

In performing the simulations, the lattice size of 80×80 spins with periodic boundary conditions on all edges were prepared (where results from larger systems were not significantly different for the considered parameters in this study). Then, the non-magnetic sites with concentration c ranging from 0 to 20 percent were included into the structure. In this way, the normal Ising spins were randomly substituted by the non-magnetic sites. In dilute structure, the Hamiltonian in Eq. (1) still holds but one has to substitute the normal Ising spins from original values ± 1 to 0 for the non-magnetic sites. Next, an initial magnetic configuration was set with all available spins pointing into the up direction (+1). To update the configuration, the single spin flip Metropolis algorithm [4] was used where the spin at site i (s_i) was flipped to its opposite direction with a probability $p = \exp(-\Delta E_i(t)/k_B T)$. The energy difference $\Delta E_i(t) = 2s_i \left[\sum_j s_j(t) + h(t) \right]$ is due to the update at site i and time t . During the simulation, the s_i was flipped (updated) if $\Delta E_i \leq 0$ or a uniform random number $r \in [0,1]$ is less than probability p . The unit time step is defined from one full scan all sites of the Ising lattice, i.e., 1 Monte Carlo step per site (mcs). From the magnetic configuration at time t , after the steady state of the hysteresis loop had been reached, the magnetization per spin at time t was measured i.e. $m(t) = (1/N) \sum_i s_i$ where N is the total number of available Ising. Next, hysteresis loop (m - h relation) was drawn and the loop area $A = \oint m dh$ was calculated to investigate how the area A responds to the amplitude h_0 , the frequency f and the non-magnetic concentration c . In this work, f varied from 0.010 to 1.000 mcs⁻¹, h_0 varied from 2.0 to 5.0 J , and c varied from 0 to 20%. All simulations were done at temperature $T = 2 J/k_B$ which is below the Curie temperature of the two-dimensional Ising model ($T_C \approx 2.269 J/k_B$ [5]) to emphasize the effect of non-magnetic inclusion on ferromagnetic hysteresis.

Results and Discussion

From the results, the response of the magnetic hysteresis to the non-magnetic inclusion is found i.e. Figs. 1 and 2. In Fig. 1, the hysteresis loops for various f at $c = 0\%$, 10% and 20% are presented. At a fixed c , it can be seen that the hysteresis loop has a saturated s -shape and tends to increase in size with increasing f at low frequency region e.g. $f < 0.025$ mcs⁻¹. However, on further increasing f , the loop gets its maximum area and later reduces to an oval-shape with its major axis parallel to the field axis. This is the result of phase-lag between the magnetization and the field signal. At very low f , the field period is large and the magnetic spins have sufficient time to follow the field signal so the phase-lag between the magnetization and the field signal is small and the hysteresis loop looks like a slim s -shape. However, on increasing f , the field sweeps faster and the spin have less time in following the field. Thus, the phase-lag gets larger and so does the hysteresis. At one point, when the phase-lag is approaching π , the hysteresis gets its optimum size. After that, if f is still increasing, the spins feel very difficult in catching with the field so the overall magnetization does not change much as the field changes. Therefore the hysteresis turns its shape in the oval-shape with its major axis lying along the field axis. On the other hand, at a fixed f , on increasing c , the hysteresis loop becomes smaller at low f but larger at high f . This is since for the larger c , there are more non-magnetic sites in the systems which cause smaller magnetic interaction in the whole system. With a weaker magnetic interaction in the system, the phase-lag at π shifts to a higher f for larger c .

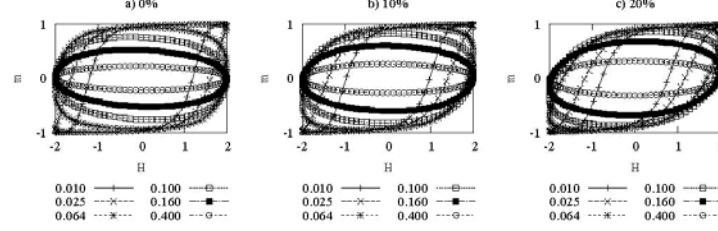


Figure 1. The hysteresis loops of the dilute Ising spins with varying frequency f from 0.010 to 0.400 mcs^{-1} at $T = 2 J/k_B$, $h_0 = 2.0 J$ and the concentration c ranges from a) 0% to b) 10% and c) 20%.

With the hysteresis trend suggested in Fig. 1, the hysteresis area A as a function of h_0 , f and c were calculated. One example is shown in Fig. 2 where it presents several peaks of A (as changing c) as a function of f . At a fixed c , A gets increasing at low f but reducing at high f . This is consistent with the hysteresis results in Fig. 1 where frequency at the peak (f_0) corresponds to the phase-lag at π . This f_0 shifts to higher f as increasing the concentration c due to the weaker magnetic interaction. Notice that, at a fixed f and on increasing c , A reduces for low f but increases for high f .

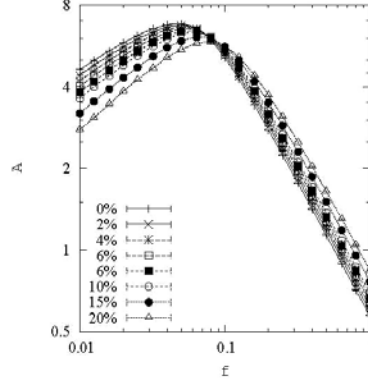


Figure 2. Hysteresis area A of the dilute Ising spins as a function of field frequency f at $T = 2 J/k_B$ and $h_0 = 2 J$ for various concentration c .

It is also of interest to consider the scaling of the area A to analytically investigate how it relates with f , h_0 and c . Therefore, the scaling relation in a power law form

$$A \propto f^\alpha h_0^\beta (1-c)^\gamma, \quad (2)$$

was considered where α , β and γ are the exponents to scaling. These exponents tell how the dissipation energy (the hysteresis area) relates to the external perturbation. Generally, since the behavior of the area A is very different between the low f and the high f regions. Therefore, in this work, the scaling relation Eq. (2) is considered to fit the hysteresis area obtained from low f and high f regions separately, where the low f region is for $f < 0.025 \text{ mcs}^{-1}$ and the high f region is for $f > 0.250 \text{ mcs}^{-1}$. The results from the fit are listed in Table 1 and quality of the fit is shown in Fig. 3.

Table 1. Exponents obtained from the fit using the scaling relation Eq. (2) and R^2 (R -square) of the corresponding fit for both hysteresis area from both high f and low f regions.

