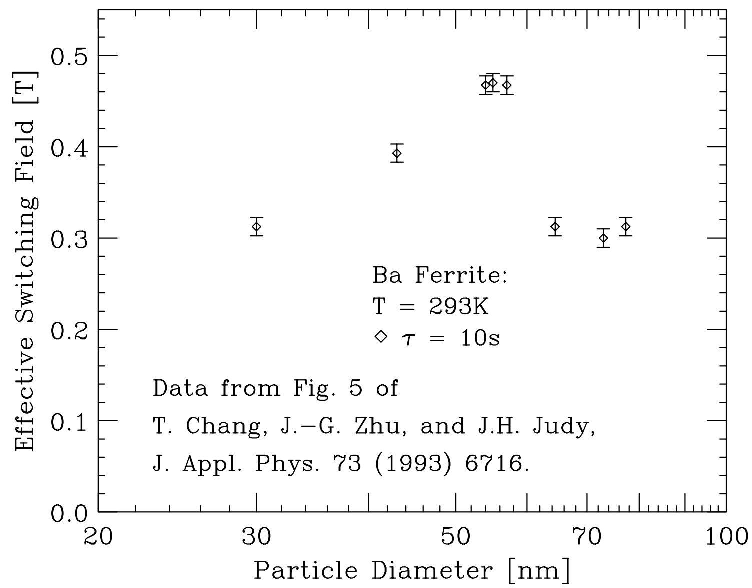
- are hot candidate materials for magnetic recording media.
- have only recently become individually observable by methods such as Magnetic Force Microscopy (MFM).
- should be single domain in equilibrium.

Why nucleation theory?

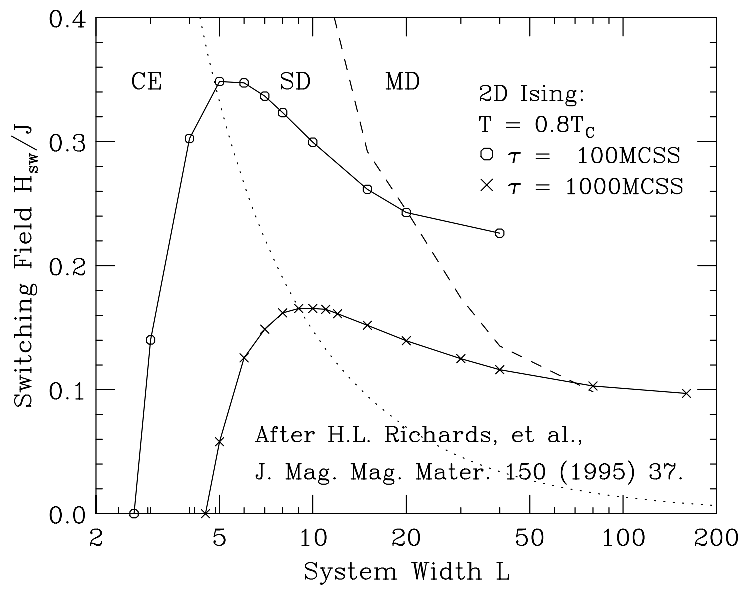
- Provides nonuniform switching mechanism for single-domain particles.

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:

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

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 $s_i \to -s_i$

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

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

Some 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

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

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

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

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

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

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.

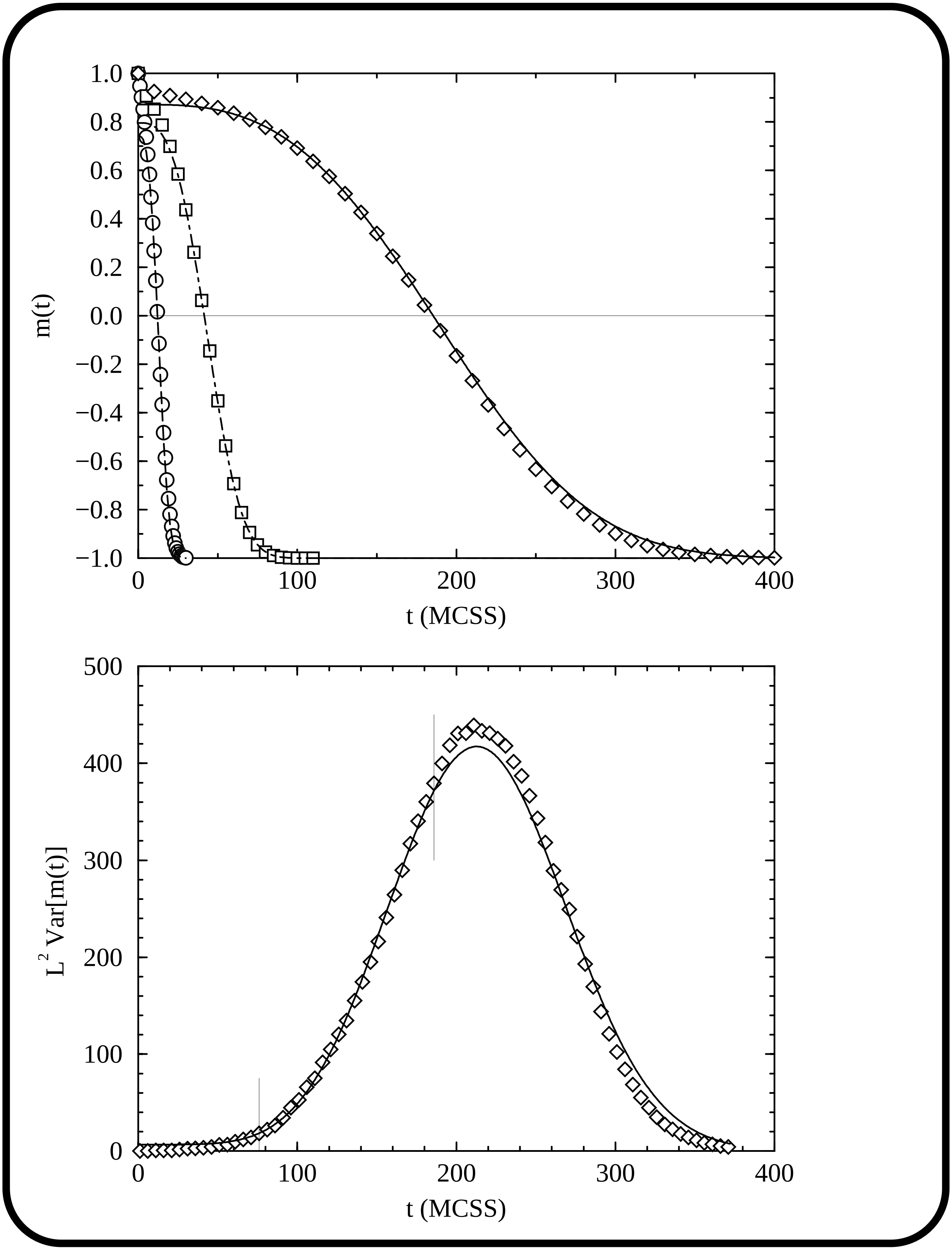
Large supercritical droplets grow at constant velocity v (Lifshitz-Allen-Cahn approximation):

