The Effect of Uniaxial Stress on the Dynamic Spin Reversal in Ferromagnetic Nano-Thickness Films : Monte Carlo Investigation

Supattra Wongsaenmai, Athipong Ngamjarurojana, Supon Ananta, Rattikorn Yimnirun and Yongyut Laosiritaworn*

Department of Physics, Faculty of Science, Chiang Mai University, Chiang Mai 50200, Thailand

**Corresponding author. E-mail: yongyut@science.cmu.ac.th*

ABSTRACT

In this work, we studied the uniaxial stress dependence of the ferromagnetic properties of nano-thickness films, i.e., bi-layered ferromagnetic films, where the films' in-plane direction is lying in the x-y plane. The Heisenberg Hamiltonian model being used in the study was modified to include the uniaxial stress effect, and both the uniaxial stress and the external magnetic field were applied on the z direction of the system. The observables, i.e., the magnetization along the out-of-plane (z) direction were taken as a function of temperatures, the magnitudes of the applied stress, the magnetic fields' period and the magnetic fields' amplitude via the dynamics of the spin reversal in the framework of the magnetic hysteresis. The study was taken by means of Monte Carlo simulations using a spin-flip algorithm. From our results, it was found that the remanent values of the hysteresis loop significantly decreased with increasing applied stress. On the other hand, the coercive field only slightly decreased. Moreover, the areas under the hysteresis loop also decreased with increased applied stress, indicating a smaller magnitude of energy dissipation. The results are in good agreement with related experiments.

Key words: Nanostructure, Magnetic thin-films, Monte Carlo, Heisenberg model, Uniaxial stress, Spin reversal, Hysteresis

INTRODUCTION

Magnetic multi-layers grown on non-magnetic substrates, especially thin-films with a thickness in nano-scale range, have recently been of wide interest in view of both technological and fundamental importance (Johnson et al., 1996). Of a particular interest is the technological applicability such as high-storage magnetic recording media which high areal densities of the recording media are in demand (Judy, 2001). Consequently, there comes an interest on the study of how to enable more data bits to be stored in a finite magnetic material while the magnetic domain switching under an influence of external magnetic field, during the read/write period, is controllable. Accordingly, to fulfill this objective, knowledge about magnetic spin reversal from one direction to its opposite direction of the magnetic multi-layers, under the effect of an external field, corresponding to specific material structures must be understood in details.

Nevertheless, for the sake of simplicity, theoretical studies on magnetic multi-layers are usually performed on an ideal structure, for instance, stress-free material. However, real materials being used in many applications especially in thin-films structures are often affected from crystalline anisotropy contributed from mechanical stress. Even in an unstrained lattice, this can be regarded as a strain on the crystal due to some slightly different atomic positions, for example, the lattice mismatch at the interfaces between the magnetic layers and the substrate. Furthermore, according to prior study by Karl et al., (2000), ferromagnetic materials under mechanical load were found to have a dimensional change and its magnetization behavior was altered. As a result, any calculation obtained from a stress-free condition, may lead to incorrect or inappropriate application designs. Therefore, it is very important to include the applied stress if we want to model real materials, and it is the objective of this study to model such a situation.

In this work, we studied the uniaxial stress dependence of the ferromagnetic dynamic properties, i.e., hysteresis, of thin-films with a thickness falling into a few nanometers range, i.e., thin-films, consisting only a few monolayers. As a prototype, the studied structure is confined into a bi-layered structure where the in-plane direction is lying in the x-y plane and the applied field and compressive stresses are acting on the out-of-plane direction (z direction). To outline, the study was firstly done by modifying the isotropic classical Heisenberg Hamiltonian to include the uniaxial stress effect. Since the spin reversal takes a form of saturated hysteresis loop only when the magnetic field amplitude h_0 and its period are sufficiently high enough, we then additionally considered how temperatures, the field's period and the field's amplitude incorporate with the uniaxial stress to affect the dynamic hysteresis properties. Then, by means of Monte Carlo simulations, the observables, i.e., the magnetization along the out-of-plane direction are investigated as a function of temperatures, the magnetic field's period and amplitude, and the magnitudes of the applied stress via the dynamics of the spin reversal, i.e., hysteresis loops. Finally, all the descriptions to those results are given in details.