	α	β	γ	R^2
High f	-0.9365	1.638671	-1.34195	0.995763
Low f	0.401094	0.607942	1.743747	0.995841

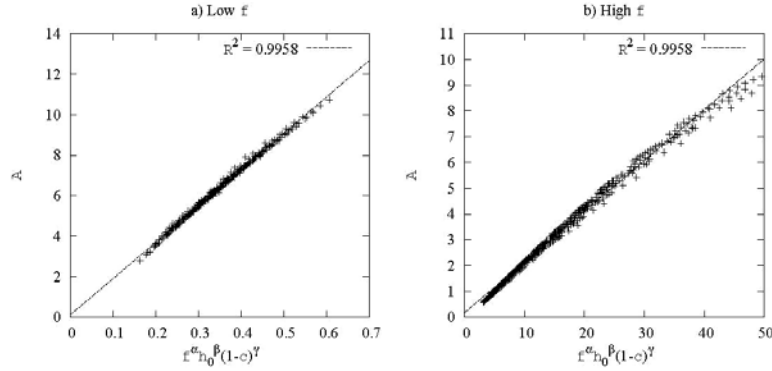


Figure 3. The scaling relation between A and $f^\alpha h_0^\beta (1-c)^\gamma$ based on Eq. (2) using the exponents listed in Table 1. The linear lines and the R^2 to the fits show that scaling relation Eq. (2) is applicable.

Summary

Monte Carlo simulation was performed on the dilute Ising ultra-thin-film to investigate the effect of field parameters and non-magnetic concentrations on hysteresis properties. With increase frequency, the hysteresis loop and its area were found to increase and decrease in low and high frequency regions respectively. Consequently, the area results in peak over frequency domain. On considering the non-magnetic inclusion, the weaker magnetic interaction shifts the low and high frequency boundary to a higher frequency since it is easier for the spins to catch the change in field signal in dilute system. Finally, the empirical scaling relation among the area, field amplitude and frequency and the non-magnetic concentration in a power law form is successfully extracted. Therefore, hysteresis properties under external field perturbation in dilute magnetic ultra-thin-film can be predicted from this scaling relation.

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References

- [1] A. Murayama, K. Hyomi, J. Eickmann and C. M. Falco: Phys. Rev. B Vol. 61 (2000), p. 8984 and references therein.
- [2] M. Plummer, J. van Ek and D. Weller: *The Physics of Ultra-High-Density Magnetic Recording* (Springer, Berlin, 2000).
- [3] M. T. Johnson, P. J. H. Bloemen, F. J. A. den Broeder and J. J. de Vries: Rep. Prog. Phys. Vol. 59 (1996), p. 1409.
- [4] N. Metropolis, A. W. Rosenbluth, M. N. Rosenbluth, A. H. Teller and E. Teller: J. Chem. Phys. Vol 21 (1953), p. 1087.
- [5] B. M. McCoy and T. T. Wu: *The Two-Dimensional Ising Model* (Harvard University Press, Cambridge, MA, 1973).

ภาคผนวก ง.

ต้นฉบับบทความวิชาการที่ส่งเพื่อขอรับการตีพิมพ์เรื่อง

Monte Carlo simulation on thickness dependence of hysteresis properties in
Ising thin-films

โดย

Y. Laosiritaworn

ส่งไปที่

Thin Solid Films (submitted)

Monte Carlo simulation on thickness dependence of hysteresis properties in Ising thin-films

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Abstract

In this work, Monte Carlo simulation was used to model the dynamic hysteresis behavior of ferromagnetic Ising thin-films using the spin-flip algorithm. The purpose is to investigate the thickness dependence of ferromagnetic hysteresis properties while varying frequency and amplitude of the external field. From the results, with increasing the films thickness, the calculated hysteresis properties significantly change due to the stronger ferromagnetic coupling in thicker films. In addition, the universal power law relations among the hysteresis properties, the thickness and the field parameters were found. The scaling exponents were also reported which agree well with a previous experiment on ferromagnetic thin-films.

Keywords: Monte Carlo; Ising thin-films; Hysteresis

1. Introduction

The ferromagnetic thin-films have been a subject of intensive interest due to a broad range of applications especially in recording applications [1]. For instance, one may control the films thickness to obtain the magnetic hysteresis at a right shape to suit desired technological purpose [2]. Therefore, the reasons why physical mechanisms involved in these reduced structures are different from the bulk have become a topic of frequent investigating issues. However, the description of how the hysteresis and their influences on the magnetic properties of ferromagnetic thin-films are affected by the external applied field is not quite well set up due to the underlying complexity of the reduced dimension. For example, multilayered systems are known to change from two- to three-dimensional class with increasing numbers of layers. Magnetic films, however, should belong to a two dimensional universality class owing to the magnetic correlation lengths being constrained by the films thickness. Therefore, this issue highlights the importance of the dimensional pinning to the topic. Nevertheless, as direct observations are quite difficult to obtain, this work models the dynamic magnetic hysteresis behavior using Monte Carlo simulation which is a sophisticate technique for investigating statistical physics problems [3-5].

2. Methodologies

In the study, Ising model was used to investigate the dynamic magnetic properties of the films. This is since the Ising model is known to be a model with an infinite anisotropy along its easy axis direction which is suitable for magnetic thin-films structures [6-9]. This Ising Hamiltonian can be written as

$$H = -J \sum_{\langle i,j \rangle} s_i s_j - h(t) \sum_i s_i . \quad (37)$$

In the equation, the spin $s_i (= \pm 1)$ represents the direction of an Ising spin at site i where its magnetic moment is absorbed into the exchange interaction J . In this work, the exchange interaction J is used as a unit of energy. Therefore, this redefines the unit of the external field as J and unit of temperature as J/k_B . The symbol $\langle i,j \rangle$ denotes that sites i and j appearing in the sum are nearest-neighbor pairs. The external magnetic field takes a sinusoidal form i.e. $h(t) = h_0 \sin(\omega t) = h_0 \sin(2\pi f t)$ where h_0 and f are the field amplitude and frequency respectively.

