In-plane spin reorientation transition in a two-dimensional ferromagnetic/antiferromagnetic system studied using Monte Carlo simulations

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We investigated the in-plane spin reorientation transition (SRT) in a two-dimensional ferromagnetic/antiferromagnetic system by using Monte Carlo simulation based on the Heisenberg model. The temperature-driven SRT in the ferromagnetic layer is studied for the case of that the antiferromagnetic layer has an uniaxial in-plane or fourfold in-plane anisotropy. For the case of an uniaxial in-plane anisotropy in the antiferromagnetic layer, the ferromagnetic layer spin processes a 90° in-plane SRT from perpendicular to parallel direction of the anisotropy. For the case of a fourfold in-plane anisotropy in the antiferromagnetic layer, the ferromagnetic layer spin processes a 45° in-plane SRT. We also studied the Curie temperature of the ferromagnetic layer and find a significant reduction in the Curie temperature as the Curie temperature is close to the SRT temperature.

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I. INTRODUCTION

Since the discovery of exchange bias in Co particles covered by antiferromagnetic (AF) oxide (CoO) layers,[1] the magnetic properties in ferromagnetic (F)/AF systems have been intensively studied in nanomagnetism research.[2,3] Recently, several groups reported an unusual spin reorientation transition (SRT) of the ferromagnetic layer in F/AF layered structures.[4–8] For example, the Fe spin in NiO/Fe(001) system[4] is found to be perpendicular to the NiO spin direction for NiO films thinner than a critical thickness and is parallel to the NiO spin direction above the NiO critical thickness. In FeMn/Co/Cu(001) system,[8] the antiferromagnetic order of the FeMn layer switches the Co magnetization easy axis from [110] direction to [100] direction (45°). Note that in the above two examples the ferromagnetic layer thickness and its interface with the antiferromagnetic layer is unchanged, the observed SRT has to be related to the F/AF interfacial interaction, demonstrating the importance of the F/AF interfacial interaction in the overall magnetic anisotropy of the ferromagnetic layer.

Since F/AF systems are widely applied to magnetic devices such as magnetic read heads, spin valves, and magnetic memory mediums, etc.,[9,10] understanding the underlying mechanism of the observed SRT becomes crucial to the development of future technology. Despite the extensive effort made both experimentally and theoretically, a complete understanding of this SRT has not been achieved yet. For example, it is unclear on how to determine the coupling angle between the ferromagnetic and the antiferromagnetic spins at the F/AF interface, and why there exist both perpendicular[11–13] and collinear[14,15] couplings at the F/AF interface. The existence of the SRT in the ferromagnetic layer suggests that the coupling angle depends on specific conditions of the F/AF interaction.

Although it is well recognized that the F/AF interfacial interaction plays the key role in the SRT, it remains a challenge to explore the microscopic mechanism of the SRT. In an effort to understand how the F/AF interfacial interaction generates the ferromagnetic layer SRT, we carried out a simulation study on the micromagnetic structure of a double layered two-dimensional F/AF system under various conditions. First, we modeled the system based on square grids which interact under Heisenberg spin model and have anisotropy energy in the form of the Néel's surface anisotropy model's. And we developed a computational simulation program which uses the Monte Carlo (MC) method based on the Metropolis algorithm. With the program, we simulated the F/AF system under various conditions to obtain the corresponding micromagnetic structures statistically. Next, we examined the obtained micromagnetic structures and searched for the temperature-driven SRT. Finally, we investigated the change in the spin configuration near the SRT and studied the relationship between the SRT and the Curie temperature. We find that there exists a temperature-driven SRT in F/AF system due to the change in the F/AF coupling angle and that there is a significant reduction in the ferromagnetic layer Curie temperature in the SRT region.