MATERIALS AND METHODS

Spin Hamiltonian

In this study, we considered the anisotropic classical Heisenberg Hamiltonian

$$H = - \;{}_{<ij>}\; J_{ij}(\;\; l)\hat{s}_i \cdot \hat{s}_j - \;{}_{i}\; h_i(t)s_{iz}\,, \tag{1}$$

where is a spatial unit vector, and is the unit vector's component along the out-of-plane direction of the films (z-direction). The magnetic moment magnitudes of all spins are absorbed into J_{ij} and hi. Hence, the spin si is dimensionless, but both J_{ij} and h_i have a unit of energy. In the equation, the applied magnetic field $h(t)$, which is acting on the z direction, takes a sinusoidal form as

$$h_i(t) = h_{i0} \sin\left(\frac{2\pi}{T'} t\right) \tag{2}$$

where T' is the magnetic field's period. In the model, we assume uniformity such that the field acting on the spins is site-independent, i.e., $h(t) = h_i(t)$. J_{ij} refers to the exchange interaction which is a function of lattice distortion, that is strain (l), arising from an applied mechanical stress. The sum $<ij>$ takes only first nearest-neighbour (1NN) pairs. Helical (periodic) and free-boundary conditions were used for the in-plane and the out-of-plane directions, respectively. Without any applied stresses, magnetic thin-films systems were assumed to be uniform, that is $J_{ij}(0) = J$. However, when a non-zero stress was applied, we directed the stress effect to the exchange interaction part by expanding J_{ij}(l) via a Taylor series expansion, and only the first-order term was kept, that is $J_{ij}(\;\; l) = J + (\;\; l)\, J'_{ij}$. Here, J'_{ij} is the spatial derivative of the exchange parameter between site i and j. If the applied stress is not too great, $J'_{ij} = J'$ is assumed to be uniform and linear, that is $J' = J/a$ where a is the lattice spacing. Thus, we may write the Hamiltonian as

$$H = -\sum_{<ij>} \left[J\left(s_{ix}s_{jx} + s_{iy}s_{jy}\right) + \left(J-(\Delta l)\, J/a\right) s_{iz}s_{jz} \right] - h(t) \sum_{i} s_{iz}, \tag{3}$$

where the in-plane exchange interaction are left unaltered as the compressive stress affects the out-of-plane direction the most. Minus sign to the z-component term is due to the compressive stress shortening the interlayer spacing along the out-of-plane direction. Since the films are thin, we expect the stress to affect all layers with a same magnitude as appearing in the Hamiltonian. From Young's modulus $Y = P/(\Delta l\, /\, a)$, we can write $\frac{\Delta l}{a} = \frac{P}{Y}$ where P is the pressure acting on the films' surfaces. As a result, the Hamiltonian is written as

$$H = -\sum_{<ij>} \hat{s}_i \cdot \mathbf{J} \cdot \hat{s}_j - h(t) \sum_{i} s_{iz}, \tag{4}$$

where $\mathbf{J} = \begin{bmatrix} J & 0 & 0 \\ 0 & J & 0 \\ 0 & 0 & J(1-P/Y) \end{bmatrix}$ is a second-rank tensor describing anisotropic exchange interaction.

Monte Carlo Simulation

Throughout this study, by conveniently setting $J = 1$, this re-defines the unit of temperature T as J/k_B (where k_B is the Boltzmann's constant), and magnetic field's amplitude h_0 is now in a unit of J. The simulations were done for a range of temperatures in the ferromagnetic phase (where there exists the hysteresis loops), i.e., $T = 1.0$ to 2.60 J/k_B. The uniaxial stress (pressure) to the Young's modulus ratio P/Y was varied from 0 to 0.1 to investigate how the stress affects the hysteresis properties. The simulation was done on bi-layered films with total number of spins $N = 20x20x2$. The unit time step was defined from one full scan all sites of the Ising lattice, that is, 1 Monte Carlo step per site (mcs). Then, we varied the magnetic field's period in the simulations from 20 mcs to 1000 mcs and the field's amplitude from $h_0 = 1$ to 16 J.

