The Effect of Nano-Defects on Ising Hysteresis in Ultra-Thin-Film

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ABSTRACT

In this work, we modeled the dynamic magnetic behavior in magnetic ultra-thin-film structure. We investigated magnetic properties and their dynamic magnetization switching (hysteresis) by means of Monte Carlo simulations with the inclusion of various types of defects at nano-scale level. Types of defects being considered were the vacancy defects, the static-dipole defects and the anti-ferromagnetic dopants to ferromagnetic defects at various concentrations. The Ising model was considered and the spin-flip algorithm was used to update the magnetic configurations. The dynamic magnetic profiles, i.e., the time-dependent magnetization and magnetic field were observed as varying the defect concentrations. From the results, at a fixed temperature and magnetic field frequency, with increasing the vacancy concentration, both the coercivity and the remanence reduced due to the weaker ferromagnetic interaction in the system. On the other hand, the static contamination caused asymmetry pattern of the hysteresis loop such that the magnetization along anti-parallel direction to those static defect reduced its magnitude significantly. Finally, the anti-ferromagnetic defects gave rise to the combination behavior between the ferromagnetic and the anti-ferromagnetic hysteresis loops, leading to a promising way to control the hysteresis loop which reflected both the ferromagnetic and the anti-ferromagnetic phenomena.

Key words: Nanostructure, Hysteresis, Defects, Magnetic ultra-thin-films, Ising model, Monte Carlo

INTRODUCTION

The ferromagnetic magnetic thin-film has been a subject of intensive interest and investigation in view of a broad range of applications, especially in recording applications featuring from high-magnetic anisotropies (Johnson et al., 1996; Murayama et al., 2000; Plumer et al., 2001). In addition, in terms of fundamental interest in understanding, that the physical mechanisms involved in those nano-scale systems are quite different from bulk properties, has become a topic of frequent 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 use the magnetic thin-film's behavior to obtain the magnetic hysteresis which is caused by the relaxation delay between the external magnetic field and the response magnetization, at a right shape and suit some desired technological applications, e.g., transformer and magnetic storage media.

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 (e.g., vacancy, impurity, dislocations, etc.) cannot be avoided. This highlights the importance of the interface pinning which makes the problem very complicated. Generally, however, direct observations of defect interactions to hysteresis properties are difficult to obtain. One is therefore restricted to computer-simulation methods to model and observe the magnetic phenomena further insight.

In modeling such a magnetic thin-films structure, the magnetic system can be described by the Ising model since both theoretical (Binder and Hohenberg, 1974; Bander and Mills, 1988) and experimental (Li and Baberschke, 1992; Elmers et al., 1994; Dunlavy and Venus, 2004) investigations have shown that the magnetic behavior in nano-thickness ferromagnetic-films is an Ising-like. In our study, we tried to study the effect of defects, i.e., the vacancy defects, the static-dipole defects and the anti-ferromagnetic dopant-defects to the hysteresis loop by using the Ising model (with a lattice size of 50x50 spins) and Monte Carlo simulation. We considered the vacancy and static-dipole defects at concentrations ranging from 0 to 50 percent of all available magnetic sites. However, for the anti-ferromagnetic defects, concentrations ranged from 0 to 100 percent to observe the behavior changing from ferromagnetic phase to anti-ferromagnetic phase. Finally, for each type of the defects, we analyzed and compared the properties of hysteresis loops to observe how they depended on the percent of defects.

MATERIALS AND METHODS

In the study, we considered the use of Ising model with an inclusion of some defects. Since the Ising model is known to be a model with an infinite anisotropy along its easy axis direction, its Hamiltonian can be written as

$$H = -J \sum_{<i,j>} J_{ij} s_i s_j - h(t) \sum_{i} s_i \, . \qquad (1)$$

In the equation, s_i (= up/down or ±1) represents the direction of an Ising spin variable (along ± z direction) at site *i* where its magnetic moment is absorbed into the exchange interaction J_{ij}. The exchange interaction $J_{ij} = +J$ or $-J$ are for the ferromagnetic or the anti-ferromagnetic coupling respectively. The symbol <…> denotes that the sites *i* and *j* appearing in the sum are nearest-neighbor pairs. Including in the Hamiltonian, the external magnetic field $h(t) = h_0\sin(\omega t) = h_0\sin(2\pi f t)$, where *f* is the field's frequency, is applied to the systems on the *z* direction to extract the hysteresis properties. In general, it is usual to set $J = 1$, and both the Hamiltonian and the external field $h(t)$ are defined in a unit of *J*. In a similar way, this also changes the unit of temperature *T* to be J/k_B.