II. MODEL AND SIMULATION

Since most of the experimental F/AF thin films that exhibit the discussed in-plane SRT (e.g., Co/FeMn and Fe/NiO) are crystals with cubic symmetry and with the surface-normal direction along the [001] axis,[16,17] we used a square grid model composed of two sheets in our simulation with, one sheet representing the F layer and the other representing the AF layer [Fig. 1]. To correspond to the realistic F/AF experimental systems in which each magnetic layer consists of several sheets of atomic layers, the nearest-neighbor interaction in each grid of our sheet model has to be adjusted accordingly. For example, the interaction strength at a grid point in the F layer is actually the total interaction strength accounting both the interaction of the interfacial ferromag-

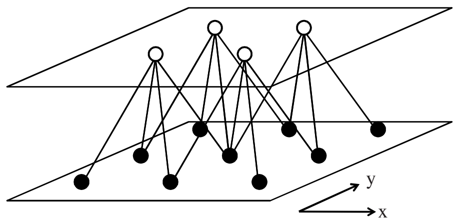

FIG. 1. Schematic drawing of the ideal two-dimensional F/AF system. Lines between the layers represent the interlayer interaction.

netic atoms and the additional interactions via above ferromagnetic layers. Hence, the normalized exchange energy factor J used in our study represent the sum of the exchange coupling energy with other atoms within its interaction range, $J=N\times J_0$, where N is the number of pairwise interaction and J_0 is a constant coupling energy of one pair. For ultrathin films, the interaction strength in our model should then be approximately proportional to the experimental film thickness $J=qJ_0[1-(n-1)/(2N_0)]$, where q is the number of pairwise interactions in a layer, n is the thickness of the film in monolayer (ML) unit, and N_0 is the thickness parameter depending on materials (for example, N_0 of Co is 2.2 ML and N_0 of Ni is 4.7 ML).[18,19] For a thick film ($n \gg N_0$), the dependency can be predicted by finite-size scaling theory and it has general form of $J\propto[(N_0+1)/2n]^{-1}$. The exchange interaction strength in the AF layer sheet of our model also accounts not only the interaction of the interfacial atoms but also bypass interaction via other AF layers.

At the (001) F/AF interface of bcc or fcc lattice, one F (or AF) interfacial atom sits right above the center of four AF (or F) atoms thus interacts with these four AF (or F) atoms with equal strength. For this reason, we shift the two square grids so that each lattice site interacts equally with four lattice sites of the other grid [Fig. 1] to represent the interfacial interaction. In addition, each lattice site interacts with four nearest-neighbor sites of its own grid. In this way, our model reasonably represents the F/AF systems of bcc or fcc films with the surface-normal direction being (001) axis. We also adopted the Heisenberg model for a free directional rotation of magnetization and added the anisotropy energy terms. We applied shape anisotropy on the F layer to force the F spins in the plane of the film to focus on the in-plane SRT.

Then the total energy of the system is given by

$$E=-J_{\mathrm{F}}\sum_{n.n.}\vec{S}_{\mathrm{F}i}\cdot\vec{S}_{\mathrm{F}i'}+J_{\mathrm{AF}}\sum_{n.n.}\vec{S}_{\mathrm{AF}i}\cdot\vec{S}_{\mathrm{AF}i'}-J_{\mathrm{int}}\sum_{n.n.}\vec{S}_{\mathrm{F}i}\cdot\vec{S}_{\mathrm{AF}i}+D_z\sum_i S_{z,\mathrm{F}i}^2-K_{y,\mathrm{F}}\sum_i S_{y,\mathrm{F}i}^2+K_{xy,\mathrm{F}}\sum_i S_{x,\mathrm{F}i}^2\cdot S_{y,\mathrm{F}i}^2-K_{y,\mathrm{AF}}\sum_i S_{y,\mathrm{AF}i}^2+K_{xy,\mathrm{AF}}\sum_i S_{x,\mathrm{AF}i}^2\cdot S_{y,\mathrm{AF}i}^2. \quad (1)$$

The normalized constants J_{F}, J_{AF}, and J_{int} are the exchange interaction energy constants. D_z represents shape anisotropy constant in the F layer and $K_{y,\mathrm{F}}$, $K_{y,\mathrm{AF}}$, $K_{xy,\mathrm{F}}$, and $K_{xy,\mathrm{AF}}$ are uniaxial and fourfold in-plane anisotropy constants in F and AF layers, respectively. Since the anisotropy originated from the symmetry breaking of the crystalline structure and that (001) fcc or bcc surface has fourfold symmetry in the xy plane, the in-plane uniaxial anisotropy exists only on a vicinal (001) surface.[20,21] Thus, the in-plane uniaxial anisotropy in our model is actually used to simulate the vicinal surface although the square grid itself is not a vicinal surface.

