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Physics Letters A 336 (2005) 216–222

PHYSICS LETTERS A

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Critical line between the first-order and the second-order phase transition for ferroelectric thin films described by TIM

Qing Jiang [a], Yong Mei Tao [a,b,*]

[a] *Department of Physics, Suzhou University, Suzhou 215006, China*
[b] *Department of Physics, Changshu Institute of Technology, Changshu 215500, China*

Received 11 January 2004; received in revised form 28 October 2004; accepted 17 December 2004

Available online 18 January 2005

Communicated by J. Flouquet

Abstract

In this Letter, we apply the transverse-field Ising model (TIM) with a four-body interaction term to ferroelectric thin films. By defining a critical value $(J'/J)_c$, the critical line between the first-order and the second-order phase transition is obtained for ferroelectric thin films. We discuss influence of the film thickness on the critical value $(J'/J)_c$. Behavior of the phase transition and the dielectric susceptibility of ferroelectric thin films are investigated within the mean-field approximation.

PACS: 77.80.-e; 77.80.Bh; 77.55.+f

Keywords: Ferroelectric thin films; Critical line; Four-body interaction; TIM

1. Introduction

The character of ferroelectric thin films has been of growing interest because of the significance in the field of microelectronics [1] and optoelectronics [2], such as dynamic random access memory [3]. Most ferroelectric thin films, having potential applications, are first-order phase transition ferroelectrics. Many researchers have focused their attention on ferroelectric thin films for their size and surface effects, in which different layers have different polarizations and susceptibility.

Early theoretical work applied Landau phenomenological theory to ferroelectric thin films [4–7]. They assumed the P^4 term was positive for the second-order phase transition, and they further supposed that the P^4 term was negative and added a positive P^6 term in the free energy expression for the first-order phase transition. In addition,

* Corresponding author.
E-mail addresses: qjiang@suda.edu.cn (Q. Jiang), ymt@cslg.cn (Y.M. Tao).

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doi:10.1016/j.physleta.2004.12.053

in this phenomenological theory two so-called 'extrapolation length' δ_2 and δ_4, were used to distinguish the surface and interior of thin films.

The transverse Ising mode (TIM) is another widely used approach to deal with ferroelectric thin films with order-disorder type, or displacive type because of their multi-site potential. The phenomenological theory can be considered as the continuum limit of TIM [8]. Previous work has shown that the first-order phase transition is possible in TIM only if the number of coupled spins is four or larger. Wang et al. [9,10] pointed out that when the first-order phase transition was discussed, the four-spin interactions must be included, but when the second-order phase transition was referred, the four-spin interactions could be neglected. They used retarded Green's function to study ferroelectrics, and found that the infinite system exhibited the first-order phase transition when the four-spin coupling strength $\tilde{J}' > 4\tilde{J}/3$, where $\tilde{J} = \sum_j J_{ij}$, $\tilde{J}' = \sum_{jkl} J'_{ijkl}$. This conclusion was in good agreement with that obtained under mean field approximation within the framework of TIM [11]. Meanwhile, in TIM the surface contribution is taken into consideration by taking the surface coupling constants of two-spin $J_{2\mathrm{s}}$ and four-spin interaction $J_{4\mathrm{s}}$, which are different from those of bulk material.

For the ferroelectric thin films, much work in TIM focused on behaviors of the second-order phase transition [12–15]. The critical temperature and driving size of thin films were discussed. However, as we pointed above, most ferroelectric thin films in practice application may undergo the first-order phase transition. Relation between behavior of the first-order phase transition and the film thickness is worthwhile to be discussed further. In our present Letter, critical behaviors of the ferroelectric thin films are given a thorough research under mean-field approximation within the framework of TIM. We investigate dependence of the critical line between the first-order and second-order phase transition on the thickness of thin film. By defining a critical value $(J'/J)_c$, which is valid for both infinite system and finite system, we discuss effect of the four-body interaction coupling on characters of the phase transition and the thermodynamic properties. The results show that $(J'/J)_c$ strongly depends on layer-number N, and changes character of the phase transition. Simultaneously, surface effects are also taken into account.

2. Theory

We consider ferroelectric thin films in which each layer is defined on the x–y plane, the orientation of thickness is z-axis, and pseudo-spins site on a cubic lattice. The Hamiltonian within the framework of TIM is given by

$$H = -\Omega \sum_i S_i^x - \frac{1}{2}\sum_{ij} J_{ij} S_i^z S_j^z - \frac{1}{4}\sum_{ijkl} J_{ijkl} S_i^z S_j^z S_k^z S_l^z - 2\mu E \sum_i S_i^z, \tag{1}$$

where Ω is the tunneling frequency, μ is the dipole moment on single ion and E is the external electric field. S_i^x, S_i^z are the x and z components of pseudo-spin ($S = 1/2$) in the ith site. J_{ij} and J_{ijkl} are the two-spin and four-spin interaction coupling constants, respectively. In order to distinguish the surface from the bulk, we define coupling constants as

$$J_{ij} = \begin{cases} J_{2\mathrm{s}}, & i, j \text{ on the surface}, \\ J_{2\mathrm{b}}, & \text{otherwise}, \end{cases} \tag{2}$$

$$J_{ijkl} = \begin{cases} J_{4\mathrm{s}}, & i, j, k, l \text{ on the surface}, \\ J_{4\mathrm{b}}, & \text{otherwise}. \end{cases} \tag{3}$$

Due to the translation symmetry in x–y plane, all the average pseudo-spins in the same layer are identical. The average pseudo-spins vary with different layers. Under mean-field approximation, the average pseudo-spin in the ith layer can be expressed as

$$m_i = \langle S_i^z \rangle = \frac{\langle H_i^z \rangle}{2|H_i|} \tanh \frac{|H_i|}{2k_B T}, \quad 1 \leqslant i \leqslant N, \tag{4}$$