In making the simulation, the lattice size of 50x50 spins with periodic boundary conditions on all edges were prepared. Then, we included 3 different types of the defects which were:-

- The vacancy type defect: The vacancy concentration being used in the simulation varies from 0 to 50 percent. Then, during the spin exchanging in the simulation, the normal Ising spins were randomly substituted by the vacancy sites. The Hamiltonian in Eq. (1) still holds but one has to substitute the normal Ising spins from original values ±1 to 0 for the vacancy sites.
- The static type defect: The static magnetic dipole-moment site is a site that does not change in time. In another word, the static defect has a built-in infinite anisotropic energy that prefers only 1 direction. In the simulation, we set all the static sites to point to the up direction ($s_i = +1$ or $+z$ direction) and these sites will not flip no matter how large the applied magnetic field is. The static concentration being considered in

the work varies from 0 to 50 percent.

- The anti-ferromagnetic defect: This type of defect prefers anti-ferromagnetic exchange interaction. Actually, there appear to be three types of interactions among magnetic spins which are ferromagnetic to ferromagnetic interactions, anti-ferromagnetic to anti-ferromagnetic interactions and the ferromagnetic to anti-ferromagnetic interaction. Therefore, we proposed an approximation such that the ferromagnetic to ferromagnetic sites are of the ferromagnetic type i.e. $J_{ij} = +1$. On the other hand, the ferromagnetic to anti-ferromagnetic and the anti-ferromagnetic to anti-ferromagnetic are of anti-ferromagnetic types i.e. $J_{ij} = -1$. In this type of defect, the concentration varies from 0 to 100 percent to provide a way to observe the changing trend from ferromagnetic to anti-ferromagnetic hysteresis.

Next, with an inclusion of defects into the system, we setup an initial magnetic configuration by setting all available spins to the up direction (+1). To update the configuration, we used the Metropolis single spin flip dynamics (Metropolis et al., 1953) where the spin at site i (s_i) was updated (flipped to its opposite direction) with a probability proportional to

$$\exp\left[-\frac{1}{k_B T}\ E\ _i(t)\right], \qquad (2)$$

where the energy difference between before update and after update at site i is

$$E\ _i(t) = 2s_i\left[\ _j\left(\mathrm{sgn}\ (J_{ij})\ \mathrm{x}\ s_j\,(t)\right) + h(t)\right], \qquad (3)$$

where sgn(J_{ij}) is (1 depending on the sign of the interaction J_{ij}. During the simulation, the spin at site i is flipped if the change in energy of the flipping spin is less than zero or a uniform random number [0,1) is less than probability of spin updating in Eq. (2). Nevertheless, the flipping procedure discards the vacancy and the static sites. Then, 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 of Ising spins at time t, after the steady state of the hysteresis loop had been reached, we calculated the response magnetization per site at time t by

$$m(t) = \frac{1}{N}\ _i\ s_i(t), \qquad (4)$$

where N is the total number of spins in Ising lattice (in this study N is 2500 or 50x50) and the sum takes on all available spins in entire lattice. From the magnetization per site m, a plot between m and the external magnetic field h leads to hysteresis loops. Next, we considered the hysteresis loop area

$$A = \oint m\,dh \qquad (5)$$

to investigate how the area responds to the type and percent of defects. In the simulations, for all types of defects, the simulated parameter that are the temperature, the field's frequency and the field's magnitude were chosen at $T = 1\ J/k_B$, $f = 0.01$ mcs^{-1}, and $h_0 = 8$ J respectively. This set of parameters was chosen from where the hysteresis loops, from all defect conditions, became saturated.