In preparing the systems, the lattice sizes of $L \times L \times l$ spins were considered with periodic boundary conditions along the in-plane (xy) directions, but free boundary condition along the out-of-plane (z) direction. In this work the films thickness l ranges from 1 to 8 layers and $L = 120$ was considered. Results obtained from larger L (e.g. 240) were not significantly different for the range of parameters used in this study. Next, an initial magnetic configuration was set with all available spins pointing into the up direction (+1). In updating the configuration, the single spin flip algorithm [10] was used where the spin at site i (s_i) was updated (flipped to its opposite direction) with a probability

$$p = \exp(-\Delta E_i(t) / k_B T). \quad (38)$$

The energy difference $\Delta E_i(t) = 2s_i \left[\sum_j s_j(t) + h(t) \right]$ is due to the update at site i and time t . During the simulation, s_i was flipped (updated) if $\Delta E_i \leq 0$ or a uniform random number $r \in [0,1)$ is less than the probability p . The unit time step is defined from one full visit of all Ising spins, i.e. 1 Monte Carlo step per site (mcs). From the magnetic

configuration at time t , after the steady state of the hysteresis loop had been reached, the response magnetization per spin at time t was measured i.e.

$$m(t) = (1/N) \sum_i s_i \quad (39)$$

where N is the total number of Ising spins. Next, hysteresis loop (m - h relation) was drawn and the loop area

$$A = \int m dh, \quad (40)$$

the magnetic coercivity h_c and the remnant magnetization m_r were calculated to investigate how the hysteresis properties respond to the amplitude h_0 , the frequency f and the thickness l , where f ranges from 0.010 to 1.000 mcs⁻¹ and h_0 ranges from 4.0 to 10.0 J . All simulations were performed at temperature $T = 2.0 J/k_B$ which is below the Curie temperatures of all considered films [11] to emphasize the effect of thickness on ferromagnetic hysteresis.

3. Results and Discussions

From the results, the response of the hysteresis loops to external fields for various Ising thin-films were found. For instance, Fig. 1 shows examples of hysteresis loops for various frequencies f at thickness $l = 1, 2$ and 8 layers. At a fixed l , it can be seen that the hysteresis loop has a saturated s -shape and tends to increase in size with increasing f at low frequency region e.g. $f < 0.025$ mcs⁻¹. However, on further increasing f , the loop gets its maximum area and later reduces to an oval-shape with its major axis parallel to the field axis. This is the result of phase-lag between the magnetization and the field signal. At very low f , the field period is large and the magnetic spins have sufficient time to follow the field signal so the phase-lag between the magnetization and the field signals is small and the hysteresis loop looks like a slim s -shape. However, on increasing f , the field

sweeps faster and the spins have less time in following the field. Consequently, the phase-lag gets larger and so does the hysteresis. At one point, when the phase-lag is approaching π , the hysteresis gets its maximum size. After that, if f is still increasing, the spins feel very difficult in following the field so the overall magnetization does not change much as the field changes. Therefore the hysteresis turns its shape in the oval-shape with its major axis lying along the field axis. On the other hand, at a fixed f but on increasing l , the hysteresis loop becomes larger at low f but slightly smaller at high f . This is since for the larger l , there are more neighboring per magnetic-sites in the systems which cause larger magnetic interaction in the whole system. With a stronger magnetic interaction in the system, it becomes more difficult for spins to follow the field, so the phase-lag at π reduces to a lower f for larger l .

Next, the hysteresis area A , the magnetic coercivity h_c and the remnant magnetization m_r as functions of h_0 , f and l were calculated to investigate relations among parameters. An example is shown in Fig. 2 where it presents several peaks of A (as changing l) as a function of f for amplitudes $h_0 = 4.0$ and 10.0 J. At a fixed l , with increasing f , A gets increasing at low f but reducing at high f in good agreement with those observed in experiments [12,13]. This is consistent with the hysteresis results in Fig. 1 where frequency at the peak (f_0) corresponds to the phase-lag at π . This f_0 shifts to lower f as increasing the thickness l due to the stronger magnetic interaction. With a same reason, at a fixed f , A increases (especially at low f) with increasing l .

In addition, in Fig. 2, the area A increases with increasing the field amplitude h_0 and its peak moves to a higher f . This is since the higher amplitude provides higher magnetic energy to the system and this higher energy provides more magnetic force in causing the spins to follow the field. As a result, the frequency at the peak (f_0) shifts to

higher f as the phase-lag between magnetization and field signals is smaller for the higher amplitude.

It is also of interest to consider the scaling of the area A to analytically investigate how it relates with f , h_0 and l . Therefore, the empirical scaling relations in power law forms

$$A \propto h_0^\alpha f^\beta l^\gamma, \quad (5)$$

$$h_c \propto h_0^\alpha f^\beta l^\gamma, \quad (6)$$

$$\text{and } m_r \propto h_0^\alpha f^\beta l^\gamma, \quad (7)$$

were considered where α , β and γ are the exponents to the scaling. These exponents tell how the hysteresis properties relate to the external perturbation and the system geometry. Generally, the behavior of the hysteresis is very different between the low f and the high f regions. Therefore, in this work, the scaling relation Eqs. (5-7) were considered to fit the hysteresis area obtained from low f and high f regions separately, where the low f region is for $f \leq 0.050 \text{ mcs}^{-1}$ and the high f region is for $f \geq 0.250 \text{ mcs}^{-1}$. Results from the fit and their R^2 are listed in Table 1. Note that, exponents for m_r are only presented for the high f as the non-linear fits for low f do not converge. However, as can be seen from Table 1, at low f , the exponents for both A and h_c are somewhat of the same magnitude. Therefore, based on the assumption that $A \propto m_r h_c$, the exponents of m_r should be close to 1. This is in accordance with hysteresis loop results where m_r does not change much with changing the films' thickness and field parameters (e.g. see Fig. 1). On the other hand, for the high f , the assumption $A \propto m_r h_c$ has proved its validity as $\alpha_A \approx \alpha_{h_c} + \alpha_{m_r}$, and so do β and γ . Furthermore, the quality of the fit e.g. $A \propto h_0^\alpha f^\beta l^\gamma$ is shown in Fig. 3 where its good R^2 shows that scaling equations are applicable. Furthermore, there was an experiment on thin Fe/Au (001) films (at low frequencies) which give $\alpha = 0.59 \pm 0.07$ and $\beta = 0.31 \pm 0.05$ [13]

while this study reports $\alpha = 0.543 \pm 0.026$ and $\beta = 0.302 \pm 0.018$. This good agreement (within error bars) confirms the validity of this work and implies its success on modeling ferromagnetic hysteresis in thin-films via Monte Carlo simulation.

4. Summary

In this work, Monte Carlo simulation was used to investigate the dynamic magnetic hysteresis behavior of Ising thin-films using the spin-flip algorithm. As varying the thickness, the frequency and the amplitude of the external field, the dynamic hysteresis was extracted, discussed and compared with previous works. In addition, the empirical power law relations among the hysteresis properties, the films thickness and the field parameters are suggested. Therefore, based on these scaling relations and its agreement with experiments, hysteresis properties under external perturbation can be predicted which provide another successful step in modeling ferromagnetic materials.