$$v \propto |H|$$

Time evolution of magnetization
(randomly placed, freely overlapping droplets):

$$\begin{aligned} m(t) &\approx m_{\rm s}(T)\left\{2\exp\left[-\Gamma\int_0^t \Omega_d (vs)^d \mathrm{d}s\right]-1\right\} \\ &= m_{\rm s}(T)\left\{2\exp\left[-\frac{\Omega_d}{d+1}\left(\frac{t}{\tau}\right)^{d+1}\right]-1\right\} \end{aligned}$$

$\tau = (v^d\Gamma)^{-\frac{1}{d+1}}$ is average metastable lifetime.


1.0
0.8
0.6
0.4
0.2
0.0
−0.2
−0.4
−0.6
−0.8
−1.0
m(t)
0
100
200
300
400
t (MCSS)
500
400
300
200
100
0
L² Var[m(t)]
0
100
200
300
400
t (MCSS)

With τ is associated the

characteristic distance of free growth:

$$R_0 = v\tau$$

Recall nucleation rate:

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

Using this, we have:

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

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, $L \gg R_0 \gg R_c$

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

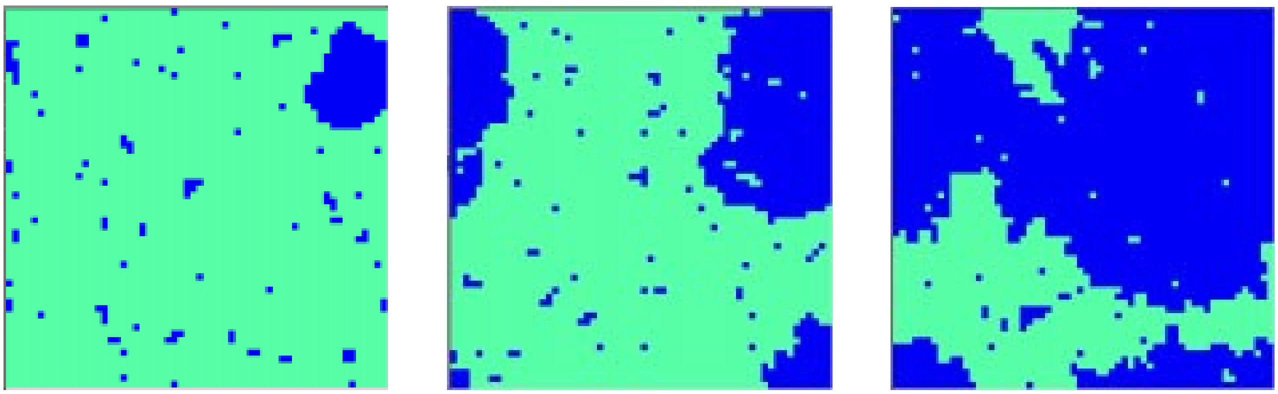
Single-droplet regime, $R_0 \gg L \gg R_c$

