Impact of in-plane anisotropic strains on the dielectric and pyroelectric properties of Ba$_{0.7}$Sr$_{0.3}$TiO$_3$ thin films

Hai-Xia Cao
Department of Applied Physics, The Hong Kong Polytechnic University, Hong Kong, China and Department of Physics, Suzhou University, Suzhou 215006, China

Veng Cheong Lo
Department of Applied Physics, The Hong Kong Polytechnic University, Hong Kong, China

Zhen-Ya Li
CCAST (World Laboratory), P.O. Box 8730, Beijing 100080, China and Department of Physics, Suzhou University, Suzhou 215006, China

(Received 18 July 2006; accepted 29 October 2006; published online 11 January 2007)

A modified Landau-Devonshire phenomenological thermodynamic theory is used to describe the influence of in-plane anisotropic strains on the dielectric and pyroelectric properties of epitaxial Ba$_{0.7}$Sr$_{0.3}$TiO$_3$ thin films grown on dissimilar tetragonal substrates. The in-plane anisotropic strain factor-temperature phase diagram is developed. The in-plane anisotropic strains play a crucial role in the dielectric and pyroelectric properties of BST thin films. The theoretical maximum dielectric tunability approaching 100% can be attained at the critical anisotropic strain factor corresponding to the structural phase transformation from $c_1$ to $a_1$ phase. Moreover, the anisotropic strain factor has an opposite effect on the figure of merit and pyroelectric coefficient, respectively. Furthermore, in the case of isotropic strains, our theoretical results are well consistent with the experimental results.


I. INTRODUCTION

During the past decade, ferroelectric thin films have been extensively investigated due to their physical properties and promising applications in various fields of microelectronics. In particular, Ba$_{1-x}$Sr$_x$TiO$_3$ (BST) thin films have long been recognized as the potential candidates for use in tunable microwave devices such as phase shifter, bandpass filter, and delay line, as well as the well-known capacitor applications such as storage capacitor in dynamic random access memory and decoupling capacitor integrated into monolithic circuit.\cite{1,2,3,4} These applications rely strongly on the excellent ferroelectric and dielectric properties of BST films including a high dielectric permittivity, reasonably low dielectric loss, and high dielectric tunability.\cite{1,2,4-6} The dielectric tunability (i.e., the degree of variation in dielectric permittivity as a function of applied electric field) is one of the key design parameters of tunable microwave devices. It is desirable to accomplish a large tunability with a small dielectric loss. On the other hand, the application of ferroelectric materials in infrared detectors is still important, such as economical pyroelectric detectors and thermal imaging devices. One major advantage is that they can operate at room temperature, thereby eliminating the need for expensive cooling systems.\cite{7,8,9,10} Moreover, the integration of hybrid arrays of ferroelectric thin films detectors with silicon readout integrated circuits can offer high-performance infrared imaging. BST thin films are also considered as the candidate materials for pyroelectric sensors because of their relatively large non-linear pyroelectric response at room temperature, good reliability, good sensitivity, and low cost.

The fundamental problem that limits the use of BST films is that they have inferior dielectric and pyroelectric properties compared to their bulk counterparts, which are usually ascribed to compositional and microstructural inhomogeneities, defects, and internal strains. In homogeneous epitaxial single-domain ferroelectric thin films, internal strains arise due to various reasons, including the lattice mismatch between the film and the substrate, the difference in thermal expansion coefficients of the film and the substrate, the self-strain induced by the paraelectric-ferroelectric phase transformation, and defects such as dislocations and vacancies. Although such strains often lead to degradation of film properties, if judicious use is made of substrates and growth parameters, strains can offer the opportunity to enhance particular properties of a chosen material in thin film form, namely, strain engineering.\cite{11,12} A great progress has been achieved in the experimental study of the isotropic misfit strain effect, induced in the ferroelectric thin films grown on cubic substrates.\cite{13-16} The internal strains have a pronounced impact on the dielectric and pyroelectric behaviors of BST thin films through the electrostrictive effect and phase transitions. It has been shown that the dielectric permittivity and the pyroelectric coefficient of epitaxial BST thin films can be tuned by varying the misfit strain. The misfit strain can be controlled through the selection of a substrate material and by the variation of the film thickness. Besides, if the ferroelectric thin films are grown on tetragonal or orthorhombic substrates, the misfit strain along a crystalline axis will obviously differ from that along the other crystalline axis, which is called anisotropic misfit strains. Recent experiments have demonstrated that the in-plane anisotropic strain can be induced in (Pb, Sr)TiO$_3$ thin film by using orthorhombic...
NdGaO$_3$ (110) as a substrate and may significantly affect dielectric properties of the film. Moreover, in-plane dielectric properties of (110) oriented epitaxial (Ba$_{0.60}$Sr$_{0.40}$)TiO$_3$ thin films have been experimentally studied under the influence of anisotropic epitaxial strains from (100) NdGaO$_3$ substrates. The anisotropic misfit strains may result in different material properties and thus open up other possibilities for the design of electronic devices.