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References

- [1] T. Osaka, T. Asahi, J. Kawaji, T. Yokoshima, *Electrochim. Acta* 50 (2005) 4576.
- [2] J-S Suen, M. H. Lee, G. Teeter, J. L. Erskine, *Phys. Rev. B* 59 (1999) 4249.
- [3] M. E. J. Newman, G. T. Barkema, *Monte Carlo Methods in Statistical Physics*, Oxford University Press, Oxford, 1999.
- [4] D.P. Landau, K. Binder, *A Guide to Monte Carlo Simulations in Statistical Physics*, Cambridge University Press, Cambridge, 2000.

- [5] K. Binder, D.W. Heermann, Monte Carlo Simulation in Statistical Physics (4th Edition), Springer-Verlag, Berlin, 2002.
- [6] M. Bander, D.L. Mills, Phys. Rev. B 38 (1988) 12015.
- [7] M. J. Dunlavy, D. Venus, Phys. Rev. B 69 (2004) 094411.
- [8] H. J. Elmers, J. Hauschild, H. Höche, U. Gradmann, H. Bethge, D. Heuer, U. Köhler, Phys. Rev. Lett. 73 (1994) 898.
- [9] K. Binder, P. C. Hohenberg, Phys. Rev. B 9 (1974) 2194.
- [10] N. Metropolis, A.W. Rosenbluth, M.N. Rosenbluth, A.H Teller, E. Teller, J. Chem. Phys. 21 (1953) 1087 .
- [11] Y. Laosiritaworn, J. Poulter, J. B. Staunton, Phys. Rev. B 70 (2004) 104413.
- [12] Q. Jiang, H.-N. Yang, G.-C. Wang, Phys. Rev. B 52 (1995) 14911.
- [13] Y.-L. He, G.-C. Wang, Phys. Rev. Lett. 70 (1993) 2336.

Table 1. Exponents obtained from the fit using the scaling relation Eqs. (5-7) and the R^2 (R -square) of the corresponding fit for hysteresis area A , magnetic coercivity h_c and remnant magnetization m_r for both high f and low f regions. However, exponents for m_r at low f are not available as the fit does not converge.

		α	β	γ	R^2
A	Low f	0.543±0.026	0.302±0.018	0.142±0.005	0.9655
	High f	1.260±0.009	−0.907±0.007	−0.017±0.004	0.9954
h_c	Low f	0.465±0.027	0.303±0.018	0.152±0.005	0.9657
	High f	0.976±0.003	0.021±0.002	0.006±0.001	0.9991
m_r	High f	0.334±0.009	−0.873±0.007	−0.029±0.004	0.9913

Figure 1

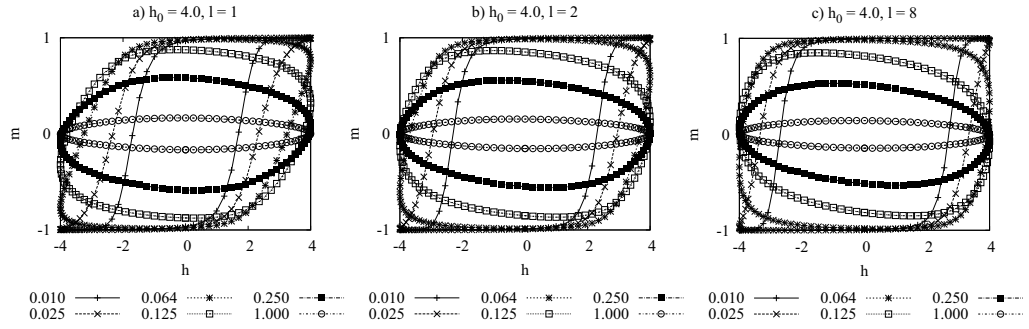


Fig. 1. The hysteresis loops of the Ising films with varying frequency f from 0.010 to 1.000 mcs $^{-1}$ at $T = 2.0 J/k_B$, $h_0 = 4.0 J$ and the thickness l ranges from a) 1 layer to b) 2 layers and c) 8 layers.

Figure 2

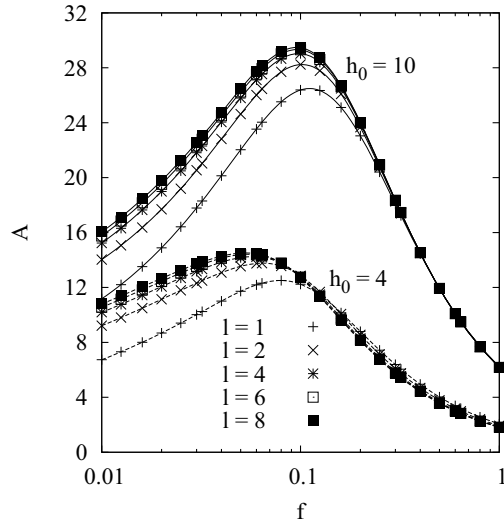


Fig. 2. Hysteresis area A of the Ising films as a function of field frequency f at $T = 2.0$ J/k_B for $h_0 = 2$ and $h_0 = 10 J$.

Figure 3

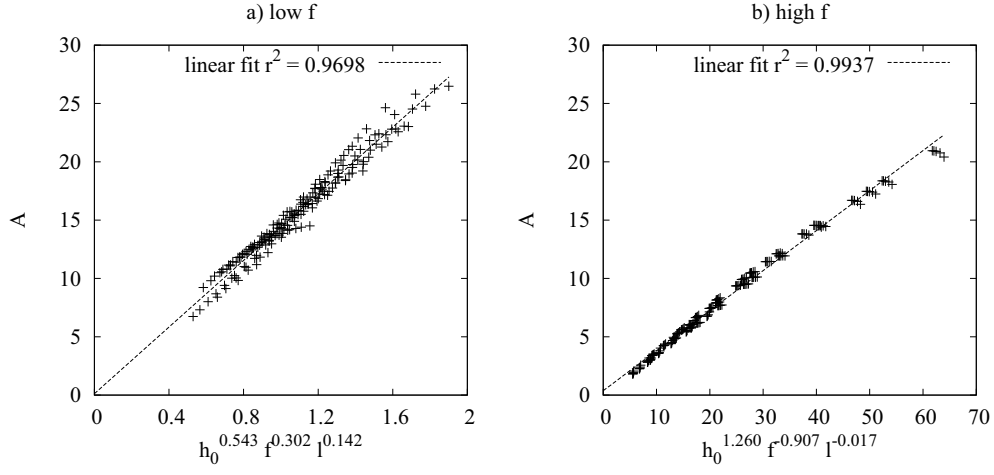


Fig. 3. The scaling relation between A and $h_0^\alpha f^\beta l^\gamma$ based on Eq. (5) using the exponents listed in Table 1. The linear dependence and good R^2 show that the scaling relation is applicable.