We used a MC method to study the effect of temperature on the spin configuration. In the MC simulation,[22] each sheet is composed of 2500 grids with a periodic boundary condition. We reassigned the spin of each grid according to the statistical probability of a canonical ensemble $P\propto\exp(-\varepsilon/T)$, where ε is the energy of one site and is a function of its spin direction. The ε was calculated through the effective local field $\vec{h}_{\mathrm{eff}}$ which contains the effect of the exchange and the anisotropy,

$$\varepsilon_{\mathrm{F}i}=-\vec{S}_{\mathrm{F}i}\cdot\vec{h}_{\mathrm{eff},i}=-\vec{S}_{\mathrm{F}i}\cdot\left[J_{\mathrm{F}}\sum_{n.n.}\vec{S}_{\mathrm{F}i'}+J_{\mathrm{int}}\sum_{n.n.}\vec{S}_{\mathrm{AF}i'}-D_zS_{z,\mathrm{F}i}\hat{z}+K_{y,\mathrm{F}}S_{y,\mathrm{F}i}\hat{y}-\frac{K_{xy,\mathrm{F}}}{2}(S_{y,\mathrm{F}i}^2S_{x,\mathrm{F}i}\hat{x}+S_{x,\mathrm{F}i}^2S_{y,\mathrm{F}i}\hat{y})\right],$$

$$\varepsilon_{\mathrm{AF}i}=-\vec{S}_{\mathrm{AF}i}\cdot\vec{h}_{\mathrm{eff},i}=-\vec{S}_{\mathrm{AF}i}\cdot\left[-J_{\mathrm{AF}}\sum_{n.n.}\vec{S}_{\mathrm{AF}i'}+J_{\mathrm{int}}\sum_{n.n.}\vec{S}_{\mathrm{F}i}+K_{y,\mathrm{AF}}S_{y,\mathrm{AF}i}\hat{y}-\frac{K_{xy,\mathrm{AF}}}{2}(S_{y,\mathrm{AF}i}^2S_{x,\mathrm{AF}i}\hat{x}+S_{x,\mathrm{AF}i}^2S_{y,\mathrm{AF}i}\hat{y})\right]. \quad (2)$$

In one iteration of a site, a random numbers r from 0 to 1 returns new spin value along H_{eff} as given below

$$S_{\mathrm{along}H_{\mathrm{eff}}}=\frac{T\,\mathrm{Log}\left[\mathrm{Exp}\left(-\frac{H_{\mathrm{eff}}}{T}\right)+2r\times\mathrm{Sinh}\left(\frac{H_{\mathrm{eff}}}{T}\right)\right]}{H_{\mathrm{eff}}}. \quad (3)$$

Then, the perpendicular component of the new assigned spin is given by $S_{\perp H_{\mathrm{eff}}}=\sqrt{1-(S_{\mathrm{along}H_{\mathrm{eff}}})^2}$.

We first iterated the algorithm until the system reached its stable state and second iterated 50 000 times to obtain the total magnetization and the susceptibility statistically; hence, we obtained the statistics over 10^8 sites. The magnetization is averaged over whole iteration and the susceptibility is obtained using the fluctuation-dissipation theorem, $\chi=\frac{1}{T}(\overline{M^2}-\overline{M}^2)$. We defined the SRT temperature where the direction of magnetization changes to the other direction. The Curie temperature in our study was defined where the fluctuation of magnetization exceeds the averaged value of the magnetization. We checked that the Curie temperature defined in this way is the same as the Curie temperature defined by the peak of the susceptibility.

