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Curie temperature of ultrathin ferromagnetic layer with Dzyaloshinskii-Moriya interaction

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We investigate the effect of the Dzyaloshinskii-Moriya interaction (DMI) on the Curie temperature of the ultrathin ferromagnetic layers. It has been known that the Curie temperature of the ferromagnet depends on the exchange interaction, and they are affected by DMI. Therefore, the ferromagnetic transition temperature of the ultrathin ferromagnetic layer must be sensitive on the DMI. We find that the Curie temperature depends on the DMI by using the double time Green’s function method. Since the DMI is arisen by the inversion symmetry breaking structure, the DMI is always important in the inversion symmetry breaking ultrathin ferromagnetic layers.

I. INTRODUCTION

Recently, the Dzyaloshinskii-Moriya interaction (DMI) is attracting a lot of interest due to its rich physics and potential applications of the nano-scale information technologies with a skyrmion. The DMI is arisen by the inversion symmetry breaking structure with a strong spin-orbit coupling (SOC), it always exist in ultrathin ferromagnetic layers with heavy metal underlayer. The DMI Hamiltonian gives an additional energy term, which prefers non-collinear spin configurations, while the isotropic inter-atomic exchange energy prefers collinear spin configurations. Intuitively, the DMI acts as an opposite side to the isotropic exchange interaction, so that DMI may reduce the Curie temperature. Therefore, it must be addressed whether the DMI reduce the Curie temperature or not. The Curie temperature is one of the fundamental physical quantities of the ferromagnetic materials, where the ferromagnetic phase transition occurs. The Curie temperature is determined by the exchange stiffness, $A_{ex}$ in bulk materials. However, the ferromagnetic ordering becomes unstable in the 2-dimensional system, and the ferromagnetic phase transition never occurs without finite anisotropy. Therefore, the Curie temperature of the ultrathin ferromagnetic layers is strongly affected by the anisotropy energy. More precisely, the Curie temperature is a result of the spin wave (SW) excitation due to the thermal agitation, since the SW excitation depends on the dispersion relations, which depends on SW energies including exchange, anisotropy, dipole interaction, and DMI. In the calculation of the Curie temperature for the ultrathin ferromagnetic layers and super-lattices, the double time Green’s function method is widely used. It is well developed technology in the statistical physics and magnetism. With the double time Green’s function method, we can calculate the SW dispersion relations and SW excitation, and determine the Curie temperature of the given system.

In this study, we developed the double time Green’s function method including the DMI Hamiltonian for the ultrathin ferromagnetic layers to investigate the effect of the DMI on the Curie temperature. Since we interested only on ultrathin ferromagnetic layers with heavy metal underlayer, we formulated the double time Green’s function for $N$-layer ferromagnetic systems with the finite DMI contribution. We clearly observed the DMI contribution in the SW dispersion relations, which is already predicted by Moon et al. They claimed that the DMI term added a linear SW wave vector $k$ dependence on the SW dispersion relations, so that the SW energy minimum shifts from zero $k$ to non-zero $k$. As a result, the SW excitation energy is lowered by the DMI contribution. Since the SW excitation energy determined the Curie temperature, it must be lowered. We also considered various cases of the bulk and surface anisotropies, since the anisotropy energies affect to the Curie temperature. We found that the DMI reduce Curie temperature and the reduction is serious when the anisotropy energy is smaller.

II. DOUBLE TIME GREEN’S FUNCTION METHOD

Let us briefly review the double time Green’s function to obtain the Curie temperature ($T_C$) of the $N$ atomic ferromagnetic layer with DMI. The Hamiltonian with DMI in terms of the spin operator is

$$H = -\mu_B H_0 \sum_i S_i^z - \sum_{\langle i,j \rangle} J_{ij} (S_i \cdot S_j) - K_u \sum_{\langle i,j \rangle} S_i^x S_j^x + \sum_{\langle i,j \rangle} D_{ij} \mathbf{S}_i \cdot \mathbf{S}_j.$$  \hspace{1cm} (1)