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

Coexistence regime, $R_c > L$

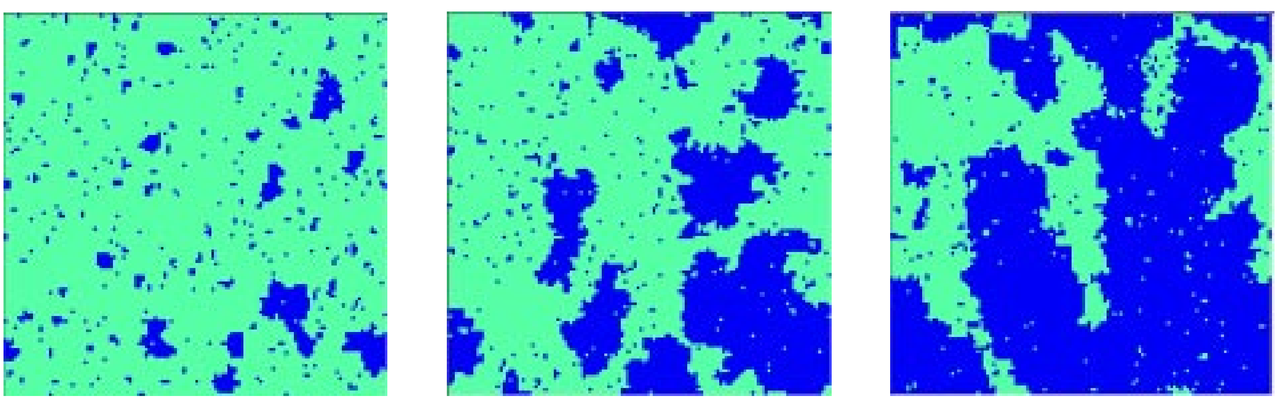
$$\tau \approx \exp\left[const \cdot L^{d-1}\right]$$

SD and MD decay snapshots



$t \ll \tau$ $t \approx \tau/2$ $t \approx \tau$

SD decay



$t \ll \tau$ $t \approx \tau/2$ $t \approx \tau$

MD decay

Crossover fields

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

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

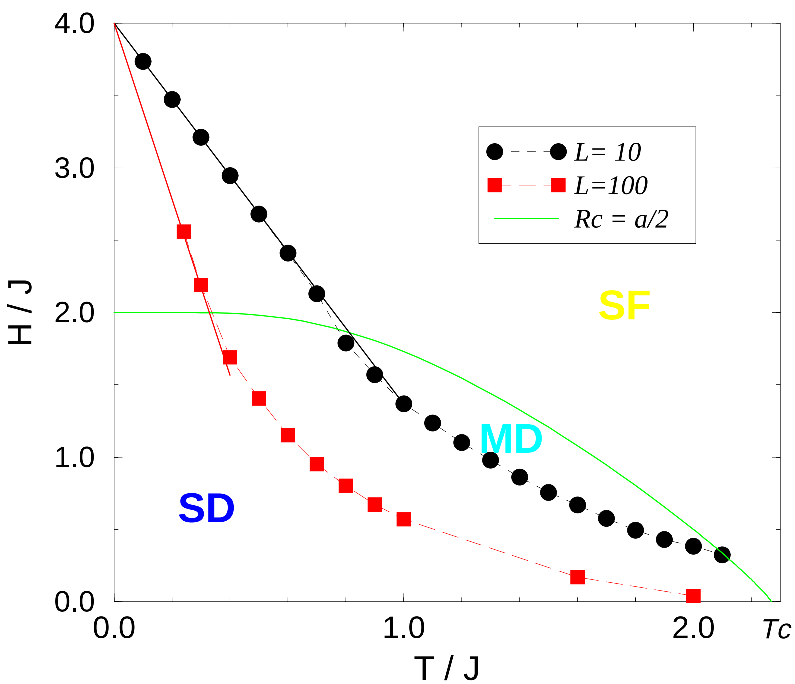
EXCEEDINGLY SLOW CONVERGENCE WITH L !!!

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

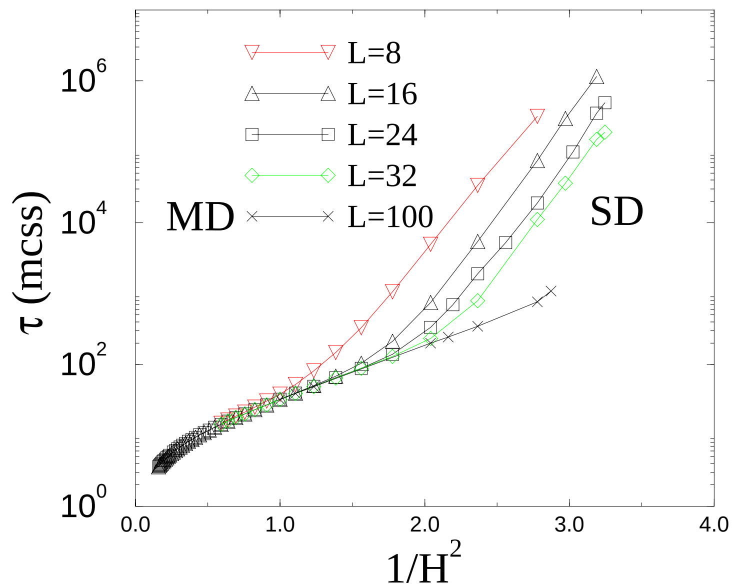
$$H_{\rm THSP} \propto \frac{1}{L} \, \frac{(d-1)\sigma_0(T)}{m_{\rm s}(T)} \, .$$

