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Critical properties of XY model on two-dimensional layered magnetic films*

Wang Yi (王 漪)†, Liu Xiao-Yan (刘晓彦), Sun Lei (孙 雷),
Zhang Xing (张 兴), and Han Ru-Qi (韩汝琦)

Institute of Microelectronics, Peking University, Beijing 100871, *China*

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Using Monte Carlo simulations, we have investigated the classical XY model on triangular lattices of ultra-thin film structures with middle ferromagnetic layers sandwiched between two antiferromagnetic layers. The internal energy, the specific heat, the chirality and the chiral susceptibility are calculated in order to clarify phase transitions and critical phenomena. From the finite-size scaling analyses, the values of critical exponents are determined. In a range of interaction parameters, we find that the chirality steeply goes up as temperature increases in a temperature range; correspondingly the value of a critical exponent for this change is estimated.

Keywords: layered XY model, critical phenomena, ultra-thin magnetic film
PACC: 7510H, 0570J, 7540C

1. Introduction

Due to the development of the epitaxy technology, it has become possible to study magnetic properties of very thin magnetic films.[1−3] However, theoretical investigations of the magnetic thin films have been carried out, which are mainly concentrated on the ground state properties by phenomenological treatments and on the finite temperature properties in the mean field approximation.[4−6]

Magnetic thin films, layered magnets or magnets on superlattices show interesting properties that are different from bulk properties. For example, interface effects exert on influence on the entire system in the thin films and the layered structures may produce new static properties and new dynamic modes. Hence many different layered structures of magnetic materials have been considered such as ferromagnetic layers with non-magnetic layers, ferromagnetic layers with ferromagnetic layers, helical magnetic layers with non-magnetic layers, antiferromagnetic layers with ferromagnetic layers and so on.[7,8] Those magnetic materials have a variety of applications including magnetoresistive heads and magnetic or magneto-optical recording.[8]

Many theoretical investigations have been performed from several viewpoints for several Hamiltonian systems by using several methods.[9−11] However, there are still many open points that have to be clarified; even in a very simple model such as an XY model or a Heisenberg model, we may have a completely different nature of phase transitions in the thin film structures from that in the two-dimensional systems or the three-dimensional bulk systems. In the experimental investigations for layered XY magnets, it has been shown that there is a spontaneous magnetization due to a finite size effect. This has also been confirmed by Monte Carlo simulations. Although there is no spontaneous magnetization in the thermodynamic limit,[12] the existence of the spontaneous magnetization is quite an interesting phenomenon. In the thermodynamic limit, there is no long-range order but there does exist the so-called Kosterlitz–Thouless (KT) transition in the two-dimensional ferromagnetic XY models.[13] We do not discuss the details for the KT transition in the present paper. For the XY model, on the other hand, there exist the KT transition and also the chirality transition.[14] However, in the layered XY models such as a 2 to 4 layer system, we find that the ferromagnetic layer has also a chiral order at low temperatures.[15] The chirality on the

*Project supported by the National Natural Science Foundation of China (Grant No 10234010).
†E-mail address: wangyi@ime.pku.edu.cn

ferromagnetic layers shows a very steep increase in a temperature range below the critical temperature of the system. However, in the present paper, we are interested in phase transitions in the layered XY model, in which middle ferromagnetic layers are sandwiched between two antiferromagnetic layers. We find that critical behaviours are common for layered systems.

We describe our model in Section 2. In Section 3, we give the results obtained by Monte Carlo simulation and discuss the nature of phase transitions in terms of finite-size scaling analysis. The concluding remarks are given in Section 4.

2. Model and simulation scheme

We investigate phase transitions of a classical XY model on lattices of ultra-thin film structures with middle ferromagnetic layers sandwiched between two antiferromagnetic layers.