Here, $J_{ij}$ and $D_{ij}$ are the isotropic inter-atomic Heisenberg and DM (Dzyaloshinskii-Moriya) exchange energies between the $i$th and $j$th spins, and $K_u$ and $K_s$ are the bulk and surface uniaxial anisotropy energies. $(i,j)$, $(i,j)^\prime$, $(i,j)^\prime\prime$ denote summations of the nearest neighbor hoods inner layers, top, and bottom most layers. The positive $K_u$ and $K_s$ imply bulk and surface perpendicular magnetic anisotropy (PMA), and negative means in-plane magnetic anisotropy (IMA). The last DMI term can be rewritten as

$$H_{DMI} = \sum_{\langle i,j \rangle} D_{ij} (S_i^x S_j^x - S_i^y S_j^y).$$  \hspace{1cm} (2)
Using the relations between the spin operators and the Pauli operators, $b_i^+ \text{ and } b_i^-,$ \cite{Haubenreisser14}

$$
\begin{align*}
S_i^+ &= \frac{1}{2} (b_i^- + b_i^+), \\
S_i^0 &= i \left( b_i^+ - b_i^- \right), \\
S_i^- &= \frac{1}{2} \left( 1 - 2 b_i^+ b_i^- \right).
\end{align*}
$$

Following Haubenreisser, \cite{Haubenreisser14} the double time Green function is defined,\cite{Yun17,Yun18}

$$
G_{ij}(t, t') = \langle \langle b_i^+(t) | b_j^-(t') \rangle \rangle.
$$

The equation of motion for $G_{ij}$ is

$$
i \frac{d G_{ij}(t, t')}{dt} = \langle [b_i^-(t), b_j^-(t')] \rangle \delta(t - t')
- \langle [\{H, b_i^-(t)\}, b_j^-(t')] \rangle.
$$

And the higher order Green’s functions are decoupled by the random phase approximations,

$$
\langle \langle S_i^+ b_j^-(t) | b_j^-(t') \rangle \rangle \simeq \langle S_i^+ \rangle \langle \langle b_j^- \rangle (t) | b_j^- \rangle (t') \rangle.
$$

The set of differential equations for $N$-atomic ferromagnetic layer are written as \cite{Yun11}

$$
(E - A_i) g_{1,m} + \mu_1 g_{2,m} = \mu_1 \delta_{1,m},
$$

$$
(E - A_p) g_{p,m} + \mu_p (g_{p+1,m} + g_{p-1,m}) = \mu_p \delta_{p,m}, \quad (2 \leq p < N)
$$

$$
(E - A_N) g_{N,m} + \mu_N g_{N-1,m} = \mu_N \delta_{N,m},
$$

where, $E = \omega / J,$ $g_{pm} = J G_{pm},$ and $\mu_p = \langle S_i^+ \rangle$ for $p = 1, ..., N,$ and

$$
A_1 = 4 \mu_1 (1 + k_{a1} - \gamma_k - \delta_k) + \mu_1 (1 + k_a),
$$

$$
A_p = 4 \mu_p (1 + k_a - \gamma_k - \delta_k)
+ (\mu_{p+1} + \mu_{p-1})(1 + k_a), \quad (2 \leq p < N)
$$

$$
A_N = 4 \mu_N (1 + k_{aN} - \gamma_k - \delta_k) + \mu_{N-1} (1 + k_a),
$$

$$
\gamma_k = \frac{1}{2} (\cos k_x a + \cos k_y a),
$$

$$
\delta_k = \frac{\delta_0}{2} (\sin k_x a + \sin k_y a).
$$

Here, the normalized energy quantities are defined as

$$
\delta_0 = D / J, k_a = K_a / J, k_{a1} = K_{a1} / J, \text{ and } k_{aN} = K_{aN} / J, \text{ respectively.}
$$

The DMI contribution were developed with the number operator, $
\hat{n}_i = b_i^+ b_i^-.$ \cite{Haubenreisser14}

$$
\sum_{ij} D_{ij} \left( S_i^0 S_j^0 - S_i^+ S_j^- \right) = \frac{1}{4} \sum_{ij} 2 i m_{ij} \left( b_i^+ b_j^- - b_i^- b_j^+ \right)
\simeq D \sum_{i} (\sin(k_x a) + \sin(k_y a)) \hat{n}_i.
$$

The set of equation of motion can be written as a matrix form

$$
\Delta(E) \cdot g_m = u_m, \quad (17)
$$

where

$$
\Delta(E) = \begin{pmatrix}
E - A_1 & \mu_1 & 0 & 0 & \cdots & 0 \\
\mu_2 & E - A_2 & \mu_2 & 0 & \cdots & 0 \\
0 & \mu_3 & \ddots & \ddots & \ddots & \vdots \\
\vdots & \vdots & \ddots & \ddots & \ddots & \mu_{N-1} \\
0 & 0 & \cdots & 0 & \mu_N & E - A_N
\end{pmatrix},
$$

$$
g_m = \begin{pmatrix}
g_{1m} \\
g_{2m} \\
\vdots \\
g_{Nm}
\end{pmatrix}, \quad u_m = \begin{pmatrix}
um_1 \\
um_2 \\
\vdots \\
um_N
\end{pmatrix}.
$$