With the Hamiltonian proposed in the last section, each bi-layered system was assigned an initial random configuration and later on was passed to the thermal Monte Carlo updates, using the Metropolis algorithm (Metropolis et al., 1953). In updating the system, each spin is assigned a new random direction, and the probability of accepting that new direction is proportional to

$$p = \exp\left(-\frac{\Delta H}{k_B T}\right) \tag{5}$$

where ΔH is the energy differences between of the original and the new direction. If the energy difference is less than zero, or a uniform random number [0,1) is less than the probability p in Eq. (5), the new direction is accepted and the system is successfully updated. On the other hand, the considered spin is left untouched. The whole procedure is repeated until the simulation ends.

Next, with varying the uniaxial stress magnitude, the applied magnetic field's period and amplitude, each simulation waited for a few cycles to obtain a steady hysteresis loop, and then the magnetization per spin along the out-of-plane direction mz was calculated, that is

$$m_z = \frac{1}{N}\left[\sum_i |s_{iz}|\right], \tag{6}$$

where z refers to the out-of-plane component of the magnetization. Since there exist systematic errors and statistical errors resulting from the finite-size effect and thermal fluctuation, we recorded at least 1000 steady hysteresis loops for making an average hysteresis loop for each condition.

RESULTS AND DISCUSSION

It is well-known that when the ferromagnetic spins are under the effect of an external time-varying magnetic field, the system cannot respond promptly due to a relaxation delay. As a result, the magnetization will lag behind the applied field, and this gives a nonzero area of the hysteresis loop, i.e., the magnetization-field loop. Then, our studies concentrated on such a case. Starting with the zero-stress case, we found a significant change to the hysteresis loop with varying the field's period, the field's amplitude and the temperatures. Figures 1 and 2 present these phenomena.