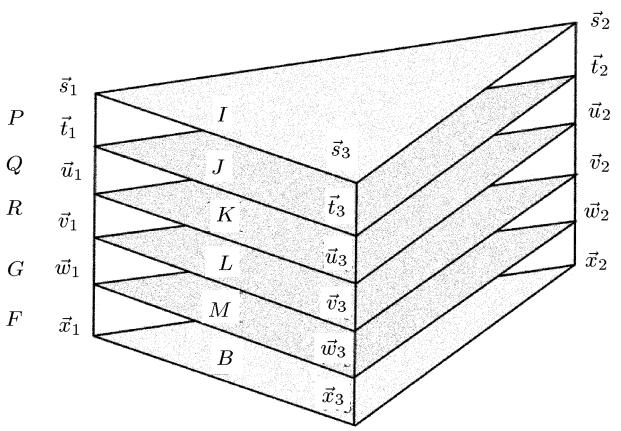


Fig.1. Unit cell of six-layer triangular lattice: $\Lambda_1, \Lambda_2, \Lambda_3, \Lambda_4, \Lambda_5$ and Λ_6. The XY spins are denoted by $\vec{s}_i$ on Λ_1, $\vec{t}_i$ on Λ_2, $\vec{u}_i$ on Λ_3, $\vec{v}_i$ on Λ_4, $\vec{w}_i$ on Λ_5 and $\vec{x}_i$ on Λ_6, respectively.

Specifically, we consider an XY model on a six-layer triangular lattice (Fig.1). The six triangular lattices are denoted by Λ_1, Λ_2, Λ_3, Λ_4, Λ_5 and Λ_6, respectively, from the top to the bottom. We assume XY spins to be denoted by $\vec{s}_i, \vec{t}_i, \vec{u}_i, \vec{v}_i, \vec{w}_i$ and $\vec{x}_i$ for $i \in \Lambda_1, \Lambda_2, \Lambda_3, \Lambda_4, \Lambda_5$ and Λ_6, respectively, where $N = |\Lambda_1| = |\Lambda_2| = |\Lambda_3| = |\Lambda_4| = |\Lambda_5| = |\Lambda_6|$. We assume that $N = N_l \times N_l$ for each layer, where N_l is the linear size of $\Lambda_k (k = 1, 2, 3, 4, 5, 6)$. Then the six-layer triangular lattice is represented by Λ:

$$\Lambda = \Lambda_1 + \Lambda_2 + \Lambda_3 + \Lambda_4 + \Lambda_5 + \Lambda_6 \,. \tag{1}$$

Hence the total number of lattice sites of the six-layer triangular lattice is equal to $6N$. The Hamiltonian is given as follows:

$$\begin{aligned}\mathcal{H} = &- I \sum_{(ij)} \vec{s}_i \cdot \vec{s}_j - J \sum_{(ij)} \vec{t}_i \cdot \vec{t}_j - K \sum_{(ij)} \vec{u}_i \cdot \vec{u}_j \\ &- L \sum_{(ij)} \vec{v}_i \cdot \vec{v}_j - M \sum_{(ij)} \vec{w}_i \cdot \vec{w}_j - B \sum_{(ij)} \vec{x}_i \cdot \vec{x}_j \\ &- P \sum_{i} \vec{s}_i \cdot \vec{t}_i - Q \sum_{i} \vec{t}_i \cdot \vec{u}_i - R \sum_{i} \vec{u}_i \cdot \vec{v}_i \\ &- G \sum_{i} \vec{v}_i \cdot \vec{w}_i - F \sum_{i} \vec{w}_i \cdot \vec{x}_i \,. \end{aligned} \tag{2}$$

Here we have assumed that intralayer interactions take place only between spins at nearest-neighbour lattice sites on each of $\Lambda_1, \Lambda_2, \Lambda_3, \Lambda_4, \Lambda_5$ and Λ_6; those interaction constants are denoted by I, J, K, L, M and B, respectively. The sum with (i, j) indicates a summation over nearest-neighbour pairs of sites on $\Lambda_1, \Lambda_2, \Lambda_3, \Lambda_4, \Lambda_5$ or Λ_6. We have also assumed interlayer exchange interactions occurring between spins at a site i on Λ_l and at its corresponding site i on Λ_{l+1} for $l = 1, 2, 3, 4$ and 5; those interaction constants are denoted by P, Q, R, G and F, respectively. The sum with i indicates a summation over pairs of sites i on $\Lambda_1 + \Lambda_2$, $\Lambda_2 + \Lambda_3$, $\Lambda_3 + \Lambda_4$, $\Lambda_4 + \Lambda_5$ or $\Lambda_5 + \Lambda_6$. We assume the periodic boundary conditions for each layer $\Lambda_1, \Lambda_2, \Lambda_3, \Lambda_4, \Lambda_5$ or Λ_6. Here we express $\vec{s}_i, \vec{t}_i, \vec{u}_i, \vec{v}_i, \vec{w}_i$ and $\vec{x}_i$ as follows:

$$\begin{aligned} &\vec{s}_i = (\cos\theta_i, \sin\theta_i)\,, \qquad \vec{t}_i = (\cos\phi_i, \sin\phi_i)\,, \\ &\vec{u}_i = (\cos\psi_i, \sin\psi_i)\,, \qquad \vec{v}_i = (\cos\omega_i, \sin\omega_i)\,, \\ &\vec{w}_i = (\cos\varphi_i, \sin\varphi_i)\,, \qquad \vec{x}_i = (\cos\xi_i, \sin\xi_i)\,. \end{aligned} \tag{3}$$