With the advancement of experimental techniques, BST films with different composition ratios Ba/Sr were fabricated by a variety of thin film deposition techniques including rf-magnetron sputtering, sol-gel, metal-organic chemical vapor deposition (MOCVD), and laser ablation process. Theoretically, phase diagrams and dielectric and pyroelectric responses of epitaxial BST films were investigated within the framework of a Landau-Devonshire phenomenological model. In addition, optimization of the tunability of BST films via epitaxial stresses was analyzed using a phenomenological model. However, the previous experimental and theoretical works were only concentrated on the effect of in-plane isotropic strains on the thermodynamic properties of BST thin films. Up to now, the influence of in-plane anisotropic strains on the phase diagram and dielectric and pyroelectric responses of BST films has not been studied theoretically. Consequently, the aim of this work is to investigate the impact of in-plane anisotropic strains on the dielectric tunability and pyroelectric response of Ba$_{0.7}$Sr$_{0.3}$TiO$_3$ thin films grown on dissimilar substrates by developing the Landau-Devonshire-type phenomenological thermodynamic theory. This theory was recently employed to predict the equilibrium polarization states and dielectric properties of BaTiO$_3$ and PbTiO$_3$ thin films.

II. THEORETICAL DEVELOPMENT

Suppose a single-domain Ba$_{0.7}$Sr$_{0.3}$TiO$_3$ thin film epitaxially grown in the (001) oriented cubic paraelectric state on a thick tetragonal substrate. If the thickness of the substrate is much larger than the film thickness, the internal stresses are concentrated in the film and the substrate is stress-free. For such a configuration, the in-plane anisotropic misfit strains can be calculated as $u_{m1}=(a_1-a_f)/a_f$ and $u_{m2}=(a_2-a_f)/a_f$, where $a_1$ and $a_2$ are the in-plane lattice parameters along the two different crystalline axes and $a_f$ the lattice constant of the cubic paraelectric phase at the stress-free state. When $u_{m1(2)}>0$, it is a tensile strain, and when $u_{m1(2)}<0$, it is compressive. The in-plane shear strain is approximately taken as zero because of the tetragonal thick substrate. We introduce an anisotropic strain factor $\beta$ as $u_{m2}/u_{m1}$, which denotes the extent of anisotropy. The thermodynamic description may be developed starting from the power-series expansion of the modified Landau-Devonshire thermodynamic potential $\tilde{G}$ in terms of polarization component $P_i$ ($i=1, 2, 3$), in-plane strain $u_{m1}$, anisotropic strain actor $\beta$, and applied field $E_i$ ($i=1, 2, 3$). The relevant general expression for this expansion reads

$$\tilde{G} = a_1^* P_1^2 + a_2^* P_2^2 + a_3^* P_3^2 + a_{11}^* (P_1^4 + P_2^4) + a_{12}^* (P_1^2 P_2^2 + P_1^2 P_3^2) + a_{13}^* (P_2^2 P_3^2) + a_{111}^* (P_1^6 + P_2^6 + P_3^6) + a_{112}^* (P_1^4 P_2^2 + P_1^4 P_3^2 + P_2^4 P_3^2) + a_{123}^* (P_1^2 P_2^4 + P_1^2 P_3^4)$$

$$+ \left( s_{11} u_{m1} (1 + \beta) - 2 s_{12} u_{m1} \beta \right) - E_1 P_1 - E_2 P_2 - E_3 P_3.$$

(1)