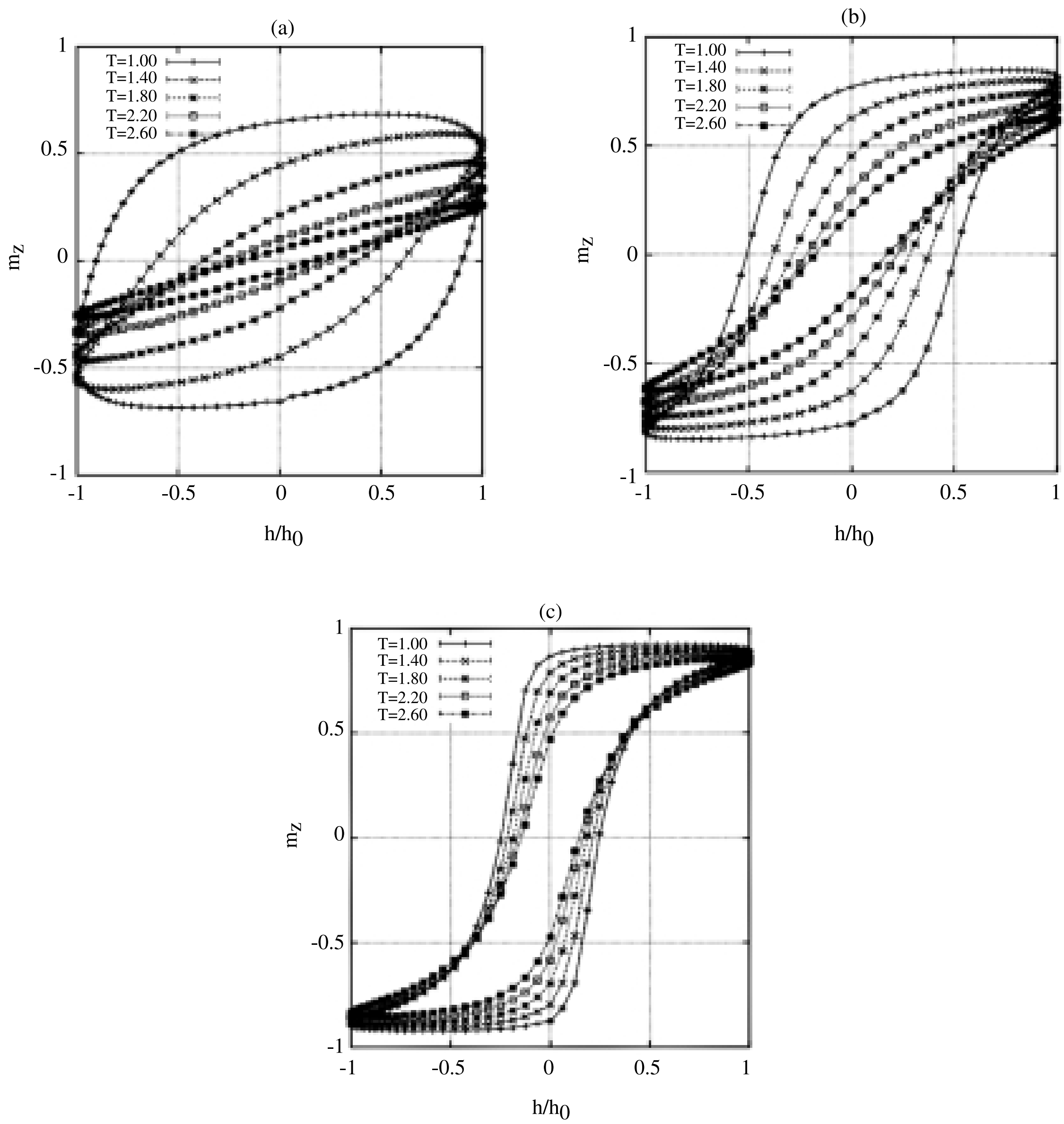

Figure 1. Hysteresis loops of the bi-layered films at zero-stress at period = 100 mcs. From (a) to (c), h_0 are 1, 8, and 16 J respectively. Unit of the temperature T is J/k_B.

In Figure 1, as increasing the temperature, it is found that the ferromagnetic hysteresis loops suggest a changing trend from the ferromagnetic phase to the paramagnetic phase, i.e., that the rhombohedra-like loop transforms to the ellipse-like loop. However, with increasing the field's magnetic from h_0 = 1 to 16 J (see Figure 1a to 3c), saturated hysteresis loops are gained even at a high temperature T = 2.60 J/k_B. This is because the higher field leads to the higher magnetic driving force to magnetic spins which stabilizes the saturated pattern.