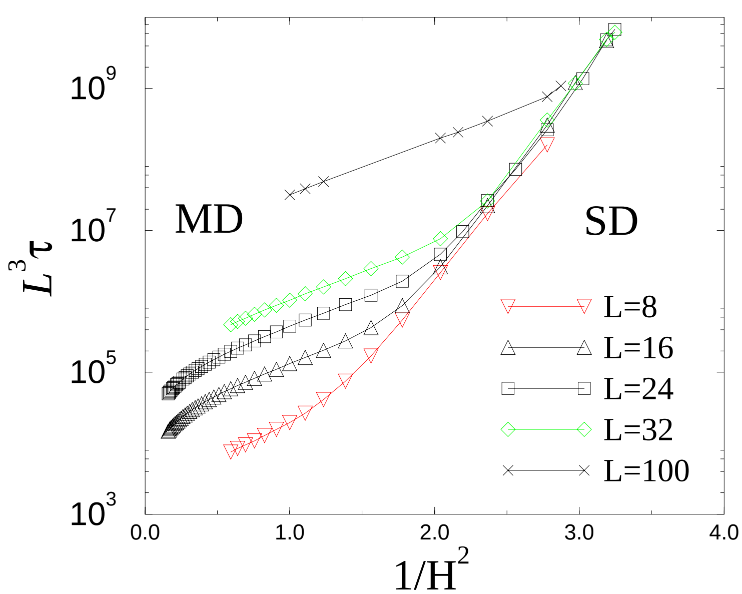
‘Cross-over Phase Diagram’

- 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 $r = \frac{1}{2}$
  - High H, $\quad H_{DSP} = 4 - T\left[\frac{3}{2}\ln(L) - 0.82\right]$



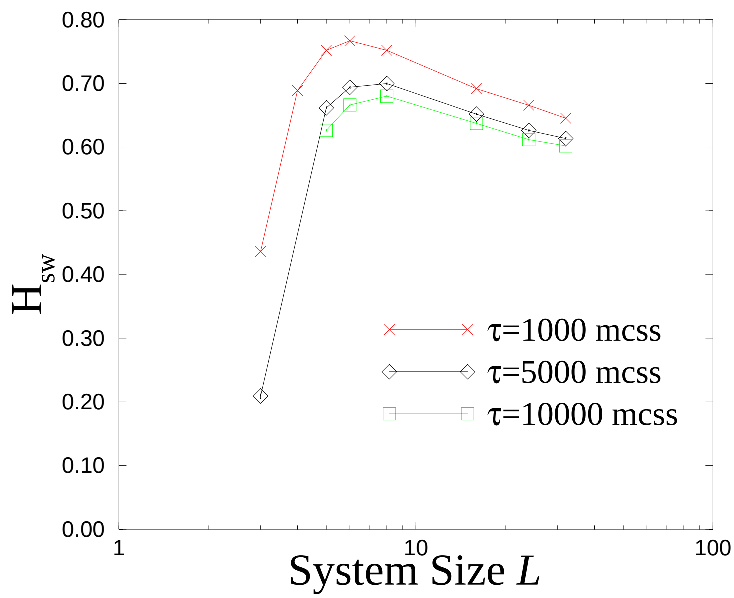
Lifetime data [$d = 3$, $T = 0.6T_c$]



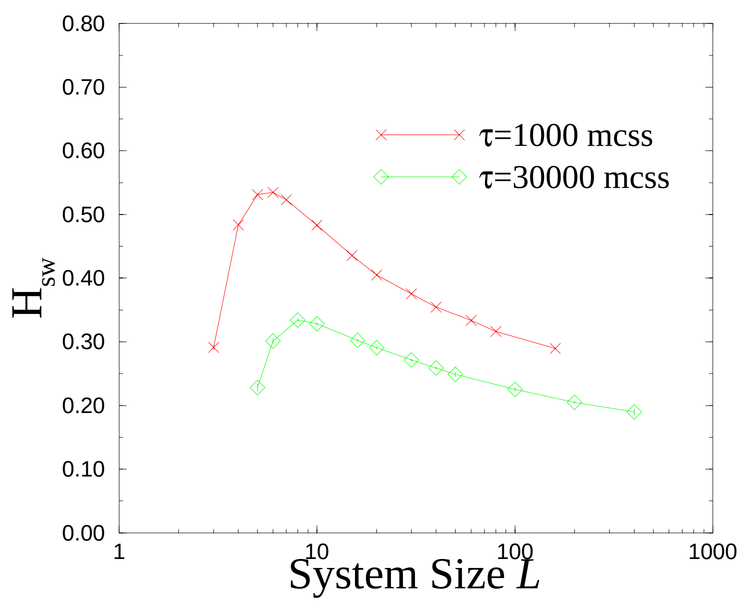


Switching Field

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.