The vector and tensor quantities are defined in a Cartesian coordinate system, for example, $P_i||(100)$, $P_2||(010)$, and $P_3||(001)$. The renormalized coefficients of the free energy expansion in Eq. (1) are

$$a_{11}^* = a_{11} + \frac{1}{2(s_{11}^2 - s_{12}^2)} [(Q_{11}^2 + Q_{12}^2)s_{11} - 2Q_{11}Q_{12}s_{12}],$$

$$a_{12}^* = a_{12} - \frac{1}{s_{11}^2 - s_{12}^2} [(Q_{11}^2 + Q_{12}^2)s_{12} - 2Q_{11}Q_{12}s_{11}] + \frac{Q_{11}^4}{2s_{44}},$$

$$a_{13}^* = a_{12} + \frac{Q_{12}^2(Q_{11} + Q_{12})}{s_{11} + s_{12}},$$

$$a_{33}^* = a_{11} + \frac{Q_{12}^2}{s_{11} + s_{12}},$$

(2)

where $a_{ij}$ is the dielectric stiffness, $a_{ij}$ and $a_{ijk}$ are higher order stiffness coefficients at constant stress, $Q_{ij}$ are the elec-
trostrictive coefficients, and $s_{ij}$ the elastic compliances of the film. The temperature dependence of the dielectric stiffness $\alpha_i$ is given by the Curie-Weiss law, $\alpha_i = (T - T_0) / 2 \varepsilon_0 C$, where $T_0$ and $C$ are the Curie-Weiss temperature and constant of a bulk ferroelectrics, respectively, and $\varepsilon_0$ is the permittivity of free space.

The polarization components as a function of the applied field can be derived from the Landau-Devonshire thermodynamic potential using the stability criterion of the first partial derivative ($\partial \tilde{G} \partial P$), as shown below.

$$\alpha_1 P_1 + 2 \alpha_{11} P_1^3 + \alpha_{12} P_1 P_2^2 + \alpha_{13} P_1 P_3^2 - \frac{E_1}{2} = 0,$$

$$\alpha_2 P_2 + 2 \alpha_{12} P_2^3 + \alpha_{11} P_1 P_2^2 + \alpha_{13} P_2 P_3^2 - \frac{E_2}{2} = 0,$$

$$\alpha_3 P_3 + 2 \alpha_{13} P_3^3 + \alpha_{11} (P_1^2 + P_2^2) P_3 - \frac{E_3}{2} = 0,$$

where the contribution of sixth-order polarization terms to the thermodynamic potential is neglected. The electric field dependent relative dielectric permittivities along [100], [010], and [001] directions can be determined by

$$\frac{\varepsilon_{11}(E_1)}{\varepsilon_0} = \left( \varepsilon_0 \frac{\partial \tilde{G}}{\partial P_1^2} \right)^{-1} = \frac{1}{2 \varepsilon_0 \left[ \alpha_1^2 + 6 \alpha_{11} P_1^2 + \alpha_{12} P_2^2 + \alpha_{13} P_3^2 \right]}$$

$$\frac{\varepsilon_{22}(E_2)}{\varepsilon_0} = \left( \varepsilon_0 \frac{\partial \tilde{G}}{\partial P_2^2} \right)^{-1} = \frac{1}{2 \varepsilon_0 \left[ \alpha_2^2 + 6 \alpha_{11} P_1^2 + \alpha_{12} P_2^2 + \alpha_{13} P_3^2 \right]}$$

$$\frac{\varepsilon_{33}(E_3)}{\varepsilon_0} = \left( \varepsilon_0 \frac{\partial \tilde{G}}{\partial P_3^2} \right)^{-1} = \frac{1}{2 \varepsilon_0 \left[ \alpha_3^2 + 6 \alpha_{13} P_3^2 + \alpha_{11} (P_1^2 + P_2^2) \right]}$$

respectively. The small-signal dielectric response along [100], [010], and [001] directions can also be determined by Eqs. (6)–(8) with the polarizations given by setting $E_i$ equal to zero in Eqs. (3)–(5). Correspondingly, we define the dielectric tunability $\Phi$ as the variation in the dielectric response with the applied field with respect to the small-signal dielectric permittivity as

$$\Phi = \begin{cases} 
1 - \varepsilon_{11}(E_1) / \varepsilon_{11}(E_1 = 0) & \text{for } E_1 \parallel [100] \\
1 - \varepsilon_{22}(E_2) / \varepsilon_{22}(E_2 = 0) & \text{for } E_2 \parallel [010] \\
1 - \varepsilon_{33}(E_3) / \varepsilon_{33}(E_3 = 0) & \text{for } E_3 \parallel [001] 
\end{cases}$$

