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Dynamic hysteresis loop in a ferroelectric heterostructure

Cui Lian*, Cui Haiying, Li Yuchun

School of Mechatronics Engineering, Daqing Normal University, Daqing 163712, China

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ABSTRACT

A Landau–Devonshire theory in combination with Landau–Khalatnikov dynamic equation has been firstly used to study the dynamic hysteresis loop of a ferroelectric heterostructure consisting of two different films. The surface transition layer within each component film and an antiferroelectric coupling at the interface between two films are considered. A parameter β is introduced to describe the differences of physical properties between two constituent films. The influence of parameterβ, surface transition layer, antiferroelectric coupling and electric field frequency on the dynamic hysteresis loop of the ferroelectric heterostructure is discussed in detail. The results show that the system can exhibit antiferroelectriclike behavior (i.e., multi-loop hysteresis) through tuning some critical factors.

1. Introduction

Increasing high demand for novel functional properties in diverse practical applications has immensely accelerated the exploration and development of advanced functional ferroelectric materials [1]. Especially the studies on the physical properties of ferroelectric heterostructures or superlattices have attracted much attention owing to their desirable functional characteristics and potential applications [2,3]. It is a widely accepted view that some outstanding properties such as enhanced polarization, dielectric, piezoresponse and multi-loop hysteresis in ferroelectric heterostructures are attributed to the interfacial coupling at the interface [4–7]. Thus, many theoretical models of ferroelectric heterostructures with interfacial coupling were established to investigate their excellent characteristics, and some abnormal phenomena observed in the experiments can be successfully explained by these models [8–10].

For designing the multi-state memories, the hysteresis loop of ferroelectric heterostructures has attracted particular attention. Initially, Ma et al. proposed that the magnitude of the coupling enhanced the antiferroelectric behavior without the applied electric field in a ferroelectric superlattice and indicated the influence of antiferroeletric coupling on polarizaton [11]. Subsequently, chew and co-workers designed some theoretical models of ferroelectric superlattice and bilayer with an antiferroelectric interfacial coupling, and studied the hysteresis loop of the system by Landau theory. The results show that there is a triple hysteresis loop pattern in the system and the loop patterns vary between typically ferroelectric and antiferroelectric depending the layer thickness and the magnitude of antiferroelectric interfacial coupling [12].

In recent years, multi-state memory is expected to achieve the simulation of human brain in the medical profession, which inspires more researchers to explore the hysteresis loop characteristics of ferroelectric heterostructures or superlattices [13]. Experimentally, Ranjith et al has demonstrated that the hysteresis loop exhibits clear size dependent ferroelectric and antiferroeletric characteristics in the multilayered of $Pb(Mg_{1/3}Nb_{2/3})O_3$ (PMN)-$PbTiO_3$ (PT) [14]. Double hysteresis loops induced by defect dipoles were also discovered in $PbZr_{0.52}Ti_{0.48}O_3/PbZr_{0.8}Ti_{0.2}O_3$ ferroelectric bilayer films by Zhang et al. in the experiment [15].

* Corresponding author.
E-mail address: cl_19830422@126.com (L. Cui).

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Theoretically, Essaoudi research team has studied the hysteresis loop of the bilayer superlattice with an antiferroelectric coupling applying the TIM, and obtained the triple-loop hysteresis [16–18]. Using the TIM theory and introducing the surface transition layer, Cui et al. investigated the combined influence of an antiferroelectric coupling and surface transition layer on the hysteresis loop of a ferroelectric bilayer film [19]. Tripe-loop hysteresis curves have been obtained. Others also observed a triple hysteresis loop pattern in a ferroelectric bilayer or superlattice with antiferroelectric coupling using the Landau theory [20].