III. RESULT AND DISCUSSION

Before studying the temperature-driven SRT, we first investigate the possible spin configurations in the lowest en-

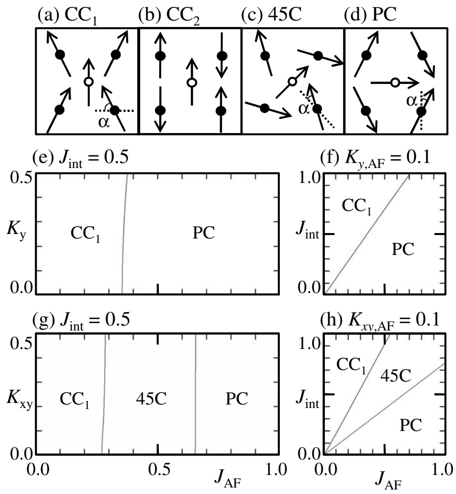

FIG. 2. Schematic diagram of the spin configurations, (a) CC_1, (b) CC_2, (c) 45C, and (d) PC. The filled and void circles represent AF and F sites each. The phase maps (e) in J_{AF}-K_y plane and (f) in J_{AF}-J_{int} plane of the system where the anisotropy in the AF layer is uniaxial. The phase maps (g) in J_{AF}-K_{xy} plane and (h) in J_{AF}-J_{int} plane of the system where the anisotropy in the AF layer is fourfold in plane.

ergy state. Figures 2(a)–2(d) show the result of the spin figurations at zero temperature for the case that the anisotropy in the AF layer is either uniaxial ($K_{y,AF}\neq 0$ and $K_{xy,AF}=0$) or fourfold ($K_{y,AF}=0$ and $K_{xy,AF}\neq 0$). In the collinear coupling (CC) configuration (CC_1 and CC_2), the spin direction of the F layer is parallel to the anisotropy direction of the AF layer. In the perpendicular coupling (PC) configuration, the spin direction of the F layer is perpendicular to the anisotropy direction of the AF layer. In the 45° coupling (45C) configuration, the spin direction of the F layer is 45° from the anisotropy direction of the AF layer. We here refer the collinear, perpendicular, and 45° couplings to CC, PC, and 45C for convenience even though the angle between AF spin and individual F does not need to be exact 0°, 90°, and 45°. The angle α in Fig. 2 defines the angle of the antiferromagnetic spin away from the perpendicular axis of the F spin and is used to show the F/AF interfacial coupling result where the total energy of the system is minimized. We then numerically calculated the energy minimums of the spin configurations of Figs. 2(a)–2(d) by varying the F and AF spin directions, and obtained the ground-state spin configurations by comparing the minimized energies of the four spin configurations.

Figure 2(e) shows a phase diagram in the J_{AF}-$K_{y,AF}$ plane under the condition of $K_{y,F}=0$ and $K_{y,AF}\neq 0$. We find that the system in this situation takes either the CC_1 phase or the PC phase. The CC_2 phase appears only when there exists the uniaxial anisotropy or temperature is not zero. We discuss the CC_2 phase later in this paper. The CC_1 and PC phases are divided by the boundary of $J_{AF}\cong 0.71\ J_{int}$. The phase boundary is not much affected by the value of $K_{y,AF}$, as far as $K_{y,AF}<J_{int}$. For J_{AF} much less than J_{int}, we find that the ground state has the CC_1 phase in which the interlayer coupling energy dominates the energy minimizing process. For J_{AF} much greater than J_{int}, we find that the ground state has the PC phase in which the AF exchange coupling energy dominates the energy minimizing process. Without the presence of the uniaxial anisotropy in the AF layer, the system is rotational invariant with respect to the surface-normal direction so that the CC_1 and PC spin configurations are actually geometrically same except different values of the deviation angle α. However, in the presence of the uniaxial anisotropy in the AF layer, the symmetry between these two configurations is broken, making the CC_1 and PC two different phases. Assuming that the y axis is the AF easy axis as shown in Figs. 2(a) and 2(d), the F spin direction will change from the y axis (CC_1 phase) to the x axis (PC phase) as the J_{AF} increases above a critical value [Fig. 2(e)], i.e., the variance of J_{AF}/J_{int} induces a SRT of the F layer [Fig. 2(f)]. The SRT found in F/AF system has usually attributed to the establishment of the AF order in the AF layer.[11,23] Our calculation shows that the F layer SRT could also exist even at zero temperature by changing the ratio of J_{AF}/J_{int}, e.g., by increasing the AF layer thickness to increase the effective J_{AF} while maintaining the interaction strength J_{int}.