ภาคผนวก จ.

เอกสารประกอบงานประชุมวิชาการที่เข้าร่วมเรื่อง

Monte Carlo investigation of hysteresis properties in ferroelectric thin-films under the effect of uniaxial stresses

นำเสนอแบบ Poster presentation

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Monte Carlo Investigation of Stress Dependence Hysteresis Properties in Ferroelectric Thin-Films

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Of a particular interest in ferroelectric ceramics is the technological applicability as ferroelectric memories, in which high areal densities and reduced access time are in demand. Consequently, the understanding of how hysteresis characteristics correspond to material structures and operating environment is important. Nevertheless, theoretical studies are usually performed on ideal stress-free conditions, whereas real materials, especially in thin-films structures, are affected from crystalline anisotropy from mechanical stress, and this may lead to inappropriate application designs. Therefore, the objective of this study is to model such a situation. The uniaxial stress dependence of the ferroelectric hysteresis properties of thin-films is studied via the DIFFOUR model and Monte Carlo simulations. The stress and electric field are applied onto the z direction of the systems. The polarization is measured via the hysteresis dynamic. The preliminary results show hysteresis properties decrease with increasing stresses. The results are in good agreement with previous experimental investigation.

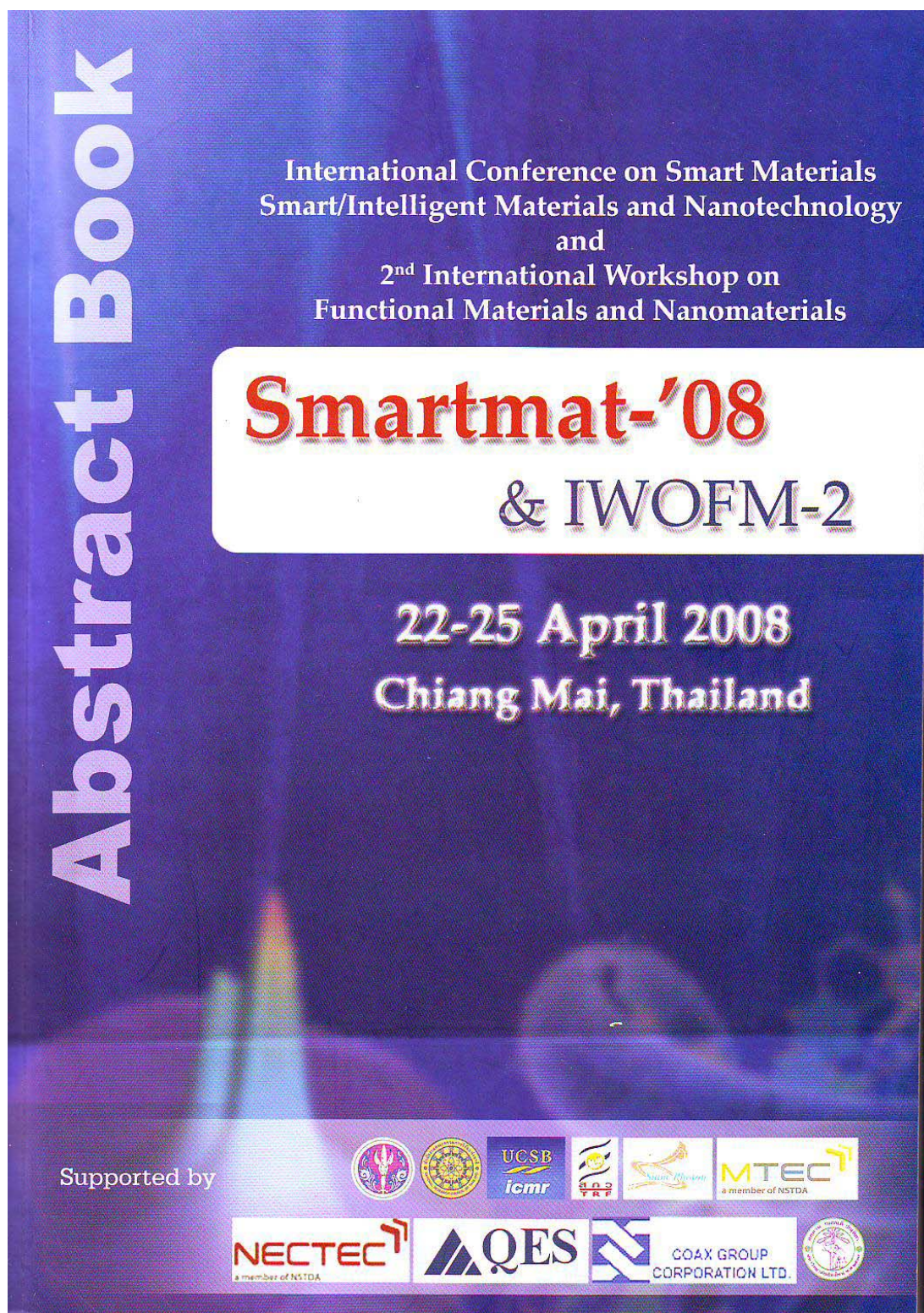
Keywords: C. Ferroelectric properties, Monte Carlo.

ภาคผนวก จ.
เอกสารประกอบงานประชุมวิชาการที่เข้าร่วมเรื่อง

Magnetic hysteresis properties in dilute Ising ultra-thin-film:
Monte Carlo investigation

นำเสนอแบบ Poster presentation
“Smart/Intelligent Materials and Nano Technology 2008 (SmartMat’08)”
22-25 April 2006
Imperial Mae Ping Hotel, Chiang Mai, Thailand.

