Critical Behaviors and Polarizations in A Transverse Ising Film

Lu Zhao-Xin
College of Mechanical Engineering
Linyi University
Linyi 276005, China
e-mail: phylzx@gmail.com

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_s 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]

$$H=-\sum_i \Omega_i S_i^x - \frac{1}{2}\sum_{i,j} J_{ij} S_i^z S_j^z \quad . \tag{1}$$

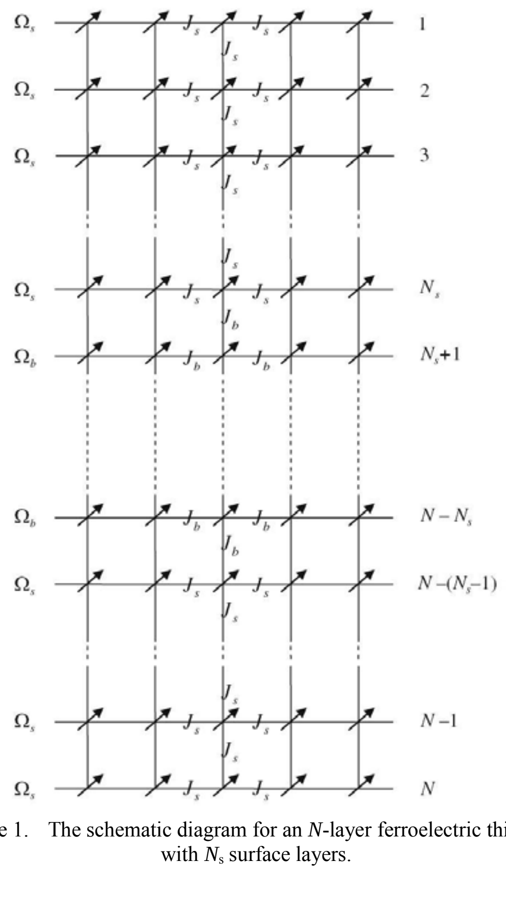

Figure 1. The schematic diagram for an N-layer ferroelectric thin film with N_s surface layers.

Where S_i^x (or S_i^z) is the component of a pseudo-spin 1/2 operator in the layer numbered i along the direction of x (or z). Ω_i is the transverse field in the layer numbered i and J_{ij} 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. Ω_s (or Ω_b) is defined as the transverse field on the surface (or bulk) layer. In the same way, J_s (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 $\langle S_i^z \rangle$ is defined as [3-11]

$$\langle S_i^z \rangle = \left(H_i^z / 2|H_i| \right) \tanh\left(|H_i| / 2k_B T \right), \tag{2}$$

where

$$H_i^z = J_{i,i-1} \langle S_{i-1}^z \rangle + 4J_{ii} \langle S_i^z \rangle + J_{i,i+1} \langle S_{i+1}^z \rangle, \tag{3}$$

$$|H_i| = \sqrt{(\Omega_i)^2 + (H_i^z)^2}. \tag{4}$$

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

$$\tau_s \langle S_1^z \rangle = 4j_s \langle S_1^z \rangle + j_s \langle S_2^z \rangle, \tag{5}$$

$$\tau_s \langle S_2^z \rangle = 4j_s \langle S_2^z \rangle + j_s \langle S_1^z \rangle + j_s \langle S_3^z \rangle, \tag{6}$$

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$$\tau_s \langle S_{N_s}^z \rangle = 4j_s \langle S_{N_s}^z \rangle + j_s \langle S_{N_s-1}^z \rangle + j_b \langle S_{N_s+1}^z \rangle, \tag{7}$$

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$$\tau_b \langle S_i^z \rangle = 4j_b \langle S_i^z \rangle + j_b \langle S_{i-1}^z \rangle + j_b \langle S_{i+1}^z \rangle, \tag{8}$$

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$$\begin{aligned}\tau_s \langle S_{N-(N_s-1)}^z \rangle = 4j_s \langle S_{N-(N_s-1)}^z \rangle + j_b \langle S_{N-N_s}^z \rangle \\ + j_s \langle S_{N-(N_s-2)}^z \rangle\end{aligned}, \tag{9}$$

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$$\tau_s \langle S_{N-1}^z \rangle = 4j_s \langle S_{N-1}^z \rangle + j_s \langle S_{N-2}^z \rangle + j_s \langle S_N^z \rangle, \tag{10}$$

$$\tau_s \langle S_N^z \rangle = 4j_s \langle S_N^z \rangle + j_s \langle S_{N-1}^z \rangle. \tag{11}$$

Where

$$\tau_s = \frac{2\Omega_s}{J} \coth\left(\frac{\Omega_s}{2k_B T} \right), \tag{12}$$

$$\tau_b = \frac{2\Omega_b}{J} \coth\left(\frac{\Omega_b}{2k_B T} \right). \tag{13}$$

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:

$$X_s B_{M-1} - B_{M-2} = 0. \tag{14}$$

2). N_s=2:

$$\left(X_s^2 - c^2 \right) B_{M-2} - X_s B_{M-3} = 0. \tag{15}$$

3). N_s=3:

$$\left(X_s^3 - 2X_s c^2 \right) B_{M-3} - \left(X_s^2 - c^2 \right) B_{M-4} = 0. \tag{16}$$

4). N_s=4:

$$\begin{aligned}&\left(X_s^4 - 3X_s^2 c^2 + c^4 \right) B_{M-4} \\ &\quad - \left(X_s^3 - 2X_s c^2 \right) B_{M-5} = 0\end{aligned}. \tag{17}$$

5). N_s=5:

$$\begin{aligned}&\left(X_s^5 - 4X_s^3 c^2 + 3X_s c^4 \right) B_{M-5} \\ &\quad - \left(X_s^4 - 3X_s^2 c^2 + c^4 \right) B_{M-6} = 0\end{aligned}. \tag{18}$$

For the ferroelectric thin film with the thickness N is an even number, $M = N/2$, and there is

$$B_M = \frac{\sinh\left[(M+1)\phi\right] - \sinh(M\phi)}{\sinh(\phi)} . \tag{19}$$

In contrast, for the ferroelectric thin film with the thickness N is an even number, $M = (N+1)/2$, and there is

$$B_M = 2\cosh(M\phi) . \tag{20}$$

Note that

$$X_s = \frac{\tau_s - 4j_s}{j_b} , \tag{21}$$

$$X_b = \frac{\tau_b - 4j_b}{j_b} , \tag{22}$$

$$c = \frac{j_s}{j_b} , \tag{23}$$

$$\cosh\phi = \frac{X_b}{2} . \tag{24}$$

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 Ω_s and the relations between Curie temperature T_c and the surface exchange interaction J_s, namely the curves of T_c : Ω_s and T_c : J_s. In this work, the curves of T_c : Ω_s are used to study the phase transition properties of ferroelectric thin films. As we know, the critical surface transverse field Ω_{sc} at which the value of Curie temperature T_c reduces to zero in the curve of T_c : Ω_s. In the following, the research emphasis is focused on the effect of surface exchange interaction J_s on the critical surface transverse field Ω_{sc} 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 Ω_{sc} for a thin film with N_s surface layers, i.e., the curves of Ω_{sc} : 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 Ω_{sc}. With the increase of the surface layer number N_s, the increase of the critical surface transverse field Ω_{sc} becomes more and more slowly. Eventually, the surface layer number N_s almost has no any effect on the critical surface transverse field Ω_{sc}. Obviously, the effect of the surface exchange interaction J_s on the critical surface transverse field Ω_{sc} 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 Ω_{sc}.

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 Ω_{sc}, 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.

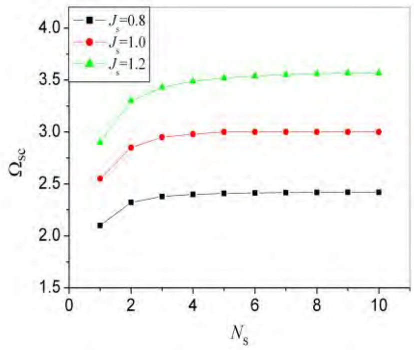

Figure 2. The effect of surface exchange interaction J_s on the critical surface transverse field Ω_{sc} for a thin film with N_s surface layers. All curves are for J_b =1.0, Ω_b =3.0, N =30.

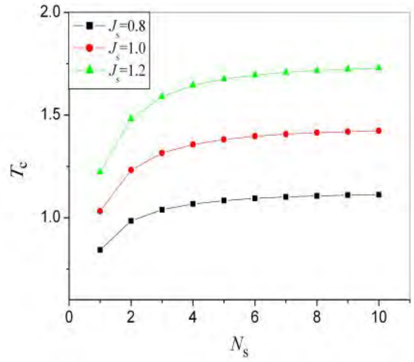

Figure 3. The effect of surface exchange interaction J_s on the Curie temperature T_c for a thin film with N_s surface layers. All curves are for J_b =1.0, Ω_s =1.0, Ω_b =3.0, N =30.

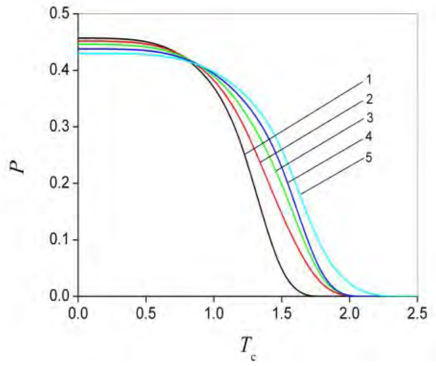

Figure 4. The dependence of polarization on the Curie temperature T_c for a ferroelectric thin film with surface layers N_s varying from 1 to 5. All curves are for J_s =2.0, J_b =1.0, Ω_s =2.0, Ω_b =1.0, N =10.

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 Ω_{sc} 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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REFERENCES

[1] J. F. Scott, “Applications of modern ferroelectrics,” Science,vol. 315, Feb. 2007, pp. 954-959, doi: 10.1126/science.1129564.

[2] M. Dawber, K. M. Rabe, and J. F. Scott, “Physics of thin-film ferroelectric oxides,” Rev. Mod. Phys., vol. 77, Oct. 2005, pp. 1083-1130, doi: 10.1103/RevModPhys.77.1083.

[3] C. L. Wang, W. L. Zhong, and P. L. Zhang, “The Curie temperature of ultra-thin ferroelectric films,” J. Phys.: Condens. Matter, vol. 4, May 1992, pp. 4743-4749, doi: 10.1088/0953-8984/4/19/014.

[4] C. L. Wang, S. R. P. Smith, and D. R. Tilley, “Ferroelectric thin films described by an Ising model in a transverse field,” J. Phys.: Condens. Matter, vol. 6, Nov. 1994, pp. 9633-9646, doi: 10.1088/0953-8984/6/45/013.

[5] H. K. Sy, “Surface modification in ferroelectric transitions,” J. Phys.: Condens. Matter, vol. 5, Mar. 1993, pp. 1213-1220, doi: 10.1088/0953-8984/5/9/006.

[6] X. G. Wang, S. H. Pan, and G. Z. Yang, “Effects of multi-surface modification on Curie temperature of ferroelectric films,”, J. Phys.: Condens. Matter, vol. 11, Aug. 1999, pp. 6581-6588, doi: 10.1088/0953-8984/11/34/310.

[7] T. Kaneyoshi, “Phase diagrams of ferroelectric thin films described by the transverse Ising model,” Physica A, vol. 319, Mar. 2003, pp. 355-361, doi: 10.1016/S0378-4371(02)01516-9.

[8] B. H. Teng and H. K. Sy, “Parameter modifications in the phase diagrams of the transverse field Ising model,” Physica B, vol. 348, May 2004, pp. 485-492, doi: 10.1016/j.physb.2004.02.006.

[9] Z. X. Lu, B. H. Teng, X. H. Lu, X. J. Zhang, and C. D. Wang, “Investigation of the crossover properties for the interaction parameters of a ferroelectric thin film,” Solid State Commun., vol. 149, Aug. 2009, pp. 1176-1179, doi: 10.1016/j.ssc.2009.04.030.

[10] Z. X. Lu, “Effects of surface modification on the critical behaviour in multiple-surface-layer ferroelectric thin films,”, Phys. Scr., vol. 87, Feb. 2013, pp. 025002, doi: 10.1088/0031-8949/87/02/025002.

[11] Z. X. Lu, “Influence of surface and bulk layers on the crossover features for interaction parameters of a ferroelectric thin film,”, PhaseTransitions, doi: 10.1080/01411594.2014.962535, in press.