Critical Behaviors and Polarizations in A Transverse Ising Film

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Abstract—Ferroelectric thin films described by the transverse field Ising model have been studied by using the usual mean-field approximation. The critical behaviors (the critical surface transverse field and Curie temperature) and polarizations in a transverse Ising film with multi-surface layers are calculated. The main emphasis of our work is laid on the effect of surface exchange interaction on the critical surface transverse field and Curie temperature as a function of the number of surface layers. At the same time, the dependence of polarization on the Curie temperature for the ferroelectric thin film with a certain layers is also discussed in detail.

Keywords—Ferroelectric thin film; Transverse Ising model; Phase diagram; Curie temperature; Polarization;

I. INTRODUCTION

In recent years, various high quality ferroelectric thin films have been successfully fabricated by different kinds of physical or chemical techniques in experiment [1, 2]. On the other hand, the ferroelectric thin film described by the transverse Ising model has also been studied by the usual mean-field approximation (MFA) [3-11]. Usually, the second-order phase transition in a transverse Ising thin film is calculated only by taking the nearest-neighbor two-spin exchange interaction into account. Effects of the surface exchange interaction and the thickness on the Curie temperature in a thin film with different numbers of surface layers have been discussed in detail. Recently, the effects of surface modification on the critical behavior in a multiple-surface-layer ferroelectric thin film have been inspected by using the usual MFA [10]. Very recently, the influence of surface and bulk layers on the crossover features for interaction parameters of a ferroelectric thin film has also been calculated under the usual MFA [11]. However, as far as we know, the effect of the surface exchange interaction on the critical behavior (the critical surface transverse field and the Curie temperature) and the polarizations in a ferroelectric thin film described by the transverse Ising model have not been reported.

In this present work, we will study the effect of surface exchange interaction on the critical behavior (the critical surface transverse field and the Curie temperature) and the dependence of polarizations on Curie temperature in a multiple surface layers ferroelectric thin film within the framework of the usual MFA. The results indicate that the critical surface transverse field and the Curie temperature can be significantly affected by the surface exchange interaction. In addition, the dependence of polarization on the Curie temperature is also obtained.

II. MODEL AND THE FORMALISM

The schematic diagram for the ferroelectric thin film is shown in Figure 1. Usually, it is assumed that the thin film is consisted of \( N \) layers along the \( z \)-direction with a three-dimensional simple cubic lattice structure. The top \( N_s \) layers and the bottom \( N_b \) layers are symmetrical and are defined as the surfaces layers. The other remaining \( N - N_s \) layers are defined as the bulk layers. The Hamiltonian of the system is [3-11]

\[
H = - \sum_i \Omega_i S_i^x - \frac{1}{2} \sum_{i,j} J_{ij} S_i^z S_j^z .
\]
Where $S'_i$ (or $S''_i$) is the component of a pseudo-spin 1/2 operator in the layer numbered $i$ along the direction of $x$ (or $z$). $\Omega_i$ is the transverse field in the layer numbered $i$ and $J_j$ is the exchange interaction between the site $i$ and $j$, where $i$ and $j$ run over all the sites in surface layers and bulk layers. $\Omega_j$ (or $\Omega_b$) is defined as the transverse field on the surface (or bulk) layer. In the same way, $J_j$ (or $J_b$) is defined as the exchange interaction on the surface (or bulk) layer. Furthermore, exchange interactions and transverse fields on these $2N_s$ surface layers are assumed to be different from those of remaining $N-N_s$ bulk layers.

Within the framework of the usual MFA [3-11], the spin average value in the layer numbered $i$ along the $z$ direction $z_i S_i$ is defined as [3-11]

$$
\langle S'_i \rangle = \frac{H'_i}{2|H'_i|} \tanh \left( \frac{|H'_i|}{2k_B T} \right),
$$

where

$$
H'_i = J_{i,i-1} \langle S'_{i-1} \rangle + 4J_{i-1} \langle S'_{i-1} \rangle + J_{i-1} \langle S'_{i-1} \rangle,
$$

$$
|H'_i| = \sqrt{\left( \Omega_i \right)^2 + \left( H'_i \right)^2}.
$$

When the temperature is close to the Curie temperature, the spin average value $\langle S'_i \rangle$ tends to zero. On the other hand, the spin average value is very small. As a result, the higher-order terms of $\langle S'_i \rangle$ tend to zero faster than the linear terms of $\langle S'_i \rangle$, we can only take into account those linear terms. Therefore, the spin average value $\langle S'_i \rangle$ for an $N$-layer ferroelectric thin film with $N_s$ surface layers can be expanded and there are $N$ linear equations [10-11]:

$$
\tau_s \langle S'_i \rangle = 4j_i \langle S'_i \rangle + j_i \langle S'_i \rangle,
$$

$$
\tau_s \langle S'_i \rangle = 4j_i \langle S'_i \rangle + j_i \langle S'_i \rangle + j_i \langle S'_i \rangle,
$$

......

$$
\tau_s \langle S'_{N-s} \rangle = 4j_i \langle S'_{N-s} \rangle + j_i \langle S'_{N-s} \rangle + j_i \langle S'_{N-s} \rangle,
$$

$$
\tau_s \langle S'_{N-s} \rangle = 4j_i \langle S'_{N-s} \rangle + j_i \langle S'_{N-s} \rangle + j_i \langle S'_{N-s} \rangle.
$$

According to [4, 10-11], the phase diagram for an $N$-layer ferroelectric thin film with different surface layers $N_s$ can be numerically calculated by the general equations as follows [4, 10-11]:

1). $N_s=1$:

$$
X_s B_{M-1} - B_{M-2} = 0.
$$

2). $N_s=2$:

$$
\left( X_s^2 - c^2 \right) B_{M-2} - X_s B_{M-3} = 0.
$$

3). $N_s=3$:

$$
\left( X_s^3 - 2X_s c^2 \right) B_{M-3} - \left( X_s^2 - c^2 \right) B_{M-4} = 0.
$$

4). $N_s=4$:

$$
\left( X_s^4 - 3X_s^2 c^2 + c^4 \right) B_{M-4} - \left( X_s^3 - 2X_s c^2 \right) B_{M-5} = 0.
$$

5). $N_s=5$:

$$
\left( X_s^5 - 4X_s^3 c^2 + 3X_s c^4 \right) B_{M-5} - \left( X_s^4 - 3X_s^2 c^2 + c^4 \right) B_{M-6} = 0.
$$
For the ferroelectric thin film with the thickness $N$ is an even number, $M = N / 2$, and there is
\[ B_m = \frac{\sinh[(M + 1)\phi] - \sinh(M\phi)}{\sinh(\phi)}. \] (19)

In contrast, for the ferroelectric thin film with the thickness $N$ is an even number, $M = (N + 1)/2$, and there is
\[ B_m = 2\cosh(M\phi). \] (20)

Note that
\[ X_s = \frac{r_s - 4 j_s}{j_s}, \] (21)
\[ X_h = \frac{r_s - 4 j_h}{j_h}, \] (22)
\[ c = \frac{j_s}{j_h}, \] (23)
\[ \cosh\phi = \frac{X_h}{2}. \] (24)

III. RESULTS AND DISCUSSION

Usually, the phase diagram for a ferroelectric thin film can be described by two different ways: the relations between Curie temperature $T_c$ and the surface transverse field $\Omega_s$ and the relations between Curie temperature $T_c$ and the surface exchange interaction $J_s$, namely the curves of $T_c : \Omega_s$ and $T_c : J_s$. In this work, the curves of $T_c : \Omega_s$ are used to study the phase transition properties of ferroelectric thin films. As we know, the critical surface transverse field $\Omega_m$ at which the value of Curie temperature $T_c$ reduces to zero in the curve of $T_c : \Omega_s$. In the following, the research emphasis is focused on the effect of surface exchange interaction $J_s$ on the critical surface transverse field $\Omega_m$ and Curie temperature $T_c$. In addition, the effects of Curie temperature $T_c$ on the polarizations in the thin film are also numerically calculated.

Fig. 2 shows the effect of surface exchange interaction $J_s$ on the critical surface transverse field $\Omega_m$ for a thin film with $N_s$ surface layers, i.e., the curves of $\Omega_m : N_s$ for different surface exchange interaction $J_s$. For a certain $J_s$, the larger the surface layer number $N_s$, the larger the critical surface transverse field $\Omega_m$. With the increase of the surface layer number $N_s$, the increase of the critical surface transverse field $\Omega_m$ becomes more and more slowly. Eventually, the surface layer number $N_s$ almost has no any effect on the critical surface transverse field $\Omega_m$. Obviously, the effect of the surface exchange interaction $J_s$ on the critical surface transverse field $\Omega_m$ can be found in Fig. 2. For a certain surface layer number $N_s$, the larger the surface exchange interaction $J_s$, the larger the critical surface transverse field $\Omega_m$.

Fig. 3 shows the effect of surface exchange interaction $J_s$ on the Curie temperature $T_c$ for a thin film with $N_s$ surface layers, i.e., the curves of $T_c : N_s$ for different surface exchange interaction $J_s$. For a selected surface exchange interaction $J_s$, with the increase of surface layer number $N_s$, the Curie temperature $T_c$ increases. On the other hand, the effect of the surface exchange interaction $J_s$ on the Curie temperature $T_c$ is similar to the critical surface transverse field $\Omega_m$, namely with the increase of the surface exchange interaction $J_s$, the Curie temperature $T_c$ also increases when the surface layer number $N_s$ is uniform.

Figure 2. The effect of surface exchange interaction $J_s$ on the critical surface transverse field $\Omega_m$ for a thin film with $N_s$ surface layers. All curves are for $J_s$ = 1.0, $\Omega_s$ = 3.0, $N$ = 30.

Figure 3. The effect of surface exchange interaction $J_s$ on the Curie temperature $T_c$ for a thin film with $N_s$ surface layers. All curves are for $J_s$ = 1.0, $\Omega_s$ = 1.0, $\Omega_s$ = 3.0, $N$ = 30.
Figure 4. The dependence of polarization on the Curie temperature $T_c$ for a ferroelectric thin film with surface layers $N_s$ varying from 1 to 5.

All curves are for $J_s=2.0$, $J_B=1.0$, $\Omega_s=2.0$, $\Omega=1.0$, $N=10$.

Fig. 4 shows the dependence of polarization $P$ on the Curie temperature $T_c$ for a ferroelectric thin film with a varying surface layers $N_s$. For a certain $N_s$, it is obvious that the polarization is monotonously decreasing with the increase of Curie temperature $T_c$. Meanwhile, Fig. 4 shows a characteristic feature, namely, there exists a common cross-point which is independent of the surface layers $N_s$. On the left side of this cross-point, with the surface layers $N_s$ increases, the polarization $P$ decreases. On the right side of this cross-point, with the surface layers $N_s$ increases, the polarization $P$ increases.

IV. CONCLUSION

In summary, the effect of surface exchange interaction $J_s$ on the critical behavior (the critical surface transverse field $\Omega_{s}$ and the Curie temperature $T_c$ ) and the dependence of polarization $P$ on the Curie temperature $T_c$ in an $N$–layer ferroelectric thin film with $N_s$ surface layers have been studied by using the usual MFA. Though our study is only a numerical calculation, we hope that this work will be useful for theoretical or experimental study of the ferroelectric thin film.

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