We notice that there are relations:

$$\begin{aligned} &\Gamma(I, J, K, L, M, B, P, Q, R, G, F) \\ &\quad = \Gamma(I, J, K, L, M, B, \pm P, \pm Q, \pm R, \pm G, \pm F)\,. \end{aligned} \tag{4}$$

for a thermodynamic quantity $\Gamma(I, J, K, L, M, B, P, Q, R, G, F)$. Then we assume that $P > 0$, $Q > 0$, $R > 0$, $G > 0$ and $F > 0$ without loss of generality.

In the present paper, we investigate the system with $I = B = -1$ and $J = K = L = M > 0$; namely the exchange interactions on the top layer Λ_1 and on the bottom layer Λ_6 are antiferromagnetic and those on the four middle layers $\Lambda_2, \Lambda_3, \Lambda_4$ and Λ_5 are ferromagnetic. We say, in this system, the XY model is on the six-layer triangular lattice with four ferromagnetic layers sandwiched between two antiferromagnetic layers.

Furthermore, we assume that the interlayer interaction constants for ferromagnetic layers are equal to

1.0 and the intralayer interaction constants for antiferromagnetic layers are -1.0. By changing the intralayer interaction constants between -1.0 and 1.0, we calculate thermodynamic quantities such as the internal energy, the specific heat, the chirality, the chiral susceptibility and so on by using Monte Carlo simulation. Phase transitions and critical phenomena are clarified for an XY model on lattices of ultrathin film structure systems (2 to 6 layers) such as $K = L = M = B = 0$, $Q = R = G = F = 0$ for a two-layer system;[15] $L = M = B = 0$, $R = G = F = 0$ for a three-layer system;[16] $M = B = 0$, $G = F = 0$ for a four-layer system;[17] and so on. The critical behaviours are clarified by using finite-size scaling analysis.

3. Results by Monte Carlo simulations

We investigate the system by standard Monte Carlo (MC) simulations. Hereafter we just mention only the values of J in order to indicate the system. We perform our MC simulations for $N = N_l \times N_l$ with $N_l = 24, 36$ and 48. We use random spin configurations as initial spin configurations in our MC simulations. An MC average, $\langle \mathcal{O} \rangle$, for a quantity $\mathcal{O}$ is calculated by

$$\langle \mathcal{O} \rangle = \frac{1}{n - n_0} \sum_{t=n_0+1}^{n} \mathcal{O}(t) , \tag{5}$$

where we choose $n_0 = 2.5 \times 10^5$ MC steps, $n = 5 \times 10^5$ MC steps, and also $n_0 = 5 \times 10^5$ MC steps and $n = 10^6$ MC steps, depending upon the system size and the value of temperature. We set the Boltzmann constant k to be 1 throughout the present paper.

We calculate the internal energy $\mathcal{E}$, the specific heat C, the chirality $\mathcal{K}$, the chiral susceptibility χ and so on. The internal energy is given by

$$\mathcal{E} = \frac{\langle \mathcal{H} \rangle}{\Xi N} , \tag{6}$$

where Ξ denotes the number of system layers ($\Xi = 2, 3, 4, 5$ and 6). Then the six-layer triangular lattice is denoted by $\Xi = 6$.

The specific heat is obtained by

$$C = \frac{\langle \mathcal{H}^2 \rangle - \langle \mathcal{H} \rangle^2}{\Xi N T^2} . \tag{7}$$