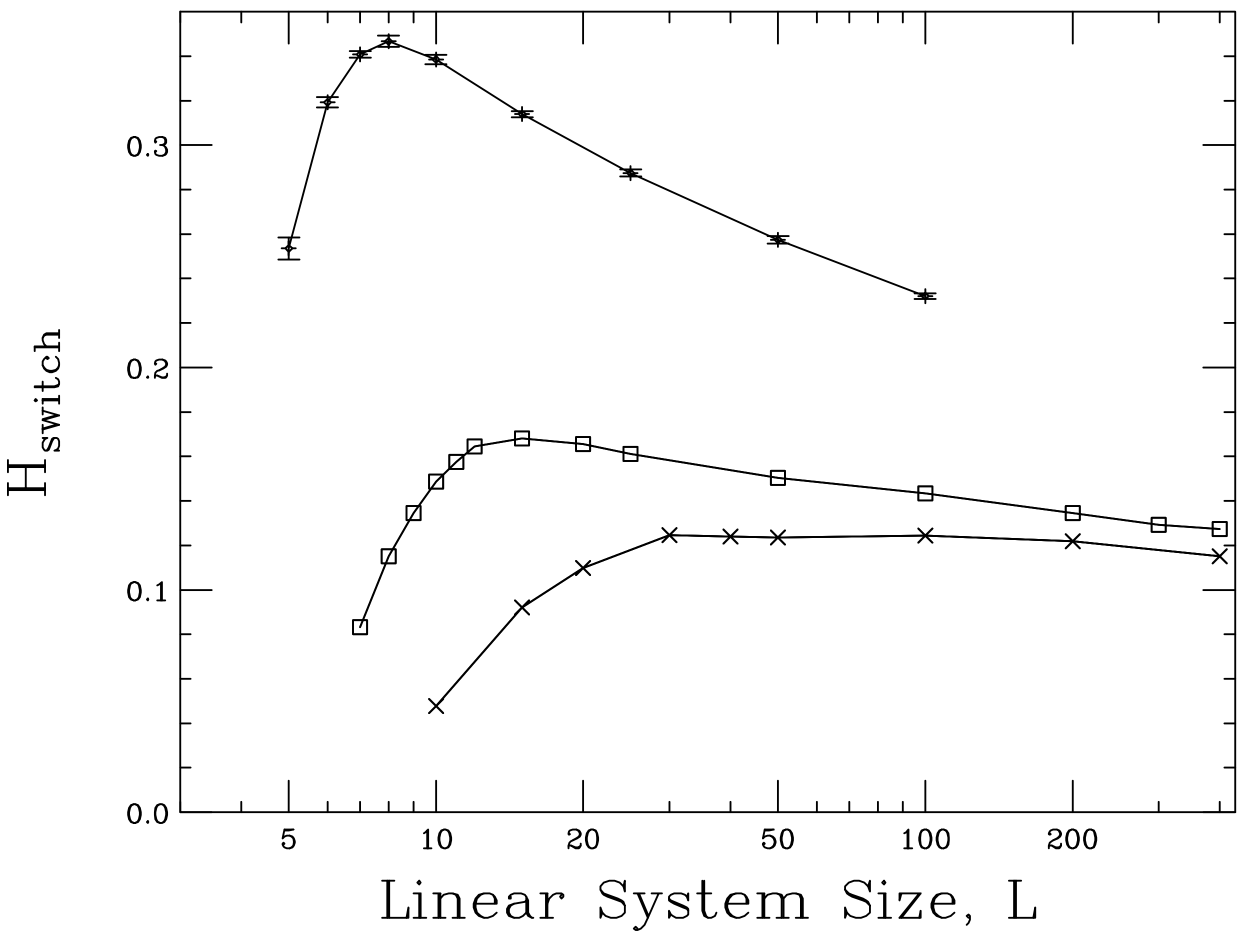
These lead to *quantitative*, but in general little *qualitative*, change. In the next few slides I will show some examples.

Different Boundary Conditions

Modified Hamiltonian with boundary interactions and fields:

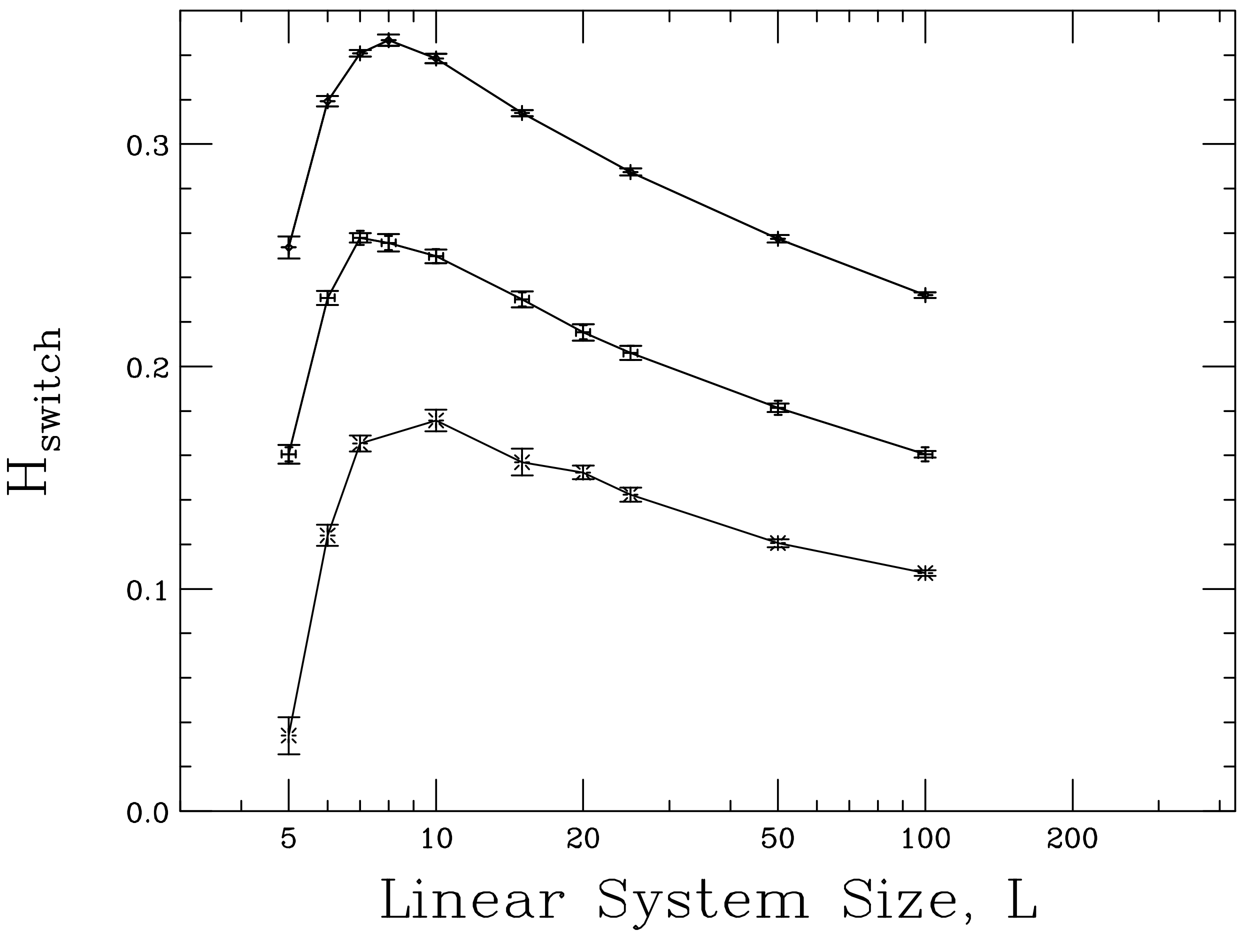
$$\mathcal{H} = -J \sum_{\langle i,j \rangle} s_i s_j - H \sum_i s_i - J_\Sigma \sum_{\langle i,j \rangle_\Sigma} s_i s_j - H_\Sigma \sum_{i_\Sigma} s_i$$