หน้าแรกของ Abstract Book





Magnetic Hysteretic Properties in Dilute Thin-films: Monte Carlo Investigation

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EP00129

The ferromagnetic thin-films has been a subject of intensive interests and investigations in view of a broad range of applications especially in recording applications featuring from high magnetic anisotropies [1-3]. In addition, in terms of fundamental interests in understanding, that the physical mechanisms involved in those reduced structure systems are quite different from bulk properties has become a topic of frequently investigating issues. For instance, the magnetic hysteresis shape of the system under an applied field in thin-films is thoroughly different from the bulk's at a set of fixed parameters. As a result, one may control the films' thicknesses to obtain the magnetic hysteresis, or the relaxation delay (lag response) between the external magnetic field and the response magnetization, at a right shape which may suit desired technological applications, e.g. transformer and magnetic storage media, fascinating lots of innovative applications [2-3]. However, the description of how the hysteresis and their influence on the magnetic properties of ferromagnetic thin-films are affected by the external applied field is not quite well set up due to the underlying complexity of the micro-structural influences. For examples, in determining the properties of real materials, the importance of defects, especially the vacancy, should not be avoided. This highlights the importance of the anisotropic interface which makes the problem very complicate. Generally, however, direct observations of defect interactions to hysteresis properties are difficult to obtain. One is therefore restricted to computer simulation methods to gain further insight. Consequently, in this study, the dynamic magnetic behavior was modeled in magnetic thin-films simplifying to ultra-thin-film structure. To understand ferromagnetic materials numerically, in this work, the magnetic properties and its dynamic magnetization switching (hysteresis) are investigated by means of Monte Carlo simulations with an inclusion of defects at nano-scale level, e.g. vacant atoms at concentrations ranging from 0 to 20 percents of all available magnetic sites. The model being used is the Ising type, which has been proved to be a useful model for magnetic thin-films [4-7], and the spin-flip algorithm is used to update the magnetic configurations. As varying the vacancy concentrations, temperatures, and the frequencies of the external field, the observables i.e. the magnetization as a function of the magnitude of magnetic field are taken. From the results, it is found that by increasing the vacancy concentration, at a fixed temperature and magnetic field frequency, both the coercivity and the remanence reduces due to the weaker ferromagnetic interaction in the system. Further investigation of how the hysteresis area varies with vacancy concentration is carrying out to extract the scaling relation at fixed temperatures and field parameters.

References:

- [1] A. Murayama, et al., Phys. Rev. B 61 (2000) 8984 and references therein.
- [2] M. Plummer (Ed.), The Physics of Ultra-High-Density Magnetic Recording, Springer, Berlin, 2000.
- [3] M. T. Johnson, P. J. H. Bloemen, F. J. A. den Broeder, and J. J. de Vries, Rep. Prog. Phys. 59, 1409 (1996).
- [4] M. Bander and D. L. Mills, Phys. Rev. B 38, 12 015 (1988).
- [5] K. Binder and P. C. Hohenberg, Phys. Rev. B 9, 2194 (1974).
- [6] H. J. Elmers, J. Hauschild, H. Hache, U. Gradmann, H. Bethge, D. Heuer, and U. Kähler, Phys. Rev. Lett. 73, 898 (1994).
- [7] Y. Li and K. Baberschke, Phys. Rev. Lett. 68, 1208 (1992).

โปสเตอร์ที่น่าสนใจ



Magnetic hysteretic properties in dilute thin-films: Monte Carlo investigation

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Abstract

Monte Carlo simulation was used to observe the magnetic behavior of Ising spins in dilute ultra-thin-filmed structure. The magnetic hysteresis properties are investigated as varying the non-magnetic-site concentration, specifying the magnitude of dilution, and both magnetic field frequencies and amplitudes close to phase transition region where the single spin flip Metropolis algorithm is used. From the results, at a fixed temperature and field amplitude, the hysteresis tends to increase in shape with increasing frequency at low frequency region but reduce at high frequency region due to the increase of the phase-lag. However, when non-magnetic inclusion is taken into account, the phase-lag tends to shift to higher frequency as a result of weaker magnetic interaction. In addition, the scaling relation among the hysteresis area, the field parameters and dilution concentration is proposed in providing general information of how hysteresis behavior responses to external field in dilute magnetic ultra-thin-film.

Introduction

- The response of a magnetic system under an external field leads to many novel physical phenomena with intriguing physics and important technical applications [1-3]
- Most studies concentrated on ideal structure whereas how external perturbation (field amplitude h_0 and frequency f) affects the dynamic hysteresis properties in dilute magnet (magnetic material with non-magnetic atoms inclusion) is less understood.
- In this work, the dynamic behavior of the hysteresis loops in dilute magnetic ultra-thin-film is investigated with vary amplitude h_0 , frequency f and non-magnetic concentration c .

Methodology

- In this study, Monte Carlo simulation was used to investigate the hysteresis properties of the Ising model with Hamiltonian

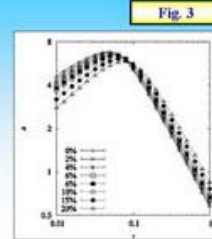
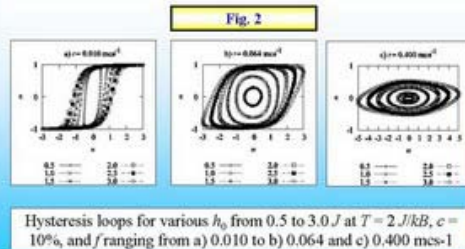
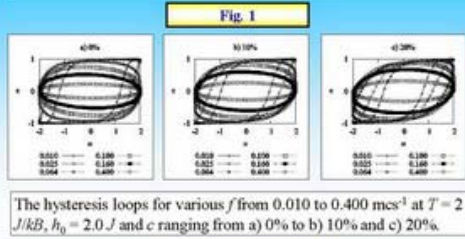
$$H = -J \sum_{\langle i,j \rangle} s_i s_j - h(t) \sum_i s_i$$

where J is the exchange interaction, $s_i (= \pm 1, 0)$ represents the Ising or non-magnetic spins at site i and $h(t)$ is the magnetic field.

- The Ising system in an external magnetic field was updated using single spin flip Metropolis algorithm [4] with varying f from 0.01 to 1.00 mcs^{-1} , h_0 from 0.5 to 5.0 J , and c from 0 to 20% at $T = 2.00 J/k_B$.
- In addition, the scaling form of how hysteresis loop area A relates to f, h_0 and $(1-c)$ is considered in the power law form i.e.

$$A \propto f^\alpha h_0^\beta (1-c)^\gamma$$

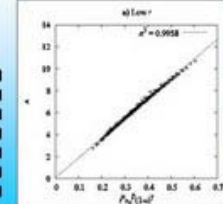
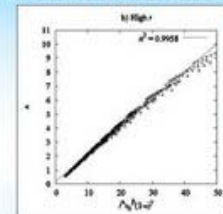
Results



The scaling relation $A \propto f^\alpha h_0^\beta (1-c)^\gamma$ using the exponents listed in Table 1.

Table 1

	α	β	γ	R^2
High f	-0.937	1.639	-1.342	0.996
Low f	0.401	0.608	1.744	0.996



Discussions and Conclusions

- With increasing f , the hysteresis loop increases at low f ($f < 0.025 \text{ mcs}^{-1}$) but decrease at high f ($f > 0.25 \text{ mcs}^{-1}$) due to the increase of phase-lag between magnetization and magnetic field signal (Fig. 1). On the other hand, with increasing h_0 , the saturated hysteresis tends to stabilize due to stronger magnetic driving force.
- With increasing c , at a fixed f , the hysteresis loop decreases at low f but increases at high f due to the weaker magnetic interaction. As a result, the frequency at the maximum area A (f_0) in Fig. 3 shifts to a higher frequency while reduces in magnitude.
- On performing scaling relation between area A and other parameters in a power law form, the exponents to the scaling are extracted with good R^2 . This indirectly tells how dissipation energy scales material density and field parameters.

References

- [1] A. Murayama, et al., Phys. Rev. B 61 (2000) 8984 and references therein.
- [2] M. Plummer (Ed.), The Physics of Ultra-High-Density Magnetic Recording, Springer, Berlin, 2000.
- [3] M. T. Johansson, P. J. H. Bloemen, F. J. A. den Broeder, and J. J. de Vries, Rep. Prog. Phys. 59, 1409 (1996).
- [4] N. Metropolis, A. W. Rosenbluth, M. N. Rosenbluth, A. H. Teller and E. Teller, J. Chem. Phys. 21, 1087 (1953).



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ภาคผนวก ข.
เอกสารประกอบงานประชุมวิชาการที่เข้าร่วมเรื่อง

Monte Carlo Simulations in Advancing Magnetic Recording Applications

นำเสนอแบบ Oral presentation
“The Eighth International Conference on Monte Carlo and Quasi-Monte Carlo
Methods in Scientific Computing (MCQMC2008)”
6 – 11 July 2008
HEC Montréal, Canada

รายละเอียดการประชุม

MCQMC'08

Eighth International Conference on Monte Carlo and Quasi-Monte Carlo Methods in Scientific Computing

July 6-11, 2008



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Program & Tutorials

July 6: Parallel advanced **tutorials** in the afternoon, three hours each.

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July 7 - 11: Five days of conference with 10 invited one-hour plenary talks, and several 30-minute talks organized in sessions of 3 or 4 talks, including some special thematic sessions, with at most three parallel sessions at a time. A selection of papers from the conference will be published after the conference, most likely as a Springer-Verlag book, as was the case for the seven previous editions.

Call for contributions

Deadlines:

- **March 4, 2008** : submissions of abstracts for contributed talks
- **March 14, 2008** : notification of acceptance
- **January 25, 2008** : proposals for special sessions
- **January 28, 2008** : notification of acceptance for special sessions

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Josef Dick (UNSW)
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Klaus Ritter (TU Darmstadt)
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CRM | Web site: www.crm.umontreal.ca/mcqm08 | Update 10.01.08 | Photo source: Université de Montréal

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Québec à Montréal

April 4, 2008

Yongyut Laosiritaworn
Department of Physics, Faculty of Science
Chiang Mai University
239 Huay Kaew Road, Suthep
Muang, Chiang Mai
Thailand 502000

Dear Yongyut Laosiritaworn,

I am pleased to invite you to give an oral presentation entitled "Monte Carlo Simulations in Advancing Magnetic Recording Applications" at the conference **Eighth International Conference on Monte Carlo and Quasi-Monte Carlo Methods in Scientific Computing**, at HEC Montréal, Canada, on July 6-11, 2008.

To attend at the conference, you will need to pay the air fares, the full registration fees and the accommodation fees by your own or by your institution.

Practical details (venue, hotels, etc.) can be found on our Website (<http://www.crm.umontreal.ca/mcqm08/>).

Please do not hesitate to contact me for any further information you may need.

I look forward to welcome you in Montréal.

Best regards,



Pierre L'Ecuyer
Université de Montréal, Canada

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บทคัดย่อ

Monte Carlo Simulations in Advancing Magnetic Recording Applications

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The ferromagnetic thin films have been a subject of intensive interests in view of both technological applications [1] and fundamental interests, where physics in reduced structure is different from those in bulk. However, the description of how the magnetic behavior in films structure are affected by the external field is not quite well set up due to complexity of the reduced dimension. For example, multilayered systems are known to change from two to three dimensional class with increasing numbers of layers [2]. Magnetic films, however, should belong to a two dimensional universality class owing to dimensional ratio. Therefore, this discrepancy highlights the importance of the dimensional pinning to the problem. Nevertheless, direct observations are difficult to obtain; consequently, many numerical techniques have been used to understand the ferromagnetic behavior e.g. the mean-field method or the first principles electronic structure calculation. However, these two methods have not yet properly taken the thermal fluctuation into account. Therefore, that the results obtained from these methods are applicable and correct for a wide range of temperatures is still of some curiosities. On the other hand, the Monte Carlo simulation (based on a stochastic method) has proved to be a useful model in cooperating with thermal disturbance. For example, the Monte Carlo simulations in two-dimension Ising model agree very well with the exact solutions. Therefore, the Monte Carlo is expected to be a promising technique when considering the effect of thermal fluctuation on magnetic properties in various structures.

In this talk, the Monte Carlo techniques used in statistical physics especially in magnetic thin-films modeling are introduced [3]. A few algorithms which follow the stochastic detailed balance and ergodicity in thermal equilibrium are given and briefly described. Then, the applications of this Monte Carlo in some ferromagnetic thin-films systems are presented. Based on its results, these have provided another fruitful step in understanding the ferromagnetic phenomena and suggest Monte Carlos role in advancing the magnetic recording applications. Finally, as an addition to ferromagnetic studies, an extension of this Monte Carlo technique to other ferroic topics such as ferroelectric applications is also suggested and discussed.

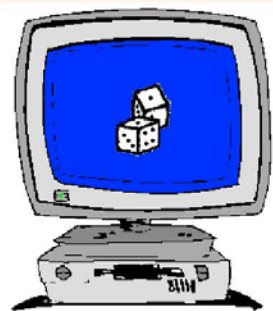
[1] T. Osaka, T. Asahi, J. Kawaji, T. Yokoshima, *Electrochim. Acta* 50, 4576 (2005).

[2] Y. Li and K. Baberschke, *Phys. Rev. Lett.* 68, 1208 (1992).

[3] M. E. J. Newman and G. T. Barkema, *Monte Carlo Methods in Statistical Physics* (Clarendon, Oxford, 1999).

Monte Carlo Simulations in Advancing Magnetic Recording Applications

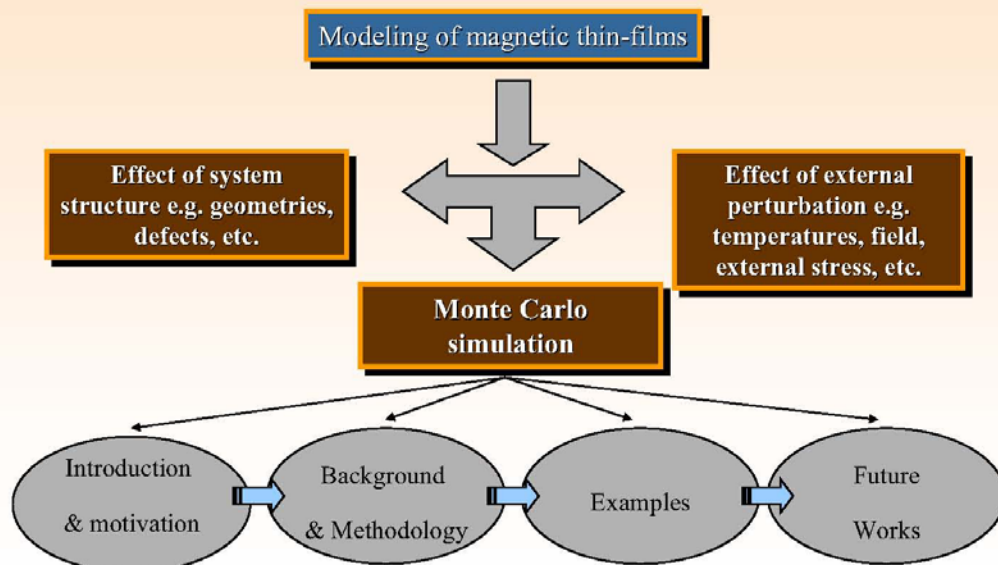
Yongyut Laosiritaworn



HEC Montréal, 7 July 2008



Outline



MCQMC'08



Introduction and motivation

- ❖ Technological and fundamental importance (Johnson *et al.* 1996)

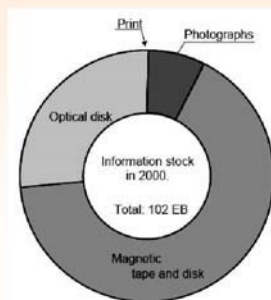


MCQMC'08



Especially in memory application.

- ❖ The blooming of information technology era.
- ❖ Among digital storage, the magnetic storage is of preferable in terms of cost-effectiveness.



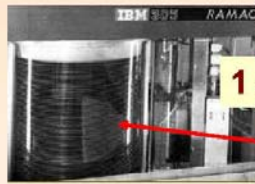
Source : Muira (2001)



MCQMC'08



Increasing the areal density



1 song

stack of 50 giant discs, 24" diameter

5 Mbyte



70 kbits/s
IBM RAMAC 1956
2 kbits/in²
50 x 24-inch diameter disks

100 songs

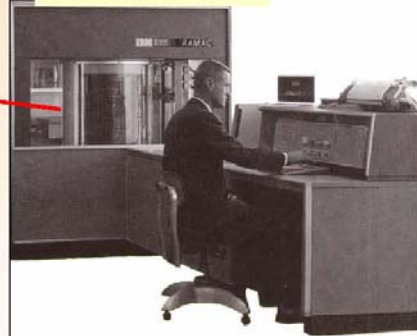


340 Mbyte

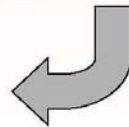


180 Mbits/s
IBM Microdrive 1999
6 Gbits/in²
1-inch diameter disk

IBM RAMAC 1956:



1956: IBM 305 RAMAC Computer with Disk Drive



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Roadmap

10 Pbit/sq.in.

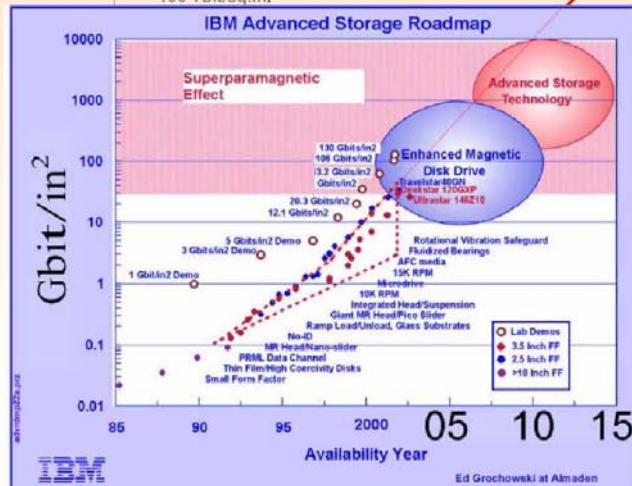
1 Pbit/sq.in.

100 Tbit/sq.in.

100% CGR

Atoms ?

Molecules ?



HDD industry aiming for 1Tbit/sq.in. storage density by 2008 to 2012

Source : IBM

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But !

“The Superparamagnetic Limit has Entered the Building.”

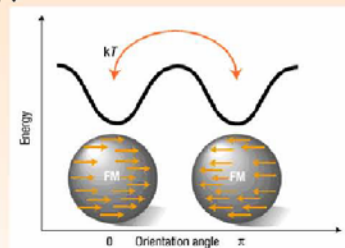
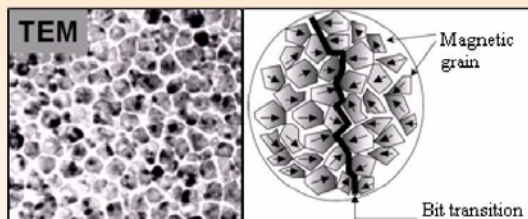
Richie Lary

MCQMC'08



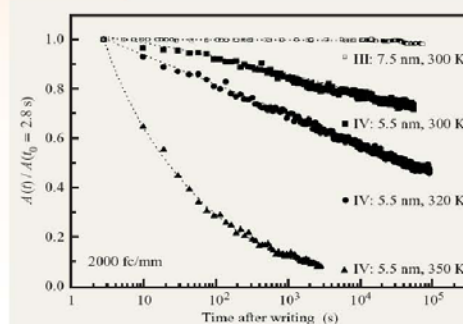
Superparamagnetic effect.

❖ Magnets get unstable if they get too small !



❖ Stability depends on:

- Magnetic domain
- Magnetic coercivity
- Temperature
- Surrounding polarity



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