In the presence of a uniform applied electric field $E_3$ normal to the film substrate interface, the pyroelectric coefficient $p_3$ is given as the sum of the variations of the spontaneous polarization and the dielectric permittivity $\varepsilon_{33}(E_3)$ with the temperature,

$$p_3 = \left. \frac{\partial \tilde{G}}{\partial T} + E_3 \frac{\partial \varepsilon_{33}(E_3)}{\partial T} \right|.$$  

### III. NUMERICAL RESULTS AND DISCUSSION

The effect of in-plane anisotropic strains on the phase diagram, dielectric tunability, and pyroelectric response in epitaxial Ba$_{0.7}$Sr$_{0.3}$TiO$_3$ thin films is discussed in this section. The parameters for the calculation of the renormalized coefficients for Ba$_{0.7}$Sr$_{0.3}$TiO$_3$ thin films are obtained by averaging the corresponding parameters of BaTiO$_3$ and SrTiO$_3$ materials shown in Table I.$^{23}$ Both $\alpha_1$ and $\alpha_1$ are temperature dependent in Ba$_{0.7}$Sr$_{0.3}$TiO$_3$ films since both are scaled with temperature in BaTiO$_3$, and the other parameters are assumed to be temperature independent.

In order to describe the transformations of equilibrium thermodynamic states that may occur in epitaxial Ba$_{0.7}$Sr$_{0.3}$TiO$_3$ films in the presence of in-plane anisotropic strains, it is useful to develop a misfit strain-temperature phase diagram. Figure 1 illustrates the anisotropic strain factor-temperature phase diagram for Ba$_{0.7}$Sr$_{0.3}$TiO$_3$ films under the short-circuited condition, at a given in-plane misfit strain $\mu_m = 0.002$. The equilibrium thermodynamic states of the film are determined by calculating all minima of the potential $\tilde{G}$ with respect to polarization components and then selecting the most energetically favorable phase. The presence of anisotropic strains may strongly affect the thermodynamic stability of various phases involved. The formation of six distinct phases due to the change in the symmetry as a result of the in-plane anisotropic misfit strains is predicted theoretically. These six phases are the paraelectric phase ($P_1 = P_2 = P_3 = 0$), the $c$ phase ($P_1 = P_2 = 0, P_3 \neq 0$), the $a_1$ phase ($P_1 \neq 0, P_2 = P_3 = 0$), the $a_2$ phase ($P_2 \neq 0, P_1 = P_3 = 0$), the $c a_1$ phase ($P_1 \neq 0, P_2 = 0, P_3 \neq 0$), and the $a_1 a_2$ phase ($P_1 \neq 0, P_3 \neq 0, P_3 = 0$). Because of the in-plane anisotropic strains, the paraelectric-to-ferroelectric transition temperature has a plateau above the $a_1$ phase, which is similar to the case of BaTiO$_3$ thin films with the in-plane anisotropic strains. It is interesting to see that the significant feature in-

---

**Table I.** The parameters for the calculation of the renormalized coefficients for Ba$_{0.7}$Sr$_{0.3}$TiO$_3$ films.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Ba$<em>{0.7}$Sr$</em>{0.3}$TiO$_3$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Curie temperature $T_c$ (°C)</td>
<td>34</td>
</tr>
<tr>
<td>Curie constant $C$ (10$^6$ °C)</td>
<td>1.29</td>
</tr>
<tr>
<td>$\alpha_{11}$ (10$^9$ m$^3$/C$^2$)</td>
<td>2.527+189 (Tm°C)</td>
</tr>
<tr>
<td>$\alpha_{12}$ (10$^9$ m$^3$/C$^2$)</td>
<td>7.21</td>
</tr>
<tr>
<td>$s_{11}$ (10$^{-12}$ m$^2$/N)</td>
<td>5.92</td>
</tr>
<tr>
<td>$s_{12}$ (10$^{-12}$ m$^2$/N)</td>
<td>−1.92</td>
</tr>
<tr>
<td>$s_{44}$ (10$^{-12}$ m$^2$/N)</td>
<td>6.7</td>
</tr>
<tr>
<td>$Q_{11}$ (m$^3$/C$^2$)</td>
<td>0.1</td>
</tr>
<tr>
<td>$Q_{12}$ (m$^3$/C$^2$)</td>
<td>−0.034</td>
</tr>
<tr>
<td>$Q_{44}$ (m$^3$/C$^2$)</td>
<td>0.029</td>
</tr>
</tbody>
</table>
duced by the anisotropic strains is the formation of the tetragonal ferroelectric phases, $a_1$ and $a_2$, which do not exist in the BST films of the same composition in the presence of isotropic strains. Under a fixed tensile strain $u_{m1}$, the $a_2$ phase is stable when the tensile strain $u_{m2}$ is large enough, and the $a_1$ phase is stable when $u_{m2}$ is either a small tensile or a small compressive strain. This indicates that the anisotropic strains may alter the type of the stable ferroelectric phase. Compared with the phase diagram of BaTiO$_3$ thin films under the anisotropic misfit strains, Fig. 1 reveals that the $c$ phase occurs when the one in-plane strain is tensile and the other is compressive in epitaxial Ba$_{0.7}$Sr$_{0.3}$TiO$_3$ films. On the other hand, the used fourth-order Landau-Devonshire polynomial cannot describe the thermodynamic properties of bulk BST at a lower temperature with the given parameters since $\gamma_2$ becomes negative at a lower temperature. Consequently, the corresponding Fig. 1 cannot be extended to a temperature below $-190 \, ^\circ$C.