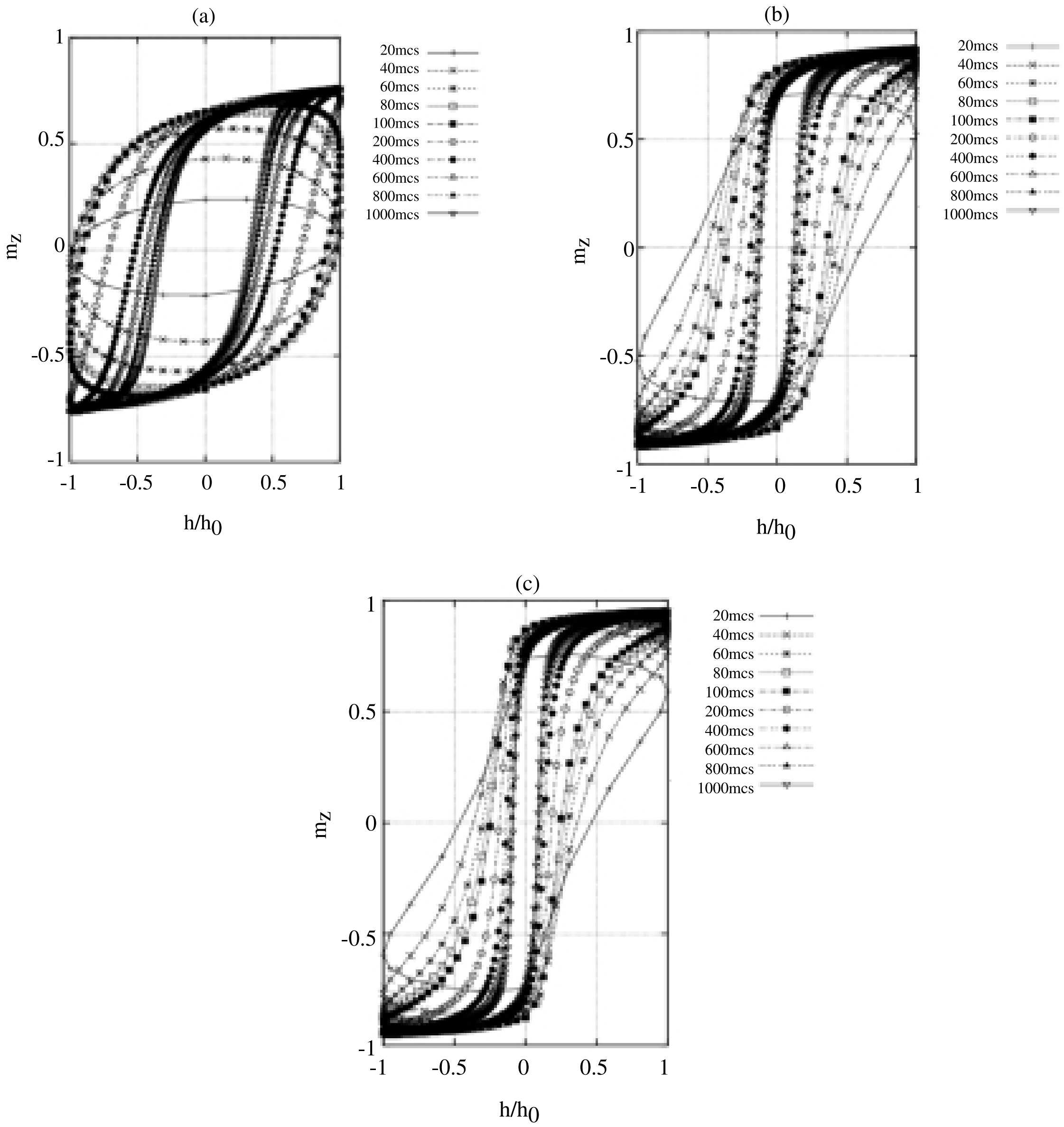

Figure 2. Hysteresis loops of the bi-layered films at zero-stress at T = 1.00 J/k_B. From (a) to (c), h_0 are 1, 8, and 16 J respectively.

Nonetheless, with varying the fields' period and amplitude, but at a fixed temperature, Figure 2 shows clear evidence of how the hysteresis responds to the field. For example, as shown in Figure 2a, the hysteresis loop at period = 20 mcs changes from an oval-like loop to the normal s-shape hysteresis loop. This is because the higher period gives the spins more time to follow the field and results in the conventional hysteresis pattern. Then again, with increasing the field's amplitude, the higher magnetic driving force assists to form the hysteresis shape even at a low magnetic field's period.

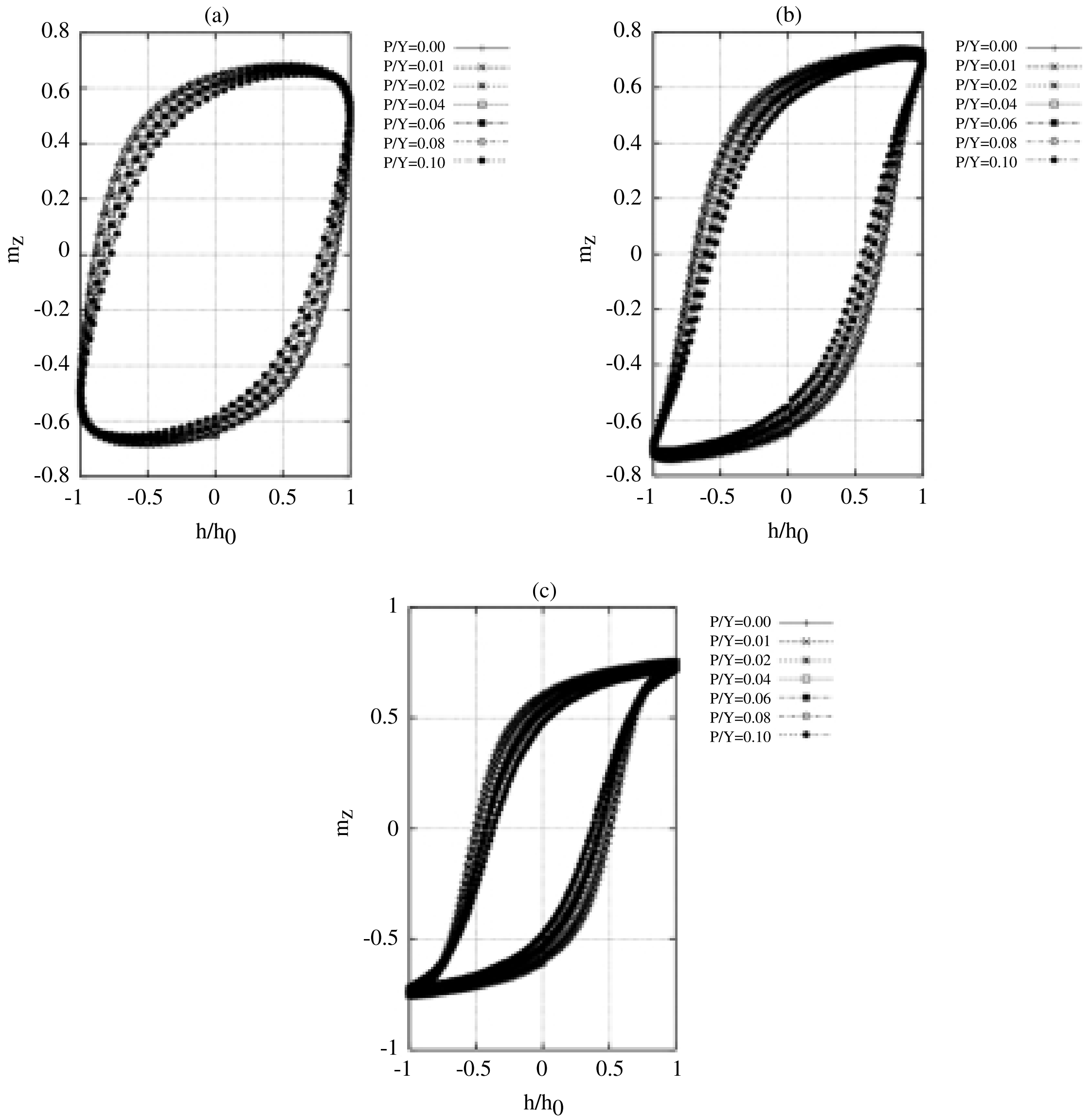

Figure 3. Stress-dependent behavior of the hysteresis loops of the bi-layered films at fixed T = 1.00 J/k_B and h_0 = 1.00 J. From (a) to (c), the field's period are 100, 200 and 400 mcs respectively.

On the other hand, with a non-zero stress applying to the films, e.g., in Figure 3, the decease of the remanent m_r, the coercivity h_c and the hysteresis loop-area are found. The reason to these phenomena is that, as can be seen in the Hamiltonian Eq. (1), the stress causes the out-of-plane direction (the z direction) to become a hard axis and the in-plane direction now becomes an easy system. As a result, the magnetic system prefers to align in the in-plane direction which has a lower energy state. Consequently, the remanent m_r along the z direction, significantly reduces in magnitude. Similarly, since the z direction is the hard axis and the magnetic spins are so grateful for leaving this direction, to bring the mz down to zero is a trivial task. The field needs not be too large to cancel the m_z which results in a smaller coercive field h_c. Based on the same description that has been given to Figure 1, the same response of the hysteresis to the field's period is found. It should also be noted that in Figure 3, the applied stress also reduces the hysteresis area. This means that the dissipation energy also reduces. The reason underlying this can be retrieved by considering the stress-inducing mechanical works. Thermodynamically, when an applied stress is given, a mechanical work is added to the system. Hence, to switch the spins from one direction to their opposite direction does not need the same magnetic work since the mechanical work has provided a help. This is why with increasing the stress, the loop-area gets smaller. In comparison with experiments, qualitatively, the decrease of the coercivity and the loop-area with increasing stress agrees well with an experiment on grain-oriented 3%-Si steel in 2D structure (Permiakov et al., 2005) and an experiment on CoNiMnP thin-films (Guan and Nelson, 2005). To summarize the results, Figure 4 provides an informative suggestion of how the uniaxial stress affects the properties of the hysteresis loop.

