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Investigation of ultra-thin ferromagnetic films with a simple cubic lattice*

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Using Green's function method, we investigate ferromagnetic films with a simple cubic lattice containing up to ten monolayers. The Hamiltonian includes the Heisenberg exchange term, surface anisotropy (SA) and dipole interaction (DI). We calculate the magnetization as a function of temperature and film thickness, and we analyse the behaviour of spin canting. The result is in agreement with experiments. We calculate phase diagrams of SA versus DI to show the conditions under which spontaneous magnetization can occur. As a special case, we discuss the Heisenberg model without SA and DI.

Keywords: ferromagnetic film, spin canting, Green's function method
PACC: 7510J, 7570F, 7540F

1. Introduction

In the last decade, the magnetic behaviour of ultra-thin films has attracted both experimental and theoretical interest due to the novel properties of the films, one of which is magnetization reorientation. There have been experimental works[1−6] which measure the magnetic behaviour of films, and theoretical works[7−12] which try to explain the magnetization reorientation in magnetic films.

Among the theoretical works based on statistical model, Moschel *et al.*[7−10] utilized molecular field theory (MFT) which neglects the correlation and fluctuation effects of the system and cannot be applied in the low-temperature limit. The Green's function method is believed to be a better method which is applicable in the whole temperature range and takes fluctuations into account, although in an approximate way. Guo *et al.*[12] have applied this method to the study of magnetic films. They have used the following Hamiltonian

$$H = -J\sum_{(i,j)} \boldsymbol{S}_i \cdot \boldsymbol{S}_j - \sum_i D_i (S_i^z)^2 + \frac{\mu^2}{2V} N_z \sum_{ij} S_i^z \cdot S_j^z. \quad (1)$$

The third term in Eq.(1) is a simplified form of the dipole interaction (DI). Unfortunately, this is an oversimplified form. In fact, the third term in Eq.(1) represents the antiferromagnetic interaction. In Eq.(1), there is no mechanism that can make spins turn around, so that, in systems described by Eq.(1), only ferromagnetism–paramagnetism or ferromagnetism–antiferromagnetism transformation might occur.

In this paper, ferromagnetic films are investigated using Green's function method. What we intend to do is to obtain a comprehensive understanding about the magnetic behaviour of ultra-thin ferromagnetic films, including spin canting, phase diagrams of surface anisotropy (SA) versus DI and the possibility of the occurrence of spontaneous magnetization in the Heisenberg model.

2. Hamiltonian and method

The film studied is a simple cubic (sc) lattice and has a thickness of L=1–10 monolayers (MLs). Its normal is the [001] direction, i.e. the perpendicular direction to the film (x–y plane). The entire Hamiltonian

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is

$$\begin{aligned} H =& H_1 + H_2 + H_3 + H_4 \\ =& - J \sum_{(i,j)} \boldsymbol{S}_i \cdot \boldsymbol{S}_j - \sum_{\mu=1}^{L} D_\mu \sum_{i\mu} (S_{i\mu}^z)^2 \\ &+ \frac{g}{2} \sum_{ij} \frac{\boldsymbol{S}_i \cdot \boldsymbol{S}_j}{r_{ij}^3} - \frac{3g}{2} \sum_{ij} \frac{(\boldsymbol{S}_i \cdot \boldsymbol{u}_{ij})(\boldsymbol{S}_j \cdot \boldsymbol{u}_{ij})}{r_{ij}^3}. \end{aligned} \quad (2)$$

Here H_1 is the Heisenberg exchange energy. Only the exchange interaction between the nearest neighbours is considered in this paper. H_2 represents SA. The anisotropy D_μ may be different from layer to layer. $i\mu$ represents the site i in the μth ML. DI is now written as $H_3 + H_4$. $\boldsymbol{u}_{ij}$ is the unit vector which connects sites i and j.

In order to make calculation possible, approximations for H_4 are necessary. The system dealt with in this paper has symmetry in the x–y plane; it is uniform and invariant under the operations $x \leftrightarrow -x$, $y \leftrightarrow -y$ and $x \leftrightarrow y$. That is to say, the lattice is symmetric about planes $x = 0$, $y = 0$ and $x = \pm y$. Now, we put $\boldsymbol{S}_i \cdot \boldsymbol{u}_{ij} = \frac{1}{2}(S_i^+ u_{ij}^- + S_i^- u_{ij}^+) + S_i^z u_{ij}^z$ and make the mean-field approximation for H_4. Because of the symmetry, some terms vanish. Finally, we have

$$\begin{aligned} H_4 =& H_\parallel + H_\perp \\ =& - \frac{3g}{8} \sum_{ij} \frac{1}{r_{ij}^3} (S_i^+ S_j^- + S_i^- S_j^+) u_{ij}^+ u_{ij}^- \\ &- \frac{3g}{2} \sum_{ij} \frac{S_i^z S_j^z (u_{ij}^z)^2}{r_{ij}^3}. \end{aligned} \quad (3)$$

Compared to Eq.(1), we see that the approximation made for DI is greatly improved. Now the Hamiltonian becomes solvable by using Green's function theory.[12,13] Let us look at the feature of each term in the Hamiltonian. H_1 and H_3 are isotropic. They do not cause spontaneous magnetization. H_2 and $H_\perp$ make spins align in the perpendicular direction. $H_\parallel$ is beneficial for spins lying in the in-plane. It is this term that is able to cause spin canting. Therefore, the Hamiltonian includes the necessary information for the discussion of magnetization reorientation.

In the calculation, we set $D_1 = D_L = D$, otherwise, $D_\mu = 0$. This case is called monolayer SA (MLSA). For comparison, we also calculate the case of $D_1 = D_2 = D_{L-1} = D_L = D$, otherwise, $D_\mu = 0$, which will be called bilayer SA (BLSA). In this paper we take $J = 1$, $D = 0.05$ and $g = 0.0005$, which are of the same magnitudes as those used in Ref.[7]. The change of the parameters dose not yield a different conclusion. All the parameters are in units of J, the exchange integral in Eq.(2). The temperature T is in units of $J/k_{\rm B}$, where $k_{\rm B}$ is the Boltzmann constant.

The definition of the retarded Green's function is[14]

$$\begin{aligned} G_{ij}(t - t') =& \langle\langle A_i; B_j \rangle\rangle \\ =& - \mathrm{i}\theta(t - t') \langle A_i B_j - B_j A_i \rangle, \end{aligned} \quad (4)$$

where

$$A_i = S_i^+, \ B_j = (S_j^z)^n S_j^-. \quad (5)$$

The Green's function is Fourier time transformed and then put into the equation of motion

$$\omega \langle\langle A_i; B_j \rangle\rangle = \frac{1}{2\pi} \langle [A_i, B_j] \rangle + \langle\langle [A_i, H]; B_j \rangle\rangle. \quad (6)$$

Higher-order Green's functions are decoupled by random phase approximation

$$\langle\langle S_{i'}^z S_i^+; (S_j^z)^n S_j^- \rangle\rangle = \langle S_{i'}^z \rangle \langle\langle S_i^+; (S_j^z)^n S_j^- \rangle\rangle \ \ i' \neq i. \quad (7)$$

For the SA, different decoupling should be adopted. Here we use Lines' approximation[15]

$$\begin{aligned} &\langle\langle S_i^z S_i^+ + S_i^+ S_i^z; (S_j^z)^n S_j^- \rangle\rangle \\ =& \Gamma_i \langle S_i^z \rangle \langle\langle S_i^+; (S_j^z)^n S_j^- \rangle\rangle, \end{aligned} \quad (8)$$

where

$$\Gamma_i = \langle 3(S_i^z)^2 - S(S+1) \rangle / \langle S_i^z \rangle^2. \quad (9)$$

Devlin[16] has shown that the Lines' decoupling is a comparatively good approximation. Note that herein we merely consider the case where the anisotropy is not too large ($D < J$).

By the commutator of S_i^+ and the Hamiltonian, we obtain the linear equations

$$\begin{aligned} &\sum_{\lambda=1}^{L} [\omega(\boldsymbol{k}) \delta_{\mu\lambda} - P_{\mu\lambda}(\boldsymbol{k})] g_{\lambda\nu}(\omega, \boldsymbol{k}) \\ =& \frac{\delta_{\mu\nu}}{2\pi} \langle [S_\mu^+, (S_\mu^z)^n S_\mu^-] \rangle, \end{aligned} \quad (10)$$

where the Greek letter subscripts label layers in the film. Now the Green's functions are further Fourier transformed about the two-dimensional real space, and their arguments become energy and two-dimensional wave vector. For $H_3 + H_4$, we have to do summations such as $\sum_{l,m=1} \cos l k_x / (l^2 + m^2 + n^2)^q$ and so on, where q is equal to 3/2 or 5/2, and n is an integer or half integer. We count both l and m up to 2000 so that the error is negligible.

For the calculation of magnetization, we have[13]

$$\begin{aligned}&\langle S(S+1)(S_\mu^z)^n-(S_\mu^z)^{n+1}-(S_\mu^z)^{n+2}\rangle\\ =&R_\nu\{\langle 2S_\mu^z(S_\mu^z-1)^n+[(S_\mu^z-1)^n\\ &-(S_\mu^z)^n][S(S+1)-S_\mu^z-(S_\mu^z)^2]\rangle\},\end{aligned}\tag{11}$$

where R_ν is the following integral

$$R_\nu=\frac{1}{4\pi^2}\iint \mathrm{d}k_x\mathrm{d}k_y\sum_{\alpha=1}^{L}\frac{U_{\nu\alpha}^2}{\mathrm{e}^{\omega_\alpha(\boldsymbol{k})/T}-1}.\tag{12}$$

Here $\omega(\boldsymbol{k})$ and $U_{\mu\nu}$ are eigenvalues and eigenvectors of matrix $P_{\mu\lambda}(\boldsymbol{k})$, respectively. The vectors $U_{\mu\nu}$ are orthogonal and normalized. The integral is carried out in the two-dimensional first Brillouin zone, and the magnetization of arbitrary S is expressed by R_ν [13]

$$\begin{aligned}\langle S_\nu^z\rangle =&\sigma_\nu\\ =&\frac{(S-R_\nu)(1+R_\nu)^{2S+1}+(1+S+R_\nu)^{2S+1}}{(1+R_\nu)^{2S+1}-{R_\nu}^{2S+1}}.\end{aligned}\tag{13}$$

Equation (13) clearly shows that $\langle S_\mu^z\rangle$ are different for different layers. However, due to the symmetry in the z-direction, we have $\langle S_\mu^z\rangle$=$\langle S_{L+1-\mu}^z\rangle$. By binomial expansion the relationship between $\langle S^z\rangle$ and R can be expressed more clearly (see Eq.(23) of chapter 35 in Ref.[13]). As $R=0$, we have $\langle S^z\rangle=S$. This is the case that all spins align in the perpendicular direction. For $R\to\infty$, we have $\langle S^z\rangle\to 0$. This means that there is no perpendicular component of magnetization. For the sake of direct visualization, the variation of $\langle S^z\rangle$ versus R is plotted in Fig.1. The smaller S is, the more rapidly $\langle S^z\rangle$ goes to zero with R.

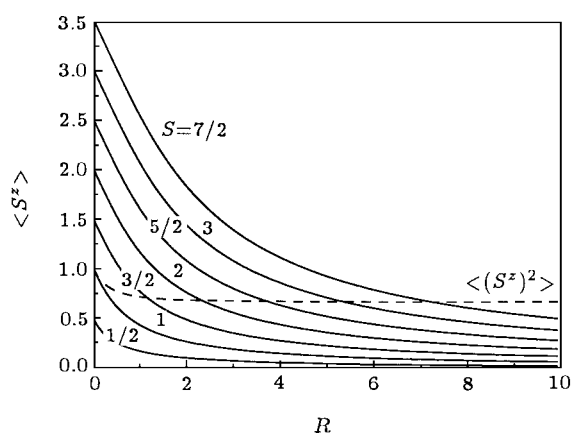


Fig.1. $\langle S^z\rangle$ versus R according to Eq.(13) for several values of S. The dashed line shows $\langle(S^z)^2\rangle$ versus R for $S=1$.

Although the above formulae are valid for any spin S, in this paper we only consider the case of $S=1$, which is the lowest spin value at which spin canting can take place. From Eq.(11), we have for $S=1$

$$\langle(S_\nu^z)^2\rangle=\frac{1+2R_\nu+2R_\nu^2}{1+3R_\nu+3R_\nu^2}.\tag{14}$$

Figure 1 also shows the variation of $\langle(S^z)^2\rangle$ versus R. As R departs from zero, $\langle(S^z)^2\rangle$ deviates from one and rapidly approaches 2/3. Hereafter we simply write $\langle S^z\rangle$ as σ.

3. Results

3.1. Magnetization as a function of temperature and film thickness

The magnetization calculated with Hamiltonian H is denoted as σ_H. Figure 2 shows σ_{H} versus temperature for various values of L in the case of MLSA. In consideration of the symmetry in the z-direction, only $[(L+1)/2]$ lines for a film with L (ML) are shown. For instance, for L=10 ML, we show the magnetization of the first to the fifth layers (as shown in the inset of Fig.2). The first layer has the lowest magnetization, and the deeper layer has a larger magnetization. This clearly suggests that the inner layers will feel a larger "inner magnetic field". Near the surface, the difference of the magnetization between adjacent layers is larger than that between the inner adjacent layers. For a ten ML film, for instance, the σ_{H} values of the fourth and fifth layers are almost the same.

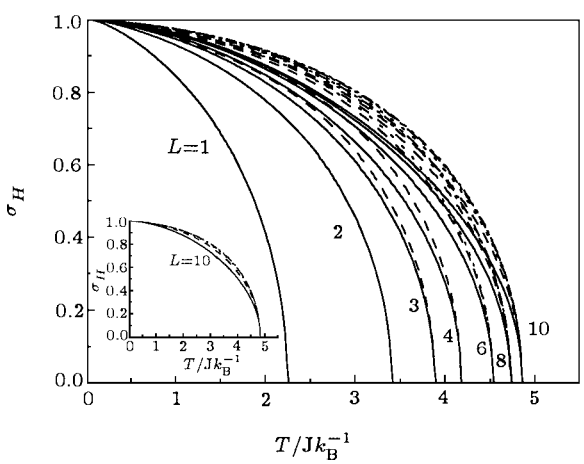


Fig.2. Magnetization σ_{H} versus temperature for the number of ML L=1 to 4, 6, 8 and 10. For clarity, the lines for L=5,7 and 9 are not shown. The inset shows the result of L=10 ML.

T_{s} is the temperature at which the magnetization is equal to zero, and $T_{\mathrm{s}}(H)$ is the temperature at which $\sigma_{\mathrm{H}}=0$. From Fig.2 it is obvious that $T_{\mathrm{s}}(H)$ increases with the thickness of the film. The open circles in

Fig.3 show the variation of $T_s(H)$ versus the film thickness. They can be fitted by $T_s(H) = 6.1 - 3.85/L^{0.5}$. It should be noted that $T_s(H)$ is not the Curie point. The reason for this will be given below.

Although in the intermediate temperature region, the magnetizations of different layers are different in a film, they reach zero at the same $T_s(H)$. If we suppose that one of the layers has a non-trivial magnetization, then the adjacent layers will be certainly affected as though they feel a magnetic field, and also exhibit non-trivial magnetizations, etc. Hence, the whole film must reach zero magnetization at the same $T_s(H)$.

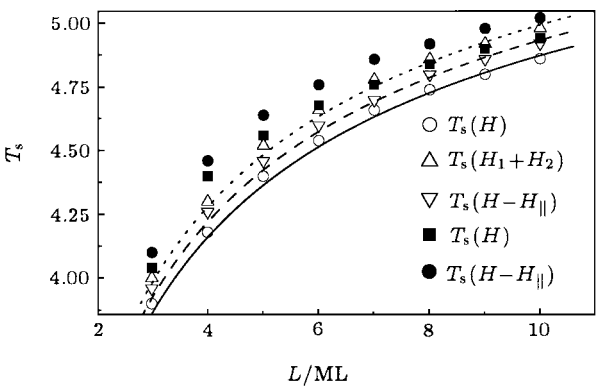


Fig.3. T_s versus film thickness for D=0.05 and g=0.0005: open symbols, MLSA; closed symbols, BLSA. The fitting lines for the open symbols are $T_s(H) = 6.1 - 3.85/L^{0.5}$, $T_s(H_1 + H_2) = 6.16 - 3.85/L^{0.5}$ and $T_s(H - H_\parallel) = 6.22 - 3.85/L^{0.5}$, respectively.

To discuss the roles of $H_\parallel$ and $H_3 + H_4$ in the Hamiltonian H, we also calculate the magnetizations $\sigma_{H-H_\parallel}$ for the Hamiltonian $H - H_\parallel$, and $\sigma_{H_1+H_2}$ for the Hamiltonian $H_1 + H_2$. These are also shown in Fig.3. Correspondingly, the temperatures at which $\sigma_{H-H_\parallel} = 0$ and $\sigma_{H_1+H_2} = 0$ are denoted as $T_s(H - H_\parallel)$ and $T_s(H_1 + H_2)$, respectively. From Fig.3 we see that $\sigma_H < \sigma_{H_1+H_2} < \sigma_{H-H_\parallel}$, and $T_s(H) < T_s(H_1 + H_2) < T_s(H - H_\parallel)$. The role of $H_\parallel$ is to turn spins to in-plane. If it is extracted from the whole Hamiltonian, the magnetization should be larger, and T_s will also become larger. The significance of the difference between σ_H and $\sigma_{H-H_\parallel}$ will be discussed in detail in section 3.2.

The curves $T_s(H - H_\parallel)$ and $T_s(H_1 + H_2)$ can also be roughly fitted by $T_s(H - H_\parallel) = 6.22 - 3.85/L^{0.5}$ and $T_s(H_1 + H_2) = 6.16 - 3.85/L^{0.5}$, respectively. It seems that up to ten ML, there is an approximate scaling law $T_s \propto -L^{-1/2}$. However, this cannot be extended to $L \to \infty$. It can be analysed by the example of $\sigma_{H_1+H_2}$ with g=0. For a bulk material where SA is negligible, the Curie point is T_C(bulk)=$4S(S + 1)/C = 5.276$ (C=1.51638 for a sc lattice).[13] T_s should approach T_C(bulk) as L goes to infinity. But according to the fitting line, as $L \to \infty$, $T_s(H_1 + H_2)$ approaches 6.16. Therefore, as $L \to \infty$, the scaling for $T_s(H_1 + H_2)$ should not be $-L^{-1/2}$, but should be slower than $-L^{-1/2}$.

One can clearly see the influence of parameters D and g on T_s. If D is fixed, $T_s(H_1 + H_2)$ is unchanged. As g increases, both the differences $T_s(H_1+H_2) - T_s(H)$ and $T_s(H - H_\parallel) - T_s(H_1+H_2)$ will increase, but the latter will increase more slowly. If we enlarge D while fixing g, all three T_s will increase.

In the case of BLSA, the values of all three σ and three T_s are larger than those in the MLSA case. This is ascribed to the stronger SA in a BLSA film. The solid symbols in Fig.3 are the results of $T_s(H)$ and $T_s(H - H_\parallel)$ for BLSA case.

3.2. The behaviour of spin canting

Now we discuss the difference between $\sigma_{H-H_\parallel}$ and σ_H. Because there is no mechanism in the Hamiltonian $H - H_\parallel$ to make spins cant, the magnetization is always in the perpendicular direction. As the temperature increases, the thermal motion increases, which leads to the decrease of $\sigma_{H-H_\parallel}$. Eventually, the spontaneous magnetization vanishes at $T_s(H - H_\parallel)$. As for Hamiltonian H, it includes a term $H_\parallel$ that forces the spins to cant. This results in an in-plane component of magnetization so that σ_H is less than $\sigma_{H-H_\parallel}$. This reduction of magnetization is not due to the thermal motion, but due to $H_\parallel$. For Hamiltonian H, we can assume that the magnetization is still $\sigma_{H-H_\parallel}$, but it is at an angle to the z-direction. The perpendicular component is $\sigma^z = \sigma_H$, while the in-plane component is $\sigma^x = \sqrt{\sigma^2_{H-H_\parallel} - \sigma^2_H}$. If a trivial magnetic field is applied in the x-direction, the component σ^x will be along the x-direction. Figure 4 shows, as an example, the three quantities of σ_H, $\sigma_{H-H_\parallel}$ and σ^x for L=10 MLs. Figure 5 shows the angle between $\sigma_{H-H_\parallel}$ and σ_H. On the whole, the Hamiltonian $H_\parallel$ results in spin canting. We have seen from Fig.3 that $T_s(H)$ is less than $T_s(H_1 + H_2)$, therefore the net effect of DI is also spin canting.

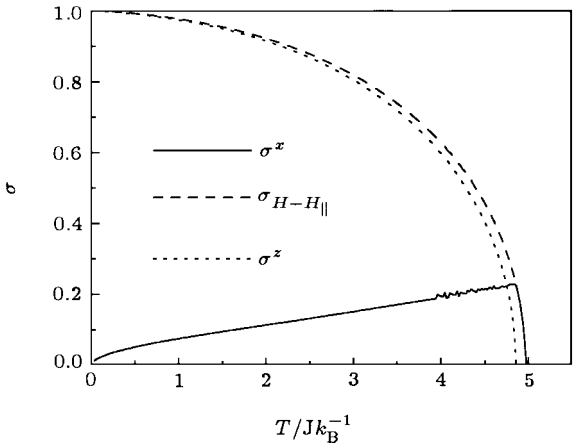


Fig.4. The perpendicular and in-plane components of magnetization versus temperature for L=10 ML.

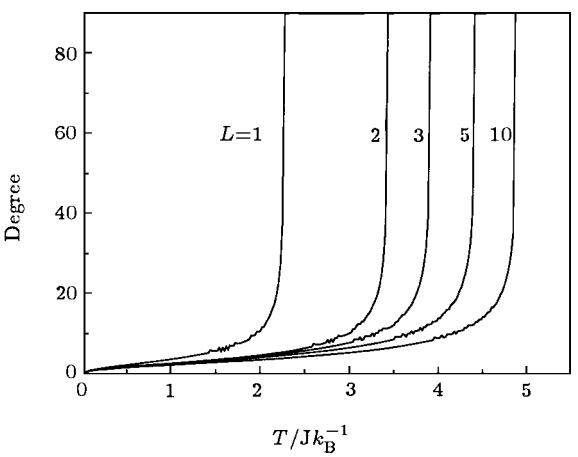


Fig.5. The angle between magnetization and perpendicular direction versus temperature for several film thicknesses.

At $T_s(H-H_\parallel)$, both σ^z and σ^x disappear. This point can be thought as the Curie point, $T_s(H-H_\parallel) = T_C$. $T_s(H)$ is the temperature where spins lie fully in the plane.

As the parameters D and g vary, the qualitative behaviour shown in Figs.4 and 5 is unchanged. This feature also remains when we study the case of BLSA.

3.3. *D-g* phase diagram

We have seen that the net effect of DI is spin canting. When g is large enough, there will be no spontaneous magnetization. To investigate the condition under which the spontaneous magnetization can occur, we have calculated the D–g phase diagram, as shown in Fig.6. Each line represents the result for a fixed film thickness. Spontaneous magnetization can occur in the lower right area from the line, while it cannot occur in the other area. Therefore, the lines are called boundary lines. They are linear unless D is close to zero.

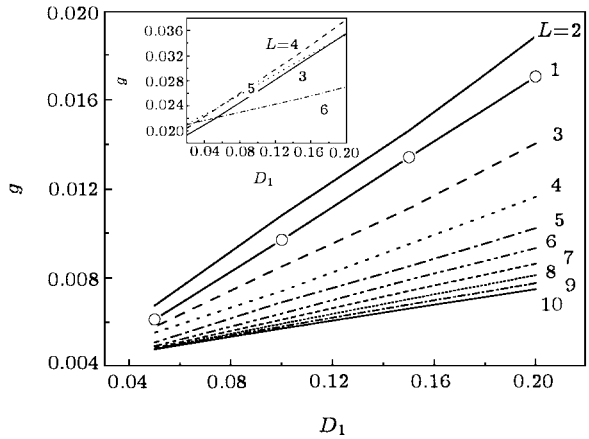


Fig.6. D–g phase diagram for the MLSA case. The inset shows the phase diagram for the BLSA case.

For MLSA, as L increases, the boundary line lowers and its slope reduces. SA is beneficial to spins aligned in the z-direction, while DI plays a role to make spins align in-plane. Layers other than the first and the Lth layers do not have SA, while DI exists in the whole system. Hence, for the same D, a smaller value of g is allowed for a thicker film to have spontaneous magnetization. If we express the lines by the equation $g_L = k_L D + g_{L0}$, the slopes k_L are shown in Fig.7.

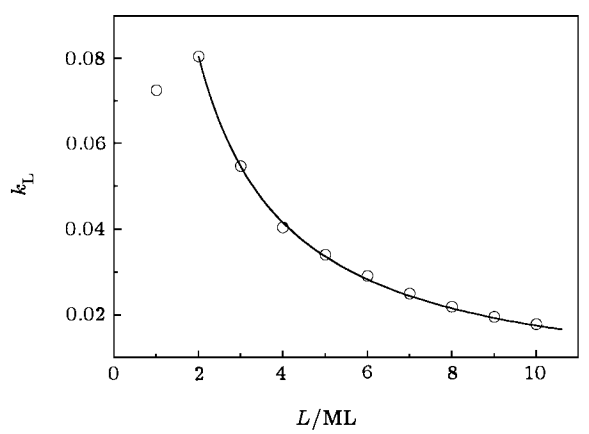


Fig.7. Slopes of the boundary lines in Fig.6 in the case of MLSA (open circles). The fitting line is $k_L = 0.155/L^{0.95}$.

The monolayer film (L=1) is an exception, since its boundary line is lower than a bilayer film (L=2) (see Fig.6). The reason for this is that, for the latter, both atomic layers have non-vanishing SA, and the force that sets spins to align in the perpendicular direction in it is stronger than that in the former. Hence, compared to the monolayer film, for the same

D, a larger value of g is permitted for the bilayer film to have spontaneous magnetization.

As long as every ML has SA, the boundary line shifts upward and its slope increases with film thickness. In the inset of Fig.6, we show the D–g diagram of L=3–6 ML for the BLSA case. Compared to an $L = 3$ film, the boundary line for an $L = 4$ film is higher and its slope is larger. For $L \geq 5$, the line shifts downward and its slope decreases, because the layers that do not have SA appear.

The linear law for the boundary lines will not be valid when D approaches zero. When both D and g go to zero, the system will not exhibit spontaneous magnetization. This case is discussed in the next subsection.

3.4. Heisenberg model

As both D and g in Hamiltonian Eq.(2) are zero, the system retrogrades to the usual Heisenberg model. It is well known that the three-dimensional Heisenberg model has spontaneous magnetization but one- and two-dimensional Heisenberg models do not. For instance, Mermin and Wagner[17] have proven that for the two-dimensional Heisenberg model with a finite-range exchange interaction there is no spontaneous magnetization. Let us consider a film with a finite thickness, i.e. the quasi two-dimensional case.

Whether there is a spontaneous magnetization or not is determined by the integral of Eq.(12). If the integral is divergent, it can be easily seen from Fig.1 that there is no spontaneous magnetization. For a pure two-dimensional plane where L=1, the dispersion relation derived from Eq.(10) is

$$\omega(\boldsymbol{k}) = -\sigma[2JQ(\boldsymbol{k}) + 8J], \tag{15}$$

where $Q(\boldsymbol{k}) = 2(\cos k_x + \cos k_y)$. The integral can be reduced to a mere computation of the Riemann ζ function

$$\zeta(1) = \sum_{n=1}^{\infty} \frac{1}{n}. \tag{16}$$

It is divergent so that there is no spontaneous magnetization.

For a bilayer film, we have $\omega_{1,2} = -\sigma[2JQ(\boldsymbol{k}) + 10J \mp 2J]$. The dispersion relationship for ω_1 is also Eq.(15), and the corresponding integral is divergent. So this system does not have spontaneous magnetization either. For a 3 ML film, we have $\omega_1 = -\sigma_1 2JQ(\boldsymbol{k}) + 8J\sigma_1 + 2J\sigma_2$, and $\omega_{2,3} = J\{-(\sigma_1 + \sigma_2)Q(\boldsymbol{k}) + 6\sigma_1 + 5\sigma_2 \mp \sqrt{[(\sigma_1 - \sigma_2)Q(\boldsymbol{k}) - 2\sigma_1 + 3\sigma_2]^2 + 8\sigma_1\sigma_2}\}$. If we set $\sigma_2 = 0$, then the integral is divergent, resulting in $\sigma_1 = 0$, and vice versa. If setting $\sigma_2 \neq 0$, we do not analytically know if the integral is convergent. It is supposed that if there is spontaneous magnetization, as temperature approaches 0K, there should be $\sigma_1 = \sigma_2 = S$. However, when $\sigma_1 = \sigma_2$, the integral including ω_2 is divergent. We therefore guess that the integral is always divergent for any presumed values of σ_1 and σ_2. Consequently, we conjecture that for any finite thickness of a sc film, there is no spontaneous magnetization.

4. Discussion

The term $H_\perp$ in the Hamiltonian H represents the antiferromagnetic effect. However, it is too small to compete with the Heisenberg term H_1. Therefore, we believe that, in such a system, no ferromagnetic–antiferromagnetic transformation can occur.

Our calculated features are qualitatively in accordance with experiments. We have calculated the value of T_s at which the perpendicular magnetization is zero and the Curie point T_C. Both of these increase with increasing film thickness. This is also in agreement with experiments. The measurement in Ref.[3] has shown that, for a monolayer Fe film, T_C is less than 125K, and is lower than that of thicker films. As shown in Ref.[18], the Curie point roughly rises with the thickness of the film. Our result shows that for any thickness there will be magnetization canting. Allenspach and Bischof[6] have clearly shown that there is not a thickness range where magnetization vanishes. Figure 4 shows that the in-plane component reaches the maximum when the perpendicular component goes to zero. This conclusion is supported by the experimental observation that, in a 4.2ML Fe/Ag(100) film, the perpendicular and in-plane magnetizations do behave in the above manner.[3]

In our model, the mechanism for spin canting is clear and reasonable. The magnetization is always turned from out-of-plane to in-plane. There are apparently two features: the first is that the spin canting occurs just as the temperature starts from 0K. This is because DI always plays a role. The second is that there is no first-order phase transition in the system. The spins cant gradually and no abrupt reorientation occurs so that only a second-order transition can occur. Both features are unchanged when we adjust the parameters D and g, no matter whether MLSA or BLSA is considered. Pappas *et al.*[2] have indicated

that there was a phenomenon that the switching is a continuous turning of the magnetization direction from perpendicular to in-plane.

We believe that our results are more reasonable compared with that of MFT. According to MFT, the spins do not cant until some finite temperature is reached.[7] As parameters vary, a first-order transition can appear (for example, in the case of BLSA).[8] In other words, MFT suggests a possibility of sudden reorientation of magnetization. Since SA is in the perpendicular direction and DI makes spins turn to in-plane, a gradual but not abrupt spin turning seems to be more reasonable.

The variations of σ^z and σ^x with temperature, as shown in Fig.4, are similar to those of the Monte Carlo simulations of Chui.[11] Though his work does not show where the in-plane magnetization vanished, Figs.8 and 11 in Ref.[11] show that the in-plane magnetization decreased slowly as $T \to 0$K. Chui also noticed that as SA was zero, for finite g, the spins were aligned in the x–y plane. Our investigation is coincident with the Monte Carlo simulations qualitatively.

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