Since the anisotropic strain-induced phase transitions may be accompanied by dielectric and pyroelectric anomalies, we discuss the impact of anisotropic strain factor on the dielectric and pyroelectric responses of Ba$_{0.7}$Sr$_{0.3}$TiO$_3$ films. A thorough examination of Fig. 1 reveals that only the $ca_1$, $a_1$, and $a_1a_2$ phases are the stable phases at room temperature ($25 \, ^\circ$C). The room temperature dielectric tunability of Ba$_{0.7}$Sr$_{0.3}$TiO$_3$ films along [100], [010], and [001] with applied fields along the same directions is calculated by using the definition of the dielectric tunability [Eq. (9)] and the dielectric response as a function of the applied field [Eqs. (6)-(8)]. The maximum applied field is taken as 100 kV/cm for $E||[100]$, [010], and [001], respectively. Figure 2 demonstrates the dielectric tunability as a function of anisotropic strain factor at $T=25 \, ^\circ$C and $u_{m1}=0.002$, (a) and (b) corresponding to the $ca_1$ phase and the $a_1a_2$ phase, respectively. It can be clearly seen that the dielectric tunability strongly depends on the anisotropic strain factor. For the $ca_1$ phase, as shown in Fig. 2(a), the dielectric tunability along [100] linearly decreases, but the dielectric tunability along [001] non-linearly increases, with decreasing the magnitude of the anisotropic strain factor. In addition, the theoretical maximum dielectric tunability approaching 100% can be attained at the critical anisotropic strain factor corresponding to the structural phase transformation from the $ca_1$ phase to the $a_1$ phase. Figure 2(b) displays the effect of anisotropic strain factor on the in-plane dielectric tunability. The dielectric tunability along [100] linearly increases, but the one along [010] non-linearly decreases with the increase of the anisotropic strain factor. In the vicinity of the phase transformations from the $a_1$ phase to the $a_1a_2$ phase, the dielectric tunability along [100] has the minimum dielectric tunability, but the corresponding value along [010] has the maximum one close.
to 80%. This indicates that the dielectric tunability can be optimized by modulating the in-plane anisotropic strains and varying the ferroelectric states.

The $a_1, a_2$ phase and the $a_1$ phase at room temperature are not suitable for applications in infrared sensors due to their in-plane polarizations. We only focus on the impact of anisotropic strain factors on the pyroelectric response along [001] in the $ca_1$ phase state, which is a more favorable state for the application in the pyroelectric sensors. Theoretical investigation has shown that the external field has little influence on the pyroelectric coefficient because of the overwhelming contribution of spontaneous polarization to the overall pyroelectric coefficient, so we do not take the external field into consideration. In the $ca_1$ phase, the out-of-plane pyroelectric coefficient as a function of temperature for a fixed $u_{m1} = 0.002$ and different anisotropic factors ($\beta=-1.0, -1.5, -2.0$) is shown in Fig. 3. For a given anisotropic strain factor, the pyroelectric coefficient increases with temperature, and then a pyroelectric coefficient peak appears in the vicinity of the phase transformation from the $ca_1$ phase to the $a_1$ phase. In addition, the peak value of the pyroelectric coefficient shifts to a higher temperature on increasing anisotropic factor. For a given temperature, the out-of-plane pyroelectric coefficient can be effectively improved by decreasing the magnitude of the anisotropic strain factor. Therefore, we can optimize the pyroelectric response by modulating the anisotropic strain factor.