RESULTS AND DISCUSSION

From out results, the response of the hysteresis loop to the types and the concentrations of the defects are found (see TABLE 1 and Fig. 1 to 3). For example, Fig. 1 shows the effects of vacancy concentration to the hysteresis profiles from 0 percent to 50 percent. Such a behavior that smaller hysteresis-loop, the smaller m_r, and the smaller h_c are found with increasing the number of vacancy is expected. This is because the number of vacancy sites has a strong effect on the averaged exchange coupling among the spins in the systems. Then, the more vacancies, the less of the averaged exchange coupling in the systems, and this strongly reduces the magnitude of the magnetization. Such a phenomena is ferromagnetic to paramagnetic phase-transition-like since the bigger number of vacancies reduces the averaged interaction among atoms in a same way as the increase of the temperature so that the thermal energy compensates the ferromagnetic interaction among spins.

Table 1. The hysteresis properties (area, coercivity and remanence) as a function of defect concentrations at fixed temperature, amplitude and frequency of magnetic field ($T = 1\ J/k_B$, $f = 0.01$ mcs^{-1}, and $h_0 = 8\ J$.).

Defect	Defect concentration	Hysteresis area	positive h_c	negative h_c	positive m_r	negative m_r
Vacancy	0%	11.48280	2.82783	-2.82953	0.99958	-0.99957
	10%	8.86928	2.44322	-2.44222	0.89720	-0.89720
	30%	4.70590	1.72385	-1.72372	0.67726	-0.67702
	50%	2.03497	1.08831	-1.08746	0.42393	-0.42401
Static-dipole	0%	11.48280	2.82783	-2.82953	0.99958	-0.99957
	10%	8.21762	1.69756	-2.90699	0.99957	-0.72585
	30%	4.07614	-0.29953	-3.16823	0.99965	0.19113
	50%	1.66844	n/a	-6.82633	0.99971	0.88402
Anti-ferromagnetic	0%	11.48280	2.82783	-2.82953	0.99958	-0.99957
	10%	9.48203	2.84609	-2.84652	0.80505	-0.80506
	30%	5.74600	2.58120	-2.57903	0.49321	-0.49292
	50%	2.87325	1.85437	-1.85330	0.25515	-0.25496
	100%	0.99985	0.10209	-0.10163	0.00587	-0.00600

Next, Figure 2 shows the response of the hysteresis loop to the static defect. Since all static spins are set to the up direction, the symmetry of the hysteresis loop is broken and the magnetization prefers to point the up direction (the static defect direction). As a result, m_r on the up direction stays very close to 1, but on the down direction m_r significantly reduces and ceases to zero at the concentration of 50 percent. On the other hand, the magnitude of the positive h_c decreases but the magnitude of the negative h_c increases. This is also caused by the static up-magnetic-spin. With the static up-spins' help to cancel the usual down-spin, the field does not need to be large to bring the magnetization to zero along the positive axis of the field, i.e., the magnitude of positive hc gets smaller with increasing concentration. Nevertheless, since the static up-spins' always point to the up-direction, hence, to bring the positive magnetization down to zero on the negative axis of the field requires a greater magnitude of the field. This results in the higher magnitude of the negative h_c.

Finally, for the anti-ferromagnetic dopants, a clear changing trend from the ferromagnetic hysteresis at 0 percent to a pure anti-ferromagnetic hysteresis at 100 percent was found

(Figure 3). On its way through, the anti-ferromagnetic hysteresis-behavior gets growing (where there exists some signal suggesting a possible double loops hysteresis) as increasing the concentration. Also, in the figure, m_r and h_c were found to reduce in magnitude due to the cancellation of magnetic spins arisen from the anti-ferromagnetic effect.

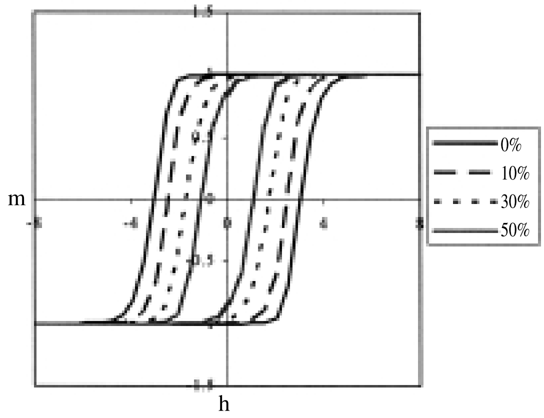

Figure 1. Hysteresis loops of the vacancy-defected systems (simulated at $T = 1\ J/k_B$, $f = 0.01$ mcs^{-1}, and $h_0 = 8\ J$) at the concentration ranging from 0% to 50%.

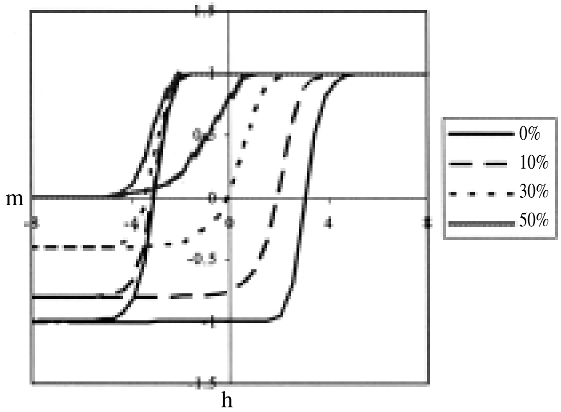

Figure 2. Hysteresis loops of the static-dipole defected systems (simulated at $T = 1\ J/k_B$, $f = 0.01$ mcs^{-1}, and $h_0 = 8\ J$) at the concentration ranging from 0% to 50%.

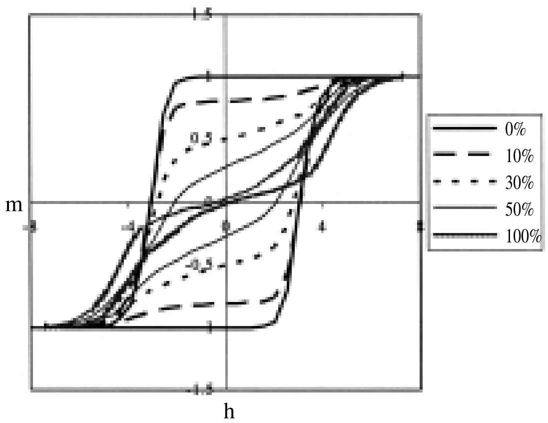

Figure 3. Hysteresis loops of the anti-ferromagnetic-dopant defected systems (simulated at $T = 1\ J/k_B$, $f = 0.01$ mcs^{-1}, and $h_0 = 8\ J$) at the concentration ranging from 0% to 100%.

CONCLUSION

We have proposed Monte Carlo simulations on the Ising ultra-thin-film system to investigate the effect of defect types and its concentrations to the dynamic hysteresis properties. As expected, for the vacancy type defect, a trend suggesting the transition from a ferromagnetic system to paramagnetic system is found even at a fixed temperature. On the other hand, the static defect provides a bias direction to the magnetization. In such case, the hysteresis loop is no longer symmetric and all hysteresis properties significantly change in response to the static defect. Finally, we consider the anti-ferromagnetic defect contamination to the ferromagnetic system. A combination behavior between the ferromagnetic and the anti-ferromagnetic phase is found in the hysteresis loop. As being evident, therefore, this works suggest a controllable way to obtain the desired hysteresis pattern by introducing the defects or impurity dopants to the system. Consequently, the study may boost up a technological development to obtain highly-efficient technological applications based on magnetic hysteresis properties in the near future.

ACKNOWLEDGEMENTS

The authors would like to express their gratitude to the Faculty of Science, Chiang Mai University and the Thailand Research Fund (TRF) for financial supports.

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