With above matrix equations, we can obtain the series of the Green’s functions as follows:

$$
g_{nm}(E) = \sum_{i=1}^{N} f_m(E_i) \cdot (E - E_i)^{-1}, \quad (20)
$$

where $f_m(E_i) = |\Delta_m(E_i)|_{\mu_i},$ and $|\Delta_m(E_i)|$ is the determinant made by replacing the $m$th column of the determinant of $|\Delta(E)|$ by $g_m.$ \cite{Yun11} And $E_i$ is the $i$th eigenvalue of $|\Delta(E)|$ normalized by $j,$ and it is the SW excitation energy for the corresponding SW vectors. The $\mu_m$ satisfy following relations and we have to solve the self-consistence equations for find $N$ unknowns $\mu_m.$ \cite{Yun11}

$$
\mu_m = \frac{1}{2} - \frac{a^2}{4\pi^2} \int_{-\pi/a}^{\pi/a} \int_{-\pi/a}^{\pi/a} d k_x d k_y \sum_{i=1}^{N} f_m(E_i) / (E_i - E_j - 1).
$$

And the $T_C$ is given by

$$
\frac{k_B T_C}{J} = \left[ \frac{2a^2}{\pi^2} \int_{-\pi/a}^{\pi/a} \int_{-\pi/a}^{\pi/a} d k_x d k_y \sum_{i=1}^{N} f_m(E_i) / E_i \right]^{-1}.
$$

III. RESULTS AND DISCUSSIONS

First, we calculated the $T_C$ as a function of number of layer $N$ for simple cubic and $S = 1/2$ case. As shown in Fig. 1, the $T_C$ approaches to bulk value as increasing number of layer $N.$ It must be noted that the bulk $T_C$ of the isotropic Heisenberg model is 1.978/J/k_B, and our $T_C$ is slightly higher due to the finite anisotropy energy. Since we interested about DMI effect, we focused our calculation on ultrathin FM, 2 monolayer (ML) case, $N = 2.$ It noted that the $T_C$ (2ML) is about 65% of bulk case. According to Eqs. (21) and (22), we must calculate SW excitation energy $E_i$ as a function of the SW $k$-vector, SW dispersion relations, for each temperature to obtain $T_C.$ Fig. 2(a) shows 3 dimensional plot of the SW
dispersion relation for the lowest SW energy $E_1 = \omega_1 / J$ in the $k$-space at $k_B T = 0.04 \text{ J}$, and we plotted SW dispersion relation again a function of $k_x$ ($k_y = 0$) for various $T$ in Fig. 2(b) without DMI. Figure 2(b) shows the typical SW dispersion relations, and the SW excitation energy decreases with increasing temperature, while the functional form does not change. When $T$ approaches to $T_C$, the SW excitation energy is lowered so that the ferromagnetism will be disappeared.

Let us consider the contribution of DMI in SW dispersion relations, Moon et al. $^{19}$ already pointed out that the DMI term manifests itself by an additional linear $k$-vector dependence term in the SW dispersion relations as follows:

$$\omega_{DMI}(k_x, k_y = 0) = \omega_0(k_x, k_y = 0) + pD^* k_x.$$  \hspace{0.9cm} (23)

Here, $\omega_{DMI}$, $\omega_0$, $p$, and $D^*$ are SW excited frequency with DMI, without DMI, polarity of the external field, and DMI energy in frequency/wave-vector unit. Details of the $\omega_0$ depend on the anisotropy energies and isotropic inter atomic exchange energy, and the Zeeman energy due to the external field, and so on. The contribution of DMI in SW dispersion can be linearly approximated always, unless the DMI term is comparable with the total energy terms. Since $\omega_0$ is approximated with a parabola as shown in Fig. 2(b) for small $k$-vector, Eq. (23) can be expressed a shifted parabola (see Fig. 3(a) in Ref. 19).