In order to compare the predictions with experimental results, we also calculate the in-plane dielectric permittivity $\varepsilon_{11}$ as a function of external field under the different strains $u_{m1} = 0.001, 0.0016, 0.003$ and a temperature $T = 25^\circ C$, in the case of the in-plane isotropic strains ($\beta = 1.0$), as depicted in Fig. 5. The in-plane isotropic strains can be regarded as a particular case of in-plane anisotropic strain distribution states. For a given temperature, the dielectric permittivity increases on decreasing the tensile strain. Besides, the influence of in-plane isotropic strain on the in-plane dielectric permittivity is more obvious when the external field is small. Interestingly, when the in-plane isotropic strain $u_{m1} = 0.0016$, our theoretical prediction of the in-plane dielectric permittivity for Ba$_{0.7}$Sr$_{0.3}$TiO$_3$ films is in good agreement with the experimental results published in the literature (see Ref. 26), as shown by the solid diamonds in the Fig. 5. Wang et al. prepared the Ba$_{0.7}$Sr$_{0.3}$TiO$_3$ films grown on MgO (001) single-crystal substrate using pulsed-laser deposition and obtained the enhanced in-plane ferroelectricity. According to the experimental data, the calculated maximum in-plane dielectric tunability is 67.8% under a moderate dc bias field of 13.3 V/µm. Our theoretical result is 66.43% under the in-plane strain $u_{m1} = 0.0016$, which is well consistent with the experimental result. It should be noted that the calculated lattice mismatch strain is $\mu_{lattice}=0.04194$, according to the lattice constants of MgO substrate and Ba$_{0.7}$Sr$_{0.3}$TiO$_3$ film, 0.4211 and 0.40344 nm, respectively. On the other hand, as

![FIG. 3. The dependence of the out-of-plane pyroelectric coefficient in the $ca_1$ phase on the temperature for a fixed $u_{m1} = 0.002$ and different anisotropic factors ($\beta=-1.0, -1.5, -2.0$).](image)

![FIG. 4. The figure of merit as a function of temperature for a given $u_{m1} = 0.002$ and different anisotropic strain factors ($\beta=-1.0, -1.5, -2.0$).](image)
the film is cooled from growth temperature $T_G$, the thermal strain can be calculated from the following expression:

$$u_{\text{thermal}} = \int_0^{T_G} (\alpha_{\text{film}} - \alpha_{\text{substrate}}) dt,$$

(11)

where $\alpha_{\text{film}}$ and $\alpha_{\text{substrate}}$ are the thermal expansion coefficients of the Ba0.3Sr0.3TiO3 thin film and the MgO substrate, respectively. According to Eq. (11), for $\alpha_{\text{film}}=10.5 \times 10^{-6} \ ^{\circ}\text{C}^{-1}$ and $\alpha_{\text{substrate}}=13.47 \times 10^{-6} \ ^{\circ}\text{C}^{-1}$, the calculated thermal strain is $u_{\text{thermal}}=-0.00215$. We can get $u_{m1} < (u_{\text{lattice}} + u_{\text{thermal}})$, which means that the actual internal strain level is not only related to the misfit strain and the thermal strain but also dependent on the other factors, such as oxygen defect, film inhomogenity, surface electrode, etc. Besides, the epitaxial strains are relaxed to a certain extent by the formation of misfit dislocations at $T_G$, which is related to the film thickness. The formation of misfit dislocations can play an important role in decreasing the internal strain level of BST thin films in the experiment.

IV. CONCLUSION

In summary, we have developed a modified thermodynamic model based on the Landau-Devonshire-type phenomenological theory to investigate the impact of in-plane anisotropic strains on the dielectric and pyroelectric responses in epitaxial Ba0.3Sr0.3TiO3 thin films. The anisotropic strain factor-temperature phase diagram has been established. The significant feature induced by the anisotropic strains is the formation of the tetragonal ferroelectric phases, $a_1$ and $a_2$, which do not exist in the BST films of the same composition under isotropic strains. In addition, the influence of anisotropic strain factor on the dielectric tunability, the pyroelectric coefficient, and the figure of merit is analyzed. The calculated results demonstrate that the in-plane anisotropic strains play an important role in the dielectric and pyroelectric properties of BST thin films. The theoretical maximum dielectric tunability approaching 100% can be attained at the critical anisotropic strain factor corresponding to the structural phