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Physical properties of ferroelectric superlattice A_3/B_3 system in electric field*

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Based on the differential operator technique, a transverse Ising model (TIM) in the effective-field theory is developed to study the physical properties of a ferroelectric superlattice A_3/B_3 system. The effects of an external electric field on the polarization, susceptibility and pyroelectric coefficient of the ferroelectric superlattice A_3/B_3 system are discussed in detail. The susceptibility of the ferroelectric superlattice A_3/B_3 system decreases with the increase of the electric field, implying that the polarization is weak.

Keywords: ferroelectric superlattice, polarization, pyroelectric coefficient, susceptibility
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1. Introduction

Ferroelectric superlattices have been widely studied in recent years owing to the advances of experimental techniques which make it possible to well prepare samples. These samples show that their various physical properties usually are very different from those of the corresponding bulk systems. Experimentally, superlattices $BaTiO_3/SrTiO_3$ and $PbTiO_3/PbZrO_3$ with perovskite-type structure consisting of two different slabs with a certain slab thickness have already been prepared.[1,2] Theoretically, efforts have been made to study the properties of ferroelectric superlattices by use of various techniques. In Ref.[3], a phonon-pseudospin coupled model in the double-time Green function theory has been developed to investigate dielectric properties of the ferroelectric strained superlattices $BaTiO_3$ /$SrTiO_3$. This issue has also been tackled by Ginzburg–Landau phenomenological theory,[4,5] as well as by transverse Ising model in mean-field approximation.[6,7] From the experimental and theoretical points of view the transverse Ising model (TIM) is a valuable model because of its potential applications. It has been applied to study the phase transitions in many systems, including order-disorder ferroelectrics, induced moment ferromagnets, and cooperative Jahn–Teller system.[8,9] In our previous work,[10,11] the TIM has been used to discuss the magnetic properties of the magnetic materials. The susceptibility has been studied by using the inverse scattering transformation.[12,13] Yet, the pyroelectric properties and polarization and susceptibility of ferroelectric superlattice A_3/B_3 have not yet been studied in the transverse Ising model with the effect of the external electric field taken into account. In this paper, we present the results of the studies using the transverse Ising model based on the effective-field theory with the differential operator technique.

2. Formulation

The model of a ferroelectric/ferroelectric superlattice A_3/B_3 system is presented as shown in Fig.1 in Ref.[6]. The system can be described by the following Hamiltonian:

$$H = -\sum_{(i,j)} J_{ij}\sigma_i^z\sigma_j^z - \sum_i \Omega_i\sigma_i^x - 2\mu E\sum_i \sigma_i^z, \quad (1)$$

where the first summation is carried out only over

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nearest-neighbor pairs of sites. The spin-1/2 with pseudo-spin moments σ_i^z and σ_i^x is at the site i in the A slab, and that with the pseudo-spin moments σ_j^z and σ_j^x is at the site j in the B slab. J_{ij} is the coupling strength between pseudo-spins at the i and j sites, with the J_1, J_2 and J_3 taken in the slab A, slab B and between the slab A and B, respectively. Ω_i represents the transverse field. μ is the effective dipole moment and E is the external electric field.

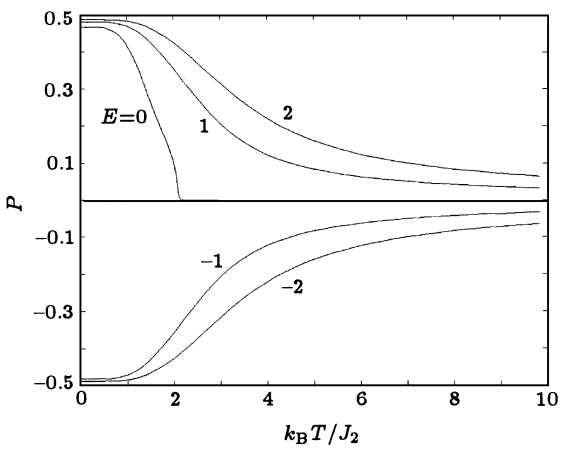


Fig.1. Temperature-dependent polarization for A_3/B_3 superlattice. The figures on the curves are the values of electric field.

Within the effective-field theory with the differential operator technique presented in Refs.[10,11,14], the polarizations P_L for each layer in one period of the superlattice are determined by

$$P_{0(4)} = \left[\cosh\left(\frac{1}{2}J_3\nabla\right) + 2P_{0(4)}\sinh\left(\frac{1}{2}J_3\nabla\right)\right]^4 \times \left[\cosh\left(\frac{1}{2}J_3\nabla\right) + 2P_{1(5)}\sinh\left(\frac{1}{2}J_3\nabla\right)\right] \times \left[\cosh\left(\frac{1}{2}J_3\nabla\right) + 2P_{7(3)}\sinh\left(\frac{1}{2}J_3\nabla\right)\right] F_i(x)|_{x=0}, \quad (2)$$

$$P_{1(5)} = \left[\cosh\left(\frac{1}{2}J_{1(2)}\nabla\right) + 2P_{1(5)}\sinh\left(\frac{1}{2}J_{1(2)}\nabla\right)\right]^4 \times \left[\cosh\left(\frac{1}{2}J_{1(2)}\nabla\right) + 2P_{2(6)}\sinh\left(\frac{1}{2}J_{1(2)}\nabla\right)\right] \times \left[\cosh\left(\frac{1}{2}J_3\nabla\right) + 2P_{0(4)}\sinh\left(\frac{1}{2}J_3\nabla\right)\right] F_i(x)|_{x=0}, \quad (3)$$

$$P_{2(6)} = \left[\cosh\left(\frac{1}{2}J_{1(2)}\nabla\right) + 2P_{2(6)}\sinh\left(\frac{1}{2}J_{1(2)}\nabla\right)\right]^4 \times \left[\cosh\left(\frac{1}{2}J_{1(2)}\nabla\right) + 2P_{3(7)}\sinh\left(\frac{1}{2}J_{1(2)}\nabla\right)\right] \times \left[\cosh\left(\frac{1}{2}J_{1(2)}\nabla\right) + 2P_{1(5)}\sinh\left(\frac{1}{2}J_{1(2)}\nabla\right)\right] F_i(x)|_{x=0}, \quad (4)$$

$$P_{3(7)} = \left[\cosh\left(\frac{1}{2}J_{1(2)}\nabla\right) + 2P_{3(7)}\sinh\left(\frac{1}{2}J_{1(2)}\nabla\right)\right]^4 \times \left[\cosh\left(\frac{1}{2}J_{1(2)}\nabla\right) + 2P_{2(6)}\sinh\left(\frac{1}{2}J_{1(2)}\nabla\right)\right] \times \left[\cosh\left(\frac{1}{2}J_3\nabla\right) + 2P_{4(0)}\sinh\left(\frac{1}{2}J_3\nabla\right)\right] F_i(x)|_{x=0}, \quad (5)$$

where $\nabla = \partial/\partial x$ is the differential operator. The function of $F_i(x)$ is given by

$$F_i(x) = \frac{(x+E)}{2\sqrt{(x+E)^2+\Omega_i^2}} \times \tanh\left(\frac{\beta\sqrt{(x+E)^2+\Omega_i^2}}{2}\right). \quad (6)$$

Then the mean polarization P of the superlattice is

$$P = \frac{1}{N}\sum_{L=1}^{N} P_L, \quad (7)$$

where N is the period of the superlattice.

The mean susceptibility and pyroelectric coefficient of the superlattices can be respectively expressed as

$$\chi = \frac{\partial P}{\partial E}, \quad (8)$$

$$p = \frac{\partial P}{\partial T}. \quad (9)$$

The following values of the parameters are used in the calculation: $\Omega_1/\Omega_2 = J_1/J_2 = 2/1$, $\Omega_3 = (\Omega_1+\Omega_2)/2$ and $J_3 = \sqrt{J_1 \cdot J_2}$, which are the same as those in Ref.[6].

3. Results and discussion

The polarization of the ferroelectric superlattice A_3/B_3 system can be calculated from Eqs.(2)–(7). The numerical result is plotted in Fig.1. The figures on the curves are the values of the electric field applied. The polarizations are a function of temperature, exchange interaction and electric field. From Fig.1, we can see that the polarization falls from a maximum down to zero with the increase of temperature when no electric field is applied. In the presence

of the electric field, the polarization falls rapidly from its maximum to a remaining polarization as temperature increases. The remaining polarization increases with the increase of the applied electric fields. The polarization curves are symmetric for both positive and negative electric field. The polarization resulting from the applied electric field has not been reported in other theoretical papers.

The susceptibility is also an interesting physical quantity that describes the property of the change in polarization under an electric field. It can reflect the position of transition temperature. In Fig.2 the temperature-dependent susceptibility for the ferroelectric superlattice A_3/B_3 system is plotted. As shown on the curves, the transition temperature shifts toward the high temperature region with the increase of the electric field. The stronger the applied electric field, the smaller the susceptibility becomes.

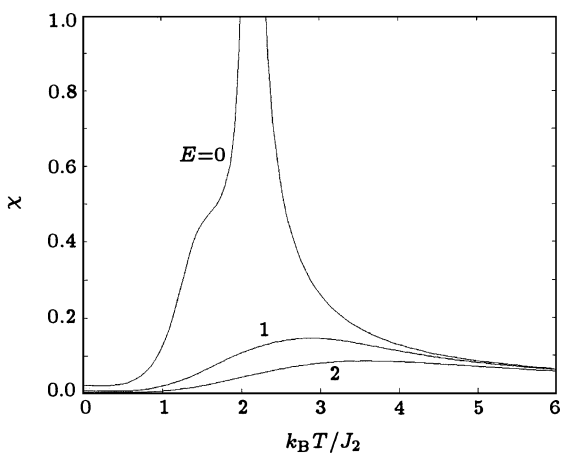


Fig.2. Temperature-dependent polarization susceptibilities for A_3/B_3 superlattice. The figures on the curves are the values of electric field.

The temperature-dependent pyroelectric coefficient for the ferroelectric superlattice A_3/B_3 system is shown in Fig.3. When the electric field is weak, two peaks appear on the curves of the pyroelectric coefficient. The first and second peaks are mainly caused by layers of slabs B and A, respectively. We can also find that when the electric field becomes stronger, two peaks of the pyroelectric coefficient disappear on the curve but a smooth peak occurs instead, and its position depends on the transition temperature and electric field. These results verify that the electric field has an important influence on the properties of the ferroelectric superlattice A_3/B_3 system.

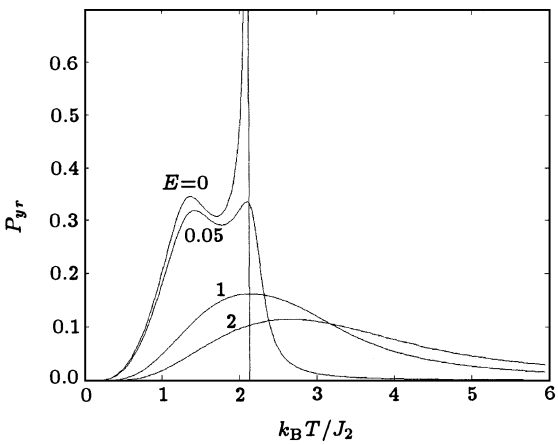


Fig.3. Temperature-dependent pyroelectric coefficient for A_3/B_3 superlattice. The figures on the curves are the values of electric field.

4. Conclusion

We have studied the properties of the ferroelectric superlattice A_3/B_3 system described by use of the transverse Ising model based on the effective-field theory with the differential technique. The polarization curves are symmetric for both positive and negative electric fields. The remaining polarization increases with the increase of the applied electric field. The transition temperature has a shift toward the high temperature region as the electric field increases. Stronger the applied electric field, the smaller the susceptibility becomes, reflecting the fact that the polarization is weaker. When the electric field is weak, two peaks appear on the curve of the pyroelectric coefficient, but when the electric field is strong, a smooth peak occurs instead.

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