The SW dispersion relations are plotted in Fig. 3(a) for $k_B T = 0.04 \text{ J}$ and (b) for $k_B T = 1.2 \text{ J} (\approx T_C)$. The SW dispersion relations for $k_y = 0$ are depicted for $\delta_0 = 0$, 0.05, and 0.1, we limited our plot for $-0.5 < k_x a < 0.5$ region. A typical parabola shape dispersion relations are shown for $\delta_0 = 0$ in Figs. 3(a) and 3(b) with the different energy scales. When the finite DMI contribution is added, the parabola shifted to right ($+k_x a$-axis) and lower energy side, and it is quite similar to the previous reports.$^{19,20}$ These shifts are more significant for the higher temperature as shown in Fig. 3(b).

Finally, we calculated the $T_C$ for various anisotropy cases. The normalized bulk anisotropy $k_u$ are set $+0.01$ or $-0.01$. Here, positive (negative) $k_u$ implies PMA (IMA), respectively. And the normalized surface anisotropy energy $k_{s1} = k_{sN}$ are varied 0.005, 0.01, and 0.05. The results are plotted in Figs. 4(a)–4(c) as a function of $\delta_0$ ($0.0 \sim 0.1$). As we already expected, $T_C$ is dropped with $\delta_0$ for most cases. First, we found that IMA have always smaller $T_C$ than PMA case. Since the $T_C$ is affected strongly by the anisotropy energy, especially for the ultrathin film, the anisotropy dependence is understandable. We set the surface anisotropy prefers PMA, the effective anisotropy of bulk IMA is partially canceled with surface anisotropy, so that the net anisotropy of PAM is always larger than IMA case. Second, the $T_C$ reduction with DMI is more significant for the smaller anisotropy cases. The reduction of $T_C$ for $k_{s1} = 0.05$ is only $\sim 1.2\%$, but it is about $\sim 9\%$ for $k_{s1} = 0.005$. Third, the DMI makes unstable phase for small IMA case as shown in Fig. 4(c). For $k_u = -0.01$ and $k_{s1} = 0.005$ case, the ferromagnetic state is no longer stable when $\delta_0 \geq 0.07$, so that we cannot

![FIG. 1. The $T_C$ dependence on the number of $N$ layer of simple cubic ferromagnetic layer.](image1)

![FIG. 2. (a) 3-dimensional plot of the SW dispersion relation as a function of $k_x a$ and $k_y a$ without DMI, and $k_B T = 0.04 \text{ J}$. (b) SW dispersion relations for $-\pi < k_x a < \pi$ with $k_y = 0$ for the various temperatures ($k_B T = 0.04 \sim 1.36 \text{ J}$).](image2)
determine $T_C$ of them. It is also observed for $k_s = 0.001$ case for $k_u = 0.01$. When $\delta_0$ over specific values, we cannot find self-consistence solutions of Eq. (21).

Before conclusion, we have to discuss about the magnitude of normalized DMI energy $\delta_0 = D/J$. The experimentally measured DMI energy $D_{DMI}$ is order of $1 \times 10^{-3}$ J/m$^2$, and exchange stiffness $A_{ex}$ of typical ferromagnet is about $0.5 \sim 0.1$ J/m depends on the materials, compositions, and fabrication conditions. Since the dimension of $D$ in our study is energy, not energy per unit area, it must be properly converted. The relevant length scale is the lattice constant $a$ (= 0.2 nm) and spin $S = 1/2$, $\delta_0 = D/J \sim f_0 (D_{DMI} S^2/a^2) \sim 0.05 f_0$, where $f_0$ is a structural constant of order of unit. Therefore, our calculation range $0.01 \sim 0.1$ is physically reasonable. Furthermore, Moon et al. estimated the frequency shift in the SW dispersion relation of order of 1 GHz. Since typical SW resonance frequency is several 10s GHz, it means $\delta_0$ of $0.01 \sim 0.1$ is quite reasonable assumptions.

IV. CONCLUSIONS

In conclusions, we investigated the Curie temperature variations due to the DMI contribution. Since the DMI modifies the SW dispersion relation by lowering system energy, SW is more easily excited by the thermal agitations. Such easier SW excitation implies that DMI lowers the $T_C$. Such reduction of $T_C$ with DMI may be a possible origin of the electric field control of the ferromagnetic phase transition, which is experimentally reported, recently. It means that if we can control DMI somehow, we can control the ferromagnetic phase transition temperature and DMI will be helpful to future developing of spin device applications.

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1T. Moriya, Phys. Rev. 120, 91 (1960).