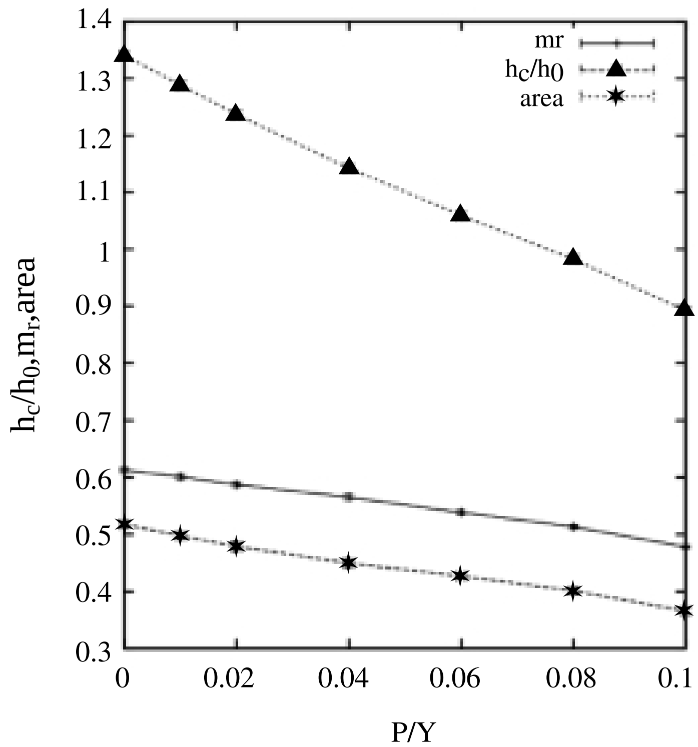

Figure 4. The stress-dependent hysteresis properties, i.e., m_r, h_c/h_0 and the area under the hysteresis-loops as a function of the compressive stress-ratio P/Y at T = 1.00 k_B/J, period = 400 mcs, and h_0 = 1 J.

CONCLUSION

In this study, we performed Monte Carlo simulations to study magnetic thin-films under the influence of mechanical uniaxial stress on the films' surfaces to the magnetic hysteresis properties at various conditions. The objective is to investigate the behavior of the spin-reversal along the out-of-plane as changing the magnitude of the stress, the temperatures, the magnetic field's period and amplitude on bi-layered films. From our studies, we found that the increase of the temperature reduces m_r, h_c and the hysteresis area since it provides a higher level of thermal fluctuation, but the longer period of the magnetic field helps stabilize the saturated hysteresis shape. On the other hand, at a fixed set of parameters, i.e., temperature, field's amplitude and period, the applied stress on the films reduces m_r, h_c and the hysteresis area. This is due to that the stress causes the out-of-plane direction to be a hard axis for the system and the induced mechanical work (caused by the stress) helps the magnetic work reduce the hysteresis loop-area, resulting in smaller energy dissipation. The results qualitatively agree well with experiments where applicable.

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 support.

REFERENCES

Guan S., and B. J. Nelson. 2005. Electrodeposition of low residual stress CoNiMnP hard magnetic thin films for magnetic MEMS actuators. J. Magn. Magn. Mater. 292: 49–58.

Johnson, M. T., P. J. H. Bloemen , F. J. A. den Broeder, and J. J. de Vries. 1996. Magnetic anisotropy in metallic multilayers. Rep. Prog. Phys. 59: 1409–1458.

Judy, J. H. 2001. Past, present, and future of perpendicular magnetic recording. J. Magn. Magn. Mater. 235: 235–240.

Karl, W. J., A. L. Powell, R. Watts, M. R. J. Gibbs, and C.R. Whitehouse. 2000. A micromachined magnetostrictive pressure sensor using magneto-optical interrogation. Sens. Actuators, A. 81: 137–141.

Metropolis, N., A. W. Rosenbluth, M. N. Rosenbluth, A. H. Teller, and E. Teller. 1953. Equation of state calculations by fast computing machines. J. Chem. Phys. 21: 1087–1092.

Permiakov V., L. Dupré , A. Pulnikov, and J. Melkebeek. 2005. 2D magnetization of grain-oriented 3%-Si steel under uniaxial stress. J. Magn. Magn. Mater. 290–291: 1495–1498.