Different from the AF spins that fluctuate from site to site, we find that all the ferromagnetic spins align exactly in the same direction. This can be easily understood because each F spin interacts with four AF spins so that their effect to the F spin due to the fluctuations is exactly canceled out. We then can understand why there is a CC_1-to-PC SRT for the F layer. When all F spins are locked to the same direction, the F/AF interfacial interaction is equivalent of applying a magnetic field of J_{int} to AF spins with the field direction pointing to the F spin direction. Under this situation, perpendicular alignment between F and AF spins should occur with the AF spins tilting toward the F spin direction. On the other hand, tilting away from the AF easy axis causes anisotropy energy. Then we should have the following two scenarios. (1) For weak J_{int}, the AF tilting angle α is very small so that the energy lowered by PC configuration is more than the increased anisotropy energy, leading to the PC spin configuration as shown in Fig. 2(d). (2) For very strong J_{int}, the AF spins tilt so much away from the easy axis ($\alpha>45°$) that the AF spins look like ferromagnetically aligned or the AF spins are parallel to the F spins. Because a rotation of both the AF and F spins around the surface-normal direction will not change the F/AF interfacial interaction, a 90° rotation of all the AF and F spins for $\alpha>45°$ (CC_1 configuration) will obviously reduce the increased anisotropy energy. That is why there is a CC_1-to-PC SRT for the F layer as the J_{AF}/J_{int} increases. In fact the SRT should occur at $\alpha=45°$ where $J_{AF}/J_{int}=1/[2\sin(\pi/4)]\cong 0.72$ which roughly agrees with the simulation result.

If there exist an uniaxial anisotropy in F layer, the energies in a unit cell containing a F grid and an AF grid in Eq. (1) as a functions of α in PC, CC phases are given by

$$U_{PC} = -2J_F + 2J_{AF}(\sin^2\alpha - \cos^2\alpha) - 4J_{int}\sin\alpha - K_{y,AF}\cos^2\alpha = -2J_F - 2J_{AF} - K_{y,AF} - \frac{J_{int}^2}{J_{AF} + (1/4)K_{y,AF}}, \quad (4)$$

$$U_{CC_1} = -2J_F + 2J_{AF}(\sin^2\alpha - \cos^2\alpha) - 4J_{int}\sin\alpha - K_{y,F} - K_{y,AF}\sin^2\alpha = -2J_F - 2J_{AF} - K_{y,F} - \frac{J_{int}^2}{J_{AF} - (1/4)K_{y,AF}}, \quad (5)$$

$$U_{CC_2} = -2J_F - 2J_{AF} - K_{y,F} - K_{y,AF}. \quad (6)$$

In the case, CC_2 phase can be the most stable state that has minimum energy and the SRT conditions with other phases are

$$K_{y,F} \cong \frac{J_{int}^2}{J_{AF}}, \quad K_{y,AF} \cong \frac{J_{int}^2}{J_{AF}}. \quad (7)$$

The SRT between CC_1 and PC can be found from the minimization condition of the energies $\frac{\partial U}{\partial \alpha}=0$ and the SRT condition $U_{PC}-U_{CC}=0$, which gives the following relations between the exchange energy constants and the anisotropy constants.

$$\frac{J_{int}}{2J_{AF}} \cong \sqrt{\frac{1}{2} - \frac{K_{y,F}}{2K_{y,AF}}}. \quad (8)$$

Next, we discuss the case that there exists only fourfold in-plane anisotropy in the F and AF layers ($K_y=0$ and $K_{xy}\neq 0$). Under this situation, we find that 45C phase could be the lowest energy state because the fourfold in-plane anisotropy energy is effectively minimized in the 45C phase. We first consider the case that only the AF layer carries the fourfold anisotropy ($K_{xy,F}=0$). We find that the 45C phase exists as $0.54 < J_{AF}/J_{int} < 1.31$, as shown in Figs. 2(g) and 2(h). The PC and CC_1 phases are actually the same in the sense that the direction of the F spin is the same as the anisotropy direction of the AF layer in the fourfold anisotropy case. It is only a matter of different α value ($\alpha < \pi/4$ for PC and $\alpha > \pi/4$ for CC_1).