The chirality is defined at a smallest up-triangle, namely an elementary upward triangle on each of planes: Λ_1, Λ_2, Λ_3, Λ_4, Λ_5 or Λ_6. For example, the chirality, $\mathcal{K}^s_{ijk}$, on the Λ_1 plane is given as follows:

$$\mathcal{K}^s_{ijk} = \frac{2}{3\sqrt{3}} (\vec{s}_i \times \vec{s}_j + \vec{s}_j \times \vec{s}_k + \vec{s}_k \times \vec{s}_i) \cdot \hat{e}_z$$
$$= \frac{2}{3\sqrt{3}} [\sin(\theta_j - \theta_i) + \sin(\theta_k - \theta_j) + \sin(\theta_i - \theta_k)] , \tag{8}$$

where $\hat{e}_z$ is the unit vector of z-component in the spin space. A set of sites $\{i, j, k\}$ express three sites labelled counterclockwise on an up-triangle of lattice Λ_1. In a similar way, we define the chiralities $\mathcal{K}^t_{ijk}$, $\mathcal{K}^u_{ijk}$, $\mathcal{K}^v_{ijk}$, $\mathcal{K}^w_{ijk}$ and $\mathcal{K}^x_{ijk}$ on lattices Λ_2, Λ_3, Λ_4, Λ_5 and Λ_6, respectively. The average chirality for the whole system is defined as

$$\mathcal{K} = \frac{1}{\Xi} \sum_{i=s}^{x} (\mathcal{K}_i) , \qquad (i = s, t, u, v, w, x) \tag{9}$$

with

$$\mathcal{K}_s = \frac{1}{N} \sum_{(i,j,k)} \langle \mathcal{K}^s_{ijk} \rangle , \tag{10}$$

where the sum with (i, j, k) is taken over all the elementary up-triangles on the lattice Λ_1. In a similar way, we define $\mathcal{K}_t$, $\mathcal{K}_u$, $\mathcal{K}_v$, $\mathcal{K}_w$ and $\mathcal{K}_x$ in Eq.(9).

The chiral susceptibility[18] is obtained by

$$\chi_s = \frac{\langle |\mathcal{K}_s|^2 \rangle - \langle |\mathcal{K}_s| \rangle^2}{T} . \tag{11}$$

In a similar way, we have defined χ_t, χ_u, χ_v, χ_w and χ_x in Eq.(11).

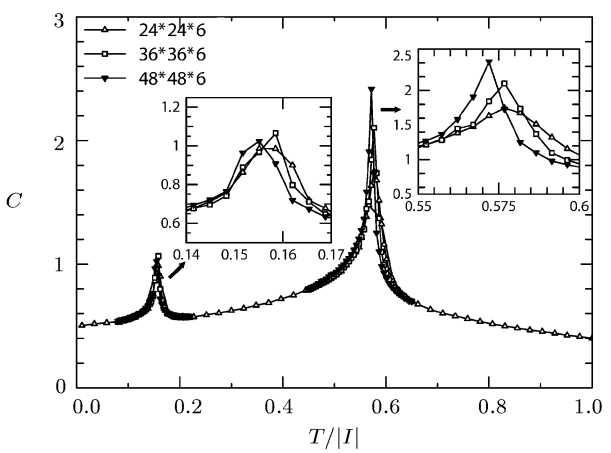


Fig.2. Specific heat C as a function of $T/|I|$ for $I = B = -1, P = Q = R = G = F = 1$ and $J = K = L = M = 0.075$. We show the results for $N_l = 24$ by open triangles, those for $N_l = 36$ by open squares and $N_l = 48$ by solid triangles. The insets show the size-dependent specific heat near $T_{\rm c1}$ and $T_{\rm cu}$.

In order to investigate the critical behaviour for the six-layer system, we set $I = B = -1, P = Q = R = G = F = 1$ and $J = K = L = M = 0.075$. We

show the specific heat respectively for $N_l = 24, 36$ and 48 in Fig.2. We denote two temperatures, at which the specific heat curve shows sharp peaks by $T_{\rm cl}$ and $T_{\rm cu}$ ($T_{\rm cl} < T_{\rm cu}$) hereafter. We notice that the behaviour of the specific heat is the same as that occurring in the 2 to 4 layer systems studied previously.[17] We calculate the chirality and the chiral susceptibility for each layer. It is expected that the chirality is responsible for the sharp peak of the specific heat at $T_{\rm cl}$. Figure 3 shows that the chiralities $\mathcal{K}_s$ on Λ_1, and $\mathcal{K}_x$ on Λ_6 are almost the same and increase as temperature decreases from $T_{\rm cu}$. Although there is a very little dip near $T_{\rm cl}$, the chiralities of middle layers ($\mathcal{K}_t$ on Λ_2, $\mathcal{K}_u$ on Λ_3, $\mathcal{K}_v$ on Λ_4 and $\mathcal{K}_w$ on Λ_5) show different behaviours from those of $\mathcal{K}_s$ and $\mathcal{K}_x$; the chiralities of middle layers show a steep decrease near and below $T_{\rm cl}$ as temperature decreases from $T_{\rm cl}$ as shown in Fig.4.

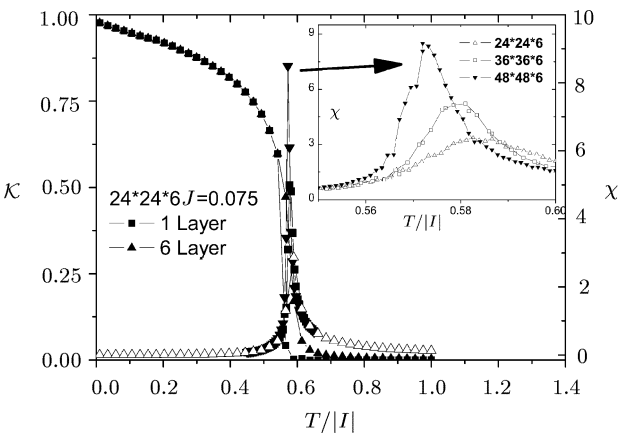


Fig.3. The chirality $\mathcal{K}$ and the chiral susceptibility χ in the top and the bottom layers as a function of $T/|I|$ for $I = B = -1$, $P = Q = R = G = F = 1$ and $J = K = L = M = 0.075$. The results for $N_l = 24$ are denoted by open triangles, those for $N_l = 36$ by open squares and those for $N_l = 48$ by solid triangles. The inset shows the size-dependent chiral susceptibility near $T_{\rm cu}$.

Figure 3 shows the chiral susceptibility χ of $\mathcal{K}_s$ on Λ_1, and $\mathcal{K}_x$ on Λ_6. The chiral susceptibility peak height goes up as the linear system size increases, for example when $N_l = 24, 36$ and 48 as shown in the inset of Fig.3. From Fig.4, we see that there are two sharp peaks of the chiral susceptibility. We find that the behaviour of height values, $\chi_{\rm top}$, of the chiral susceptibility near $T_{\rm cl}$ is different from that near $T_{\rm cu}$; we can see that $\chi_{\rm top}$ is close to $T_{\rm cl}$ as shown in the inset of Fig.4.

In order to investigate the critical behaviour of the six-layer system, we make the finite-size scaling analyses of the specific heat and the chirality at $T_{\rm cl}$ and $T_{\rm cu}$. We set $J = K = L = M = 0.075$ and then estimate $T_{\rm cl} = 0.1555$ and $T_{\rm cu} = 0.5666$.

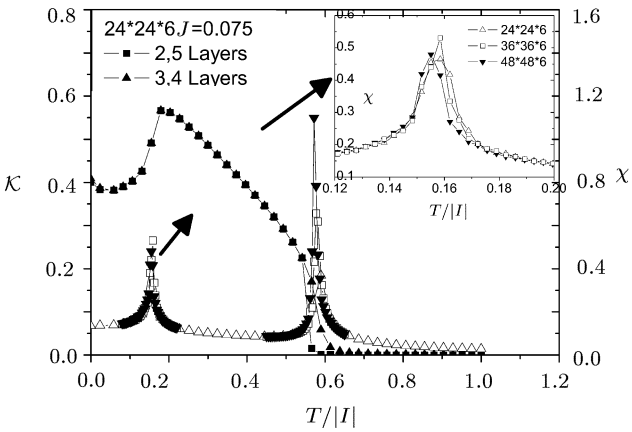


Fig.4. The chirality $\mathcal{K}$ and the chiral susceptibility χ in the middle layers as a function of $T/|I|$ for $I = B = -1, P = Q = R = G = F = 1$ and $J = K = L = M = 0.075$. The results for $N_l = 24$ are denoted by open triangles, those for $N_l = 36$ by open squares and those for $N_l = 48$ by solid triangles. The inset shows the size-dependent chiral susceptibility near $T_{\rm cl}$.

A finite-size scaling analysis of the specific heat near $T_{\rm cl}$ and $T_{\rm cu}$ indicates $\nu = 0.83 \pm 0.05$ and $\alpha = 0.28 \pm 0.03$ at $T_{\rm cl}$, and $\nu = 1.01 \pm 0.05$ and $\alpha = 0$ at $T_{\rm cu}$. At $T_{\rm cl}$, we define the critical exponent β as follows:

$$\mathcal{K}_f \sim \mathcal{K}_f^{(c)} - a(T_{\rm cl} - T)^{\beta} \qquad (T \lesssim T_{\rm cl})\,, \tag{12}$$

where $\mathcal{K}_f^{(c)}$ is a maximum of the chirality on the ferromagnetic layer (middle layers) and a is a constant. A finite-size scaling analysis of the chirality near $T_{\rm cu}$ is shown in Fig.5 and that near $T_{\rm cl}$ in the inset of Fig.5, where used are $\beta = 0.23 \pm 0.02$ and $\nu = 1.01 \pm 0.02$ at $T_{\rm cu}$ and $\beta = 0.25 \pm 0.02$ and $\nu = 0.84 \pm 0.03$ at $T_{\rm cl}$. The errors for the values of critical exponents are estimated by the fitness for the finite-size scaling.

For 2 to 4 layer systems, we find that the chirality in the middle layers with the ferromagnetic intralayer interaction increases sharply near temperature $T_{\rm cl}$ as temperature increases.[15–17] We find the usual chirality transition at temperature $T_{\rm cu}$, and we see that the chirality on the ferromagnetic layers increases very sharply in a range of temperature below the $T_{\rm cu}$ as temperature increases. Hereafter we denote the temperature by $T_{\rm cl}$ at which another sharp peak for the specific heat takes place. Hence we consider there exists a critical phenomenon at $T_{\rm cl}$.

We find a new critical behaviour due to a steep increase in the chirality as a function of temperature

for the XY model on a layered triangular lattice with antiferromagnetic layers and ferromagnetic layers in some range of interaction parameters. The peaks at $T_{\rm cl}$ in the chiral susceptibility $\chi_{\rm top}$ are not shown to be size-dependent, but the other peaks at $T_{\rm cu}$ in the chiral susceptibility $\chi_{\rm top}$ are shown to depend on size. The new chirality transition and the value of a critical exponent have not been observed over any thickness dependence of this value as far as the layers systems are concerned. The other chirality transition and the value of a critical exponent have been observed over the thickness.

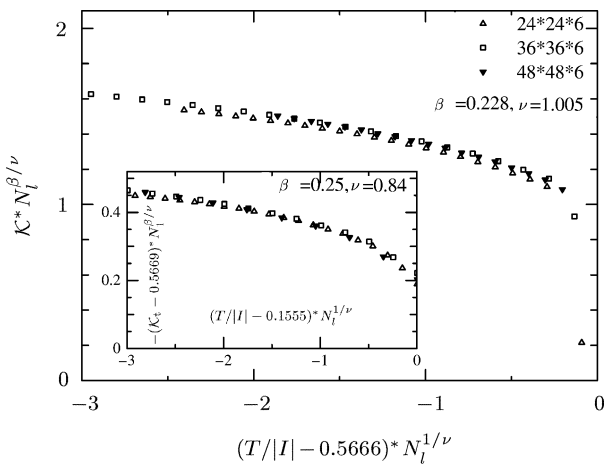


Fig.5 .Finite-size scaling analysis of the chirality for the system with $I = B = -1, P = Q = R = G = F = 1$ and $J = K = L = M = 0.075$ near $T_{\rm cu}$. The inset shows that the finite-size scaling analysis of the chirality for the same system near $T_{\rm cl}$.

4. Conclusions

In the present paper, we have investigated critical phenomena for an XY model on the 5 to 6 layer triangular lattices by using Monte Carlo simulation. We find three phases: the paramagnetic phase, the KT phase and chirality phase. The chirality in the middle layer with the ferromagnetic intralayer interaction increases sharply near temperature $T_{\rm cl}$ as temperature increases. The usual chirality transition at temperature $T_{\rm cu}$ is observed. Comparing the obtained values of critical exponents for the 2 to 6 layer systems investigated previously, we find that there is a universal behaviour for those layered XY models of the triangular lattice. However the value of the critical exponent β for the transition between the paramagnetic phase and the chirality phase is about 0.125 for the two-layer system,[15] 0.17 for the three-layer system,[16] 0.198 for the four-layer system,[17] 0.21 for the five-layer system and 0.228 for the six-layer system. Hence a crossover is observed over the thickness. We have determined the value of critical exponent β in order to see the critical behaviour on the critical line in the chirality phase. The value of β on the critical line is about 0.25 for 2 to 6 layers; we have not found any thickness dependence of this value as far as the some layered systems are concerned.

The crossover behaviour transiting from a two-dimensional system to a three-dimensional system is an interesting subject that is to be studied in future.

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