However, the aforementioned theoretical studies concerning the hysteresis loop in ferroelectric heterostructures or bilayers with an antiferroelectric coupling are all statically described, which can not really reflect the dynamic state properties of the practical applications in ferroelectric memories. The dynamic hysteresis loop is able to show the dependence of the hysteresis loop shape, remanent polarization and coercive field on the time, amplitude and frequency of driving electric field, these are the important effect factors in practical applications, particularly, the hysteresis loop is strongly dependent on the frequency [21], whereas the statically hysteresis cannot reflect it. Therefore, it is necessary to investigate the dynamical hysteresis loop of the ferroelectric systems. Based on our previous works [22–24], introducing a parameterβ which describes the differences of physical properties between two constituent films in the ferroelectric heterostructure, we design a ferroelectric heterostructure comprising two different films with an antiferroelectric coupling at the interface to expound the hysteresis behavior utilizing the Landau dynamic theory. Up to now, the study on dynamic hysteresis behavior of a ferroelectric heterostructure with an antiferroelectric coupling and surface transition layer has not been reported.

In this paper, a Landau–Devonshire theory as well as Landau–Khalatnikov dynamic equation is used to study the dynamic hysteresis loop of a ferroelectric heterostructure consisting of two different films with an antiferroelectric coupling and surface transition layer.

2. The model

Fig. 1 shows the stacking of thin layers configuration of a ferroelectric heterostructure containing two different materials 1, 2 of film thickness L_1 and L_2 with surface transition layer between two metallic electrodes. Based on our previous published work, the modified Landau – type free energy of the ferroelectric heterostructure can be expressed as the following [22]

$$G = G_1 + G_2 + G_I \tag{1}$$

where G_1, G_2 and G_I represent the free energy density of film 1, film 2 and the interfacial layer, respectively. The expressions for G_1, G_2 and G_I are given by

$$G_1 = \sum_{i=1}^{N_1} \left[\frac{1}{2}A_1(T - T_{c1})P_i^2 + \frac{1}{2}B_1\psi_1(z)P_i^2 + \frac{1}{4}C_1P_i^4 + K_1(P_i - P_{i-1})^2 - E_1P_i \right] \tag{2}$$

$$G_2 = \sum_{i=N_1}^{N} \left[\frac{1}{2}A_2(T - T_{c2})Q_i^2 + \frac{1}{2}B_2\psi_2(z)Q_i^2 + \frac{1}{4}C_2Q_i^4 + K_2(Q_i - Q_{i-1})^2 - E_2Q_i \right] \tag{3}$$

$$G_I = -\chi P(L_1)Q(L_1) \tag{4}$$

P_i and Q_i correspond to the polarization of layer i in film 1 and film 2, respectively; A_j, B_j, C_j, and K_j are positive coefficients and independent of temperature T and position z; T_{cj} is the transition temperature of the bulk ferroelectric; E_j acts as the applied electric field. The second term introduced in Eq. (2) and (3) reflects the contribution of the surface transition layer. The distribution function $\psi_j(z)$ reflects the surface effect. The $K_1(P_i - P_{i-1})^2$ and $K_2(Q_i - Q_{i-1})^2$ term represent the coupling effect between neighboring layers ($j = 1, 2$). $P(L_1)$ and $Q(L_1)$ denote the polarizations at the interfaces of layer 1 and 2, respectively. χ is the interfacial coupling constant. In this paper, we take the case of anferroelectric interfacial coupling, i.e., $\chi < 0$.

Additionally, the boundary conditions at $z = 0$, L_1 and L are [22]:

$$\left(\frac{dP}{dz}\right) = 0 \qquad (z = 0) \tag{5}$$

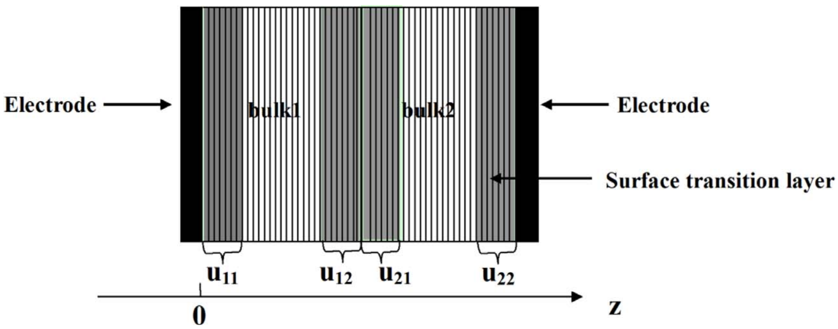

Fig. 1. Theoretical mode of a ferroelectric heterostructure.