The energies of the CC_1/PC and 45C phases are given by

$$U_{PC/CC} = -2J_F + 2J_{AF}(\sin^2\alpha - \cos^2\alpha) - 4J_{int}\sin\alpha + K_{xy,AF}\cos^2\alpha \cdot \sin^2\alpha, \quad (9)$$

$$U_{45C} = -2J_F + 2J_{AF}(\sin^2\alpha - \cos^2\alpha) - 4J_{int}\sin\alpha + K_{xy,AF}\cos^2\left(\frac{\pi}{4} - \alpha\right) \cdot \sin^2\left(\frac{\pi}{4} - \alpha\right) + \frac{1}{4}K_{xy,F}. \quad (10)$$

The SRT condition in this case is given by

$$\frac{J_{int}}{2J_{AF}} \cong \left(\frac{1}{2} \pm \frac{1}{2}\sqrt{\frac{1}{2} - \frac{K_{xy,F}}{2K_{xy,AF}}}\right)^{1/2}, \quad (11)$$

where the positive sign is for the SRT condition between PC/45C and negative sign is for the SRT condition between CC_1/45C. For $K_{xy,F}=0$, the SRT condition for CC_1/45C is $J_{AF}/J_{int} \cong 1.31$ and the SRT condition for 45C/PC is $J_{AF}/J_{int} \cong 0.54$. This result roughly agrees with our simulation result. For nonzero $K_{xy,F}$, the 45C phase window in the phase map changes slightly. If the F anisotropy direction is the same as the AF anisotropy direction, the 45C window gets narrower and if the F anisotropy direction is different from the AF anisotropy direction by 45°, the 45C window gets wider.

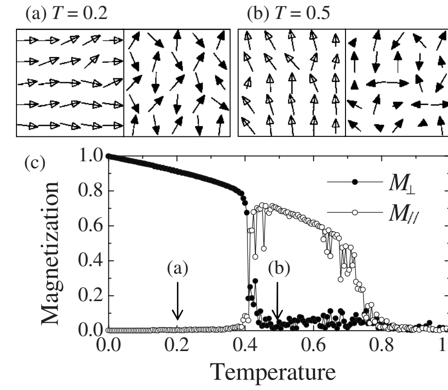

FIG. 3. Snapshots of MC simulation showing the spin configurations in the F layer (left) and the AF layer (right) for the case of an uniaxial anisotropy only in AF layer ($K_{y,F}=0$ and $K_{y,AF}\neq 0$) at (a) $T=0.2$ and (b) $T=0.5$. (c) The magnetizations of the F layer, perpendicular to the uniaxial anisotropy direction (line with filled circles) and parallel with the direction (line with void circles) as a function of temperature.

In Co/FeMn system, the Co 45° SRT from [110] to [100] was found as the FeMn thickness changes and the [100]-type atomic steps at the interface were attributed to cause this SRT.[24,25] Our simulation result shows that 45° SRT could occur even at flat interface without the interfacial roughness.

We next studied the temperature effect on the SRT for the case of an uniaxial anisotropy in the AF layer. Figures 3(a) and 3(b) show snapshot of the spin configurations from the MC simulation for the case $K_F=0$. At low temperature $T=0.2$ ($J_F=1.0$, $J_{AF}=0.6$, $J_{int}=0.5$, and $K_{y,AF}=0.1$), the F spins are mainly perpendicular to the AF anisotropy direction [Fig. 3(a)]. This result agrees with the numerical solution which shows that the PC phase has the lowest energy at $J_{AF} > 0.71 J_{int}$ [Fig. 2(e)]. At high temperature $T=0.5$, the F spins are switched to the AF anisotropy direction [Fig. 3(b)]. At high temperature, although the spin direction of the AF layer becomes more random, the AF anisotropy still affects the F spins by aligning them to the AF anisotropy direction. We find that the SRT takes place at around $T_{SRT}=0.41$ where the F magnetization in the anisotropy direction (M_y) and in the perpendicular direction (M_x) crosses each other [Fig. 3(c)]. The interesting question is why there exists a SRT by increasing the temperature. We here offer a hand waving argument. Although we start at $T=0$ with the PC phase which has a lower total energy than the CC_2 phase, flipping some AF spins to the F direction at high temperature (making the system toward the CC_2 phase) actually increases the AF entropy so to reduce the total free energy. Thus, even when the total energy of the CC_2 phase is higher than the PC phase, its free energy at high temperature could be lower than the PC phase. Another interesting feature we noticed is that the Néel temperature of the free AF layer is at $T_N=0.46$ at $J_{AF}=0.6$ and $K_{y,AF}=0.1$ from the MC simulation which is higher than the SRT temperature of $T_{SRT}=0.41$. It is

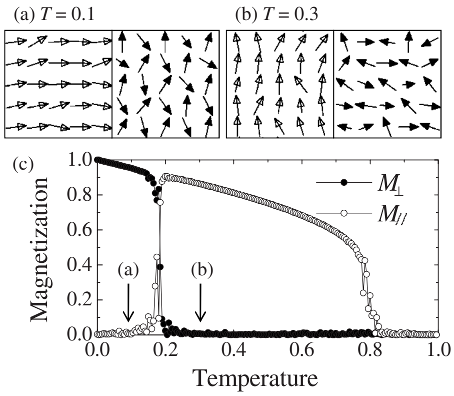

FIG. 4. Snapshots of MC simulation showing spin configurations in the F layer (left) and the AF layer (right) for the case of an uniaxial anisotropy both in F and AF layers ($K_{y,\mathrm{F}} \neq 0$ and $K_{y,\mathrm{AF}} \neq 0$) at (a) T=0.1 and (b) T=0.3. (c) The magnetizations of the F layer, perpendicular to the uniaxial anisotropy direction (line with filled circles) and parallel with the direction (line with void circles) as a function of temperature.

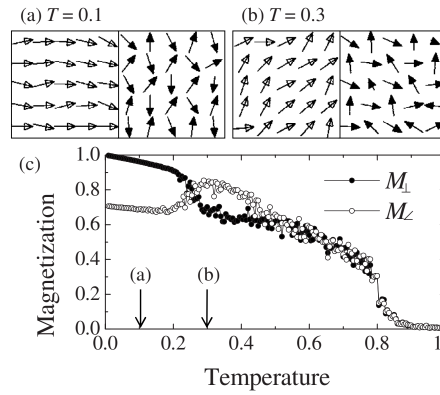

FIG. 5. Snapshots of MC simulation showing spin configurations in the F layer (left) and the AF layer (right) for the case of fourfold anisotropy ($K_{xy,\mathrm{F}}$=0 and $K_{xy,\mathrm{AF}} \neq 0$) at (a) T=0.1 and (b) T=0.3. (c) The magnetizations of the F layer, perpendicular to the uniaxial anisotropy direction (line with filled circles) and along the axis 45° from the direction (line with void circles) as a function of temperature.

interesting to observe this fact as previous studies attributed the SRT entirely to the AF order-disorder transition.

After adding an uniaxial in-plane anisotropy to the F layer while remaining the other simulation conditions, we find that the SRT position shifts due to the F anisotropy. Figure 4 shows the result of the simulation at $K_{y,\mathrm{F}}$=0.05. Figures 4(a) and 4(b) show snapshot spin configurations from the MC simulation. At low temperature T=0.1, the F spins are mainly perpendicular to the AF anisotropy direction. Though the F layer has an uniaxial anisotropy in the *y* axis, the effect of the AF anisotropy in this case is greater enough to overcome the F anisotropy. On the other hand, at T=0.3, the magnetization direction of the F layer becomes parallel to the AF anisotropy direction, leading to a CC phase of the system. The SRT from the PC phase to the CC phase takes place at about T_{SRT}=0.19 [Fig. 4(c)], which is lower than T_{SRT}=0.41 for the K_{F}=0 case.

We also find the existence of the SRT for the case of fourfold in-plane anisotropy. We here discuss K_{F}=0 case only (nonzero K_{F} only shifts the SRT to the favoring direction of the F anisotropy direction). The simulation condition is J_{F}=1.0, J_{AF}=0.7, J_{int}=0.5, and $K_{xy,\mathrm{AF}}$=0.01, where the system is close to the SRT boundary at zero temperature from Figs. 2(g) and 2(h). Therefore, the energy between the PC phase and the 45C phase is close under this condition and we expect that little fluctuation could lead to a transition between these two phases. Below T_{SRT}, we find that the spin directions of the F and AF layers are perpendicular to each other and along the AF anisotropy direction [Fig. 5(a)]. Above T_{SRT}, as shown in Fig. 5(b), the F spins switch to the direction 45° away from the AF anisotropy axis. The SRT temperature is identified in the simulation to be T_{SRT}=0.27 [Fig. 5(c)]. At higher temperature ($T > \sim 0.5$), the AF spins become random and a mixture phase of 45C and PC appears.

As the energy difference between two magnetic phases increases, we would expect the T_{SRT} also increases. Therefore, for the case of the uniaxial anisotropy in the AF layer, an increase in J_{AF} should lead to an increased T_{SRT}. We tested this speculation by tracing the T_{SRT} and T_{C} as a function of J_{AF} under the condition of J_{F}=1.0, J_{int}=0.5, and K_y=0.1. Indeed we find that the T_{SRT} increases with J_{AF} until reaching J_{AF}=0.84 where the T_{SRT} merges with T_{C}. We find that the T_{C} value is about 0.7–0.8 and varies as T_{SRT} changes. Figures 6(a)–6(c) illustrates the total magnetization and the susceptibility of the F layer as a function of temperature at J_{AF}=0.50, 0.84, and 1.40. The result shows that T_{C} is re-

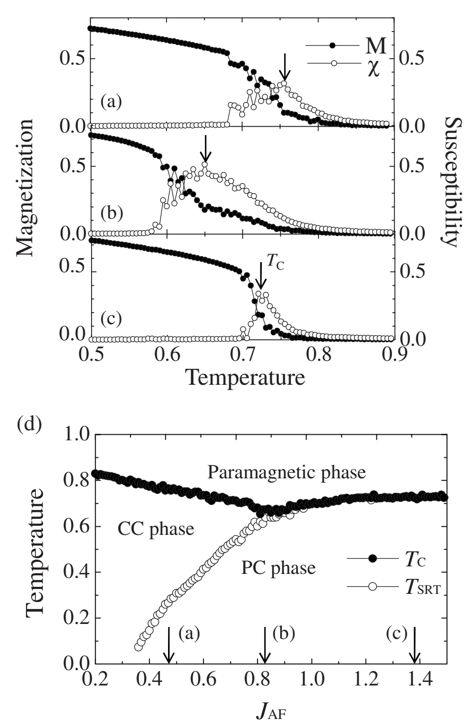

FIG. 6. Temperature dependence of the total magnetization and the susceptibility of the F layer at (a) J_{AF}=0.50, (b) J_{AF}=0.84, and (c) J_{AF}=1.40. The arrow indicates T_{C} defined at the peak of susceptibility. (d) The Curie temperature and the SRT temperature of the F layer as a function of J_{AF}.

duced when T_C and T_{SRT} are close to each other [Figs. 6(a)–6(c)].

Figure 6(d) shows a magnetic phase diagram in the J_{AF}-T plane. T_C divide the phase diagram into a ferromagnetic phase and a paramagnetic phase and T_{SRT} separates the ferromagnetic phase into PC phase and CC phase. As J_{AF} increases from 0, we find a general tendency that T_C decreases slowly, reaching a minimum value at $T_C=T_{SRT}$ and increases again after passing T_{SRT}. The reason of the Curie temperature reduction can be found from the smaller energy that is required to rotate magnetism direction around SRT where the spin degree of freedom rises. And the results partially explain the Curie temperature reduction observed in FeMn/Co bilayer system.[8]

IV. SUMMARY

As part of a research for understanding a microscopic relationship between the interfacial interaction and the SRT in crystalline F/AF thin films, we simulated the micromagnetic structure of a double layered two-dimensional F/AF system. A square grid model is used to represent the normal fcc or bcc crystalline structures of both layers. The exchange interaction among the spins is based on the Heisenberg model accounting the additional anisotropy energy. By using Monte Carlo method, we studied the spin configuration as a function of temperature according to the statistical probability of a canonical ensemble $P \propto \exp(-\varepsilon/T)$.

We studied the temperature-driven SRT in a system. For case that the AF layer has an uniaxial in-plane anisotropy, the SRT from PC phase to CC phase occurs as temperature increases. On the other hand, for the case of a fourfold in-plane anisotropy in the AF layer, there could occur a 45° SRT. We built a phase diagram among the magnetic and the coupling phases in J_{AF}-T plane and find a T_C reduction in the SRT region.

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