d=2, T=1.3J≈0.57T_c, τ=30000 MCSS



Different Amounts of Bond Disorder

***d*=2, *T*=1.3*J*, *τ*=30000 MCSS**



Effect of demagnetizing field

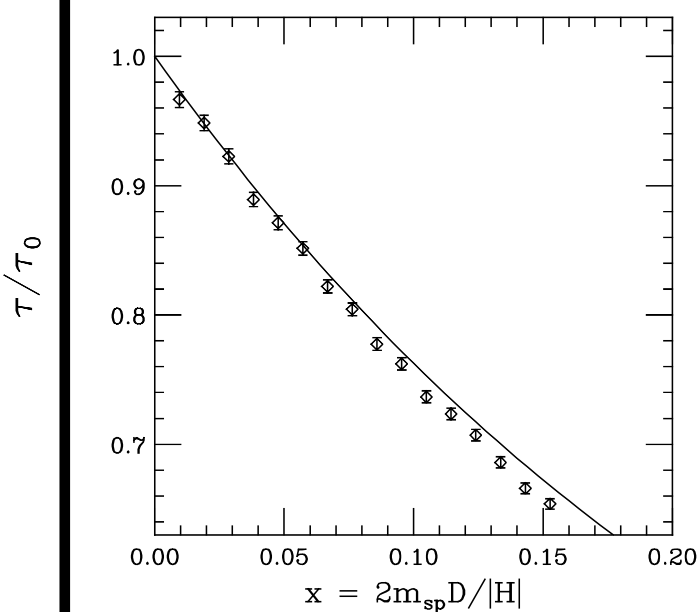
Modified Hamiltonian:

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

d=2, T=0.8T_c

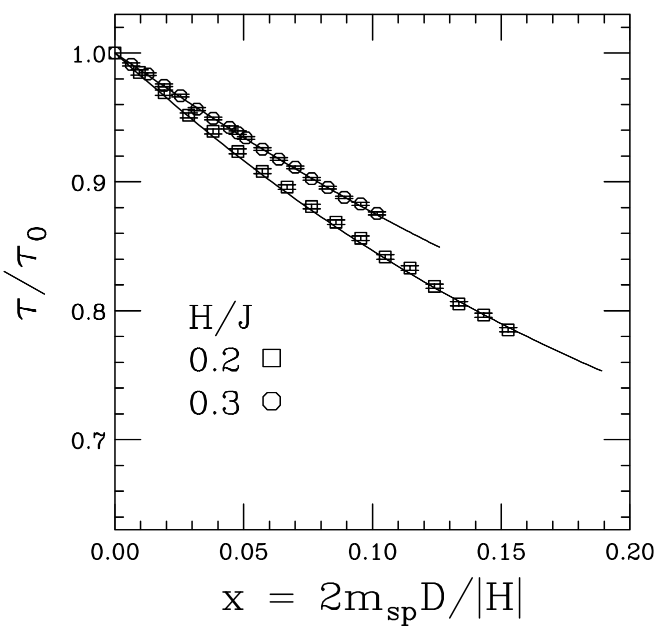
Single-droplet:

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

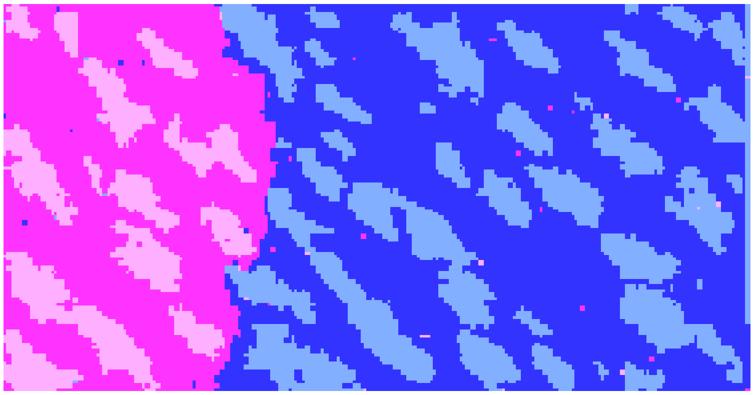


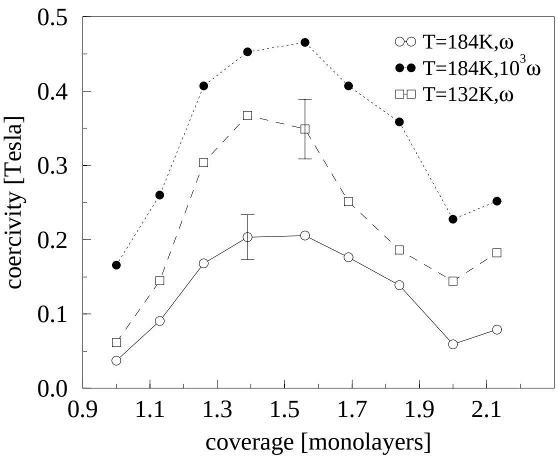
Multi-droplet:

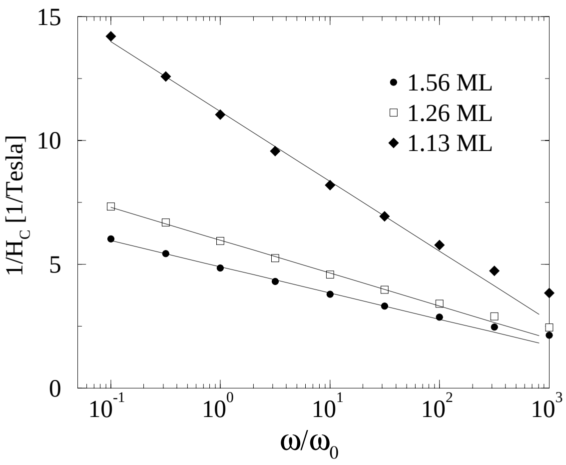
$L = 100$



Coercivity of Fe Sesquilayers on W(110)







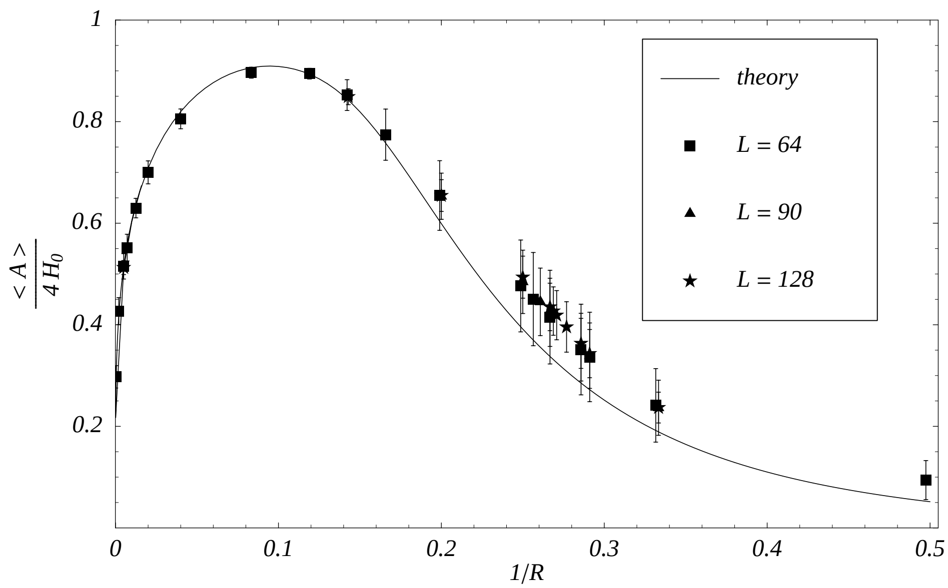
Hysteresis

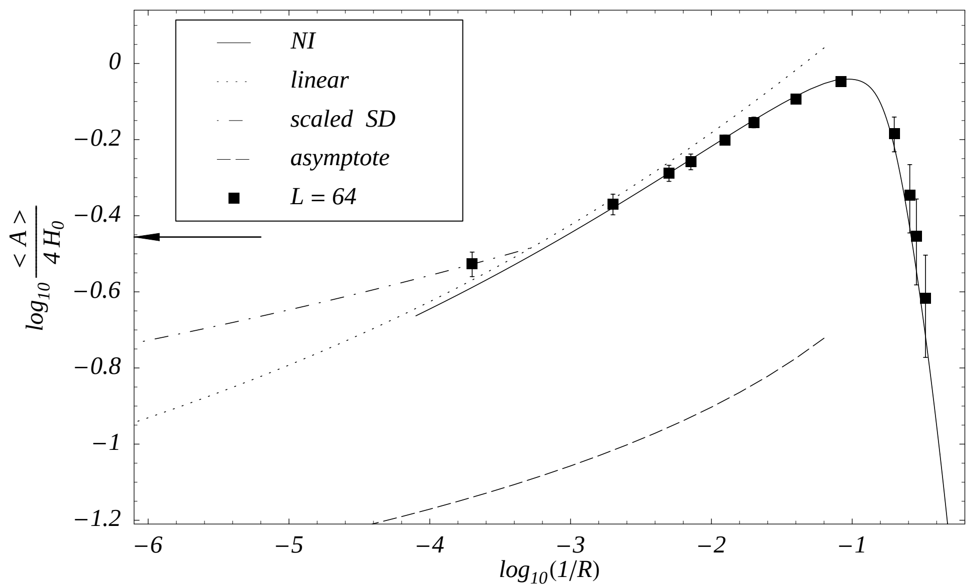
Apply oscillating magnetic field:

$$H(t) = H_0 \sin(\omega t)$$

- Loop area $A = -\oint m \, \mathrm{d}H$ important
  - Energy dissipation per cycle
  - Electric transformers and motors, ...
  - Engineering interest for more than a century:
    Ewing 1881; Warburg 1881;
    Steinmetz 1892
  - Frequency dependence: $A \propto H_0^a \omega^b$??
  - Frequency dependence:
    $A = A_0 + const.[\omega^2(H_0^2 - H_{\mathrm{sp}}^2)]^{1/3}$??
  - Frequency dependence: $A \propto -\ln(H_0\omega)$??

Average loop area





Slow crossover to $A = -\log(const. \times H_0 \omega)$!

CONCLUSIONS

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

Some relevant publications

- Metastable decay and nucleation theory
  - "Recent Results on the Decay of Metastable Phases." P. A. Rikvold and B. M. Gorman. In *Annual Reviews of Computational Physics I*, edited by D. Stauffer (World Scientific, Singapore, 1994), pp. 149–191.
  - "Metastable Lifetimes in a Kinetic Ising Model: Dependence on Field and System Size." P. A. Rikvold, H. Tomita, S. Miyashita, and S. W. Sides. *Phys. Rev. E* **49**, 5080–5090 (1994).
  - "Test of the Kolmogorov-Johnson-Mehl-Avrami Picture of Metastable Decay in a Model with Microscopic Dynamics." R. A. Ramos, P. A. Rikvold, and M. A. Novotny. *Phys. Rev. B* **59**, 9053–9069 (1999).
- Applications to magnetization switching
  - "Magnetization Switching in Nanoscale Ferromagnetic Grains: Description by a Kinetic Ising Model." H. L. Richards, S. W. Sides, M. A. Novotny, and P. A. Rikvold, *J. Magn. Magn. Mater.* **150**, 37–50 (1995).

- "Analytical and Computational Study of Magnetization Switching in Kinetic Ising Systems with Demagnetizing Fields." H. L. Richards, P. A. Rikvold, and M. A. Novotny, *Phys. Rev. B* **54**, 4113–4127 (1996).
- "Magnetization Switching in Nanoscale Ferromagnetic Grains: Simulations with Heterogeneous Nucleation." M. Kolesik, H. L. Richards, M. A. Novotny, P. A. Rikvold, and P.-A. Lindgård. *J. Appl. Phys.* **81**, 5600–5602 (1997).
- "Effects of Boundary Conditions on Magnetization Switching in Kinetic Ising Models of Nanoscale Ferromagnets." H. L. Richards, M. Kolesik, P.-A. Lindgård, M. A. Novotny, and P. A. Rikvold, *Phys. Rev. B* **55** 11521–11540 (1997).
- "Monte Carlo Simulation of Magnetization Reversal in Fe Sesquilayers on W(110)." M. Kolesik, M. A. Novotny, and P. A. Rikvold, *Phys. Rev. B* **56**, 11791–11796 (1997).
- "Nucleation Theory of Magnetization Switching in Nanoscale Ferromagnets." P. A. Rikvold, M. A. Novotny, M. Kolesik, and H. L. Richards. In *Dynamical Properties of Unconventional Magnetic Systems*, edited by A. T. Skjeltorp and D. Sherrington. (Kluwer, Dordrecht, 1998), pp. 307–316.

- Hysteresis
  - "Stochastic Hysteresis and Resonance in a Kinetic Ising System." S. W. Sides, P. A. Rikvold and M. A. Novotny. *Phys. Rev. E* **57**, 6512–6533 (1998).
  - "Kinetic Ising Model in an Oscillating Field: Finite-Size Scaling at the Dynamic Phase Transition." S. W. Sides, P. A. Rikvold, and M. A. Novotny. *Phys. Rev. Lett.* **81**, 834–837 (1998).
  - "Kinetic Ising Model in an Oscillating Field: Avrami Theory for the Hysteretic Response and Finite-Size Scaling for the Dynamic Phase Transition." S. W. Sides, P. A. Rikvold and M. A. Novotny. *Phys. Rev. E* **59**, 2710–2729 (1999).
  - "Dynamic Phase Transition and Hysteresis in Kinetic Ising Models." P. A. Rikvold, G. Korniss, C. J. White, M. A. Novotny, and S. W. Sides. In *Computer Simulation Studies in Condensed Matter Physics XII*, edited by D. P. Landau, S. P. Lewis, and H. B. Schüttler, (Springer, Heidelberg, in press). Preprints FSU-SCRI-99-20 and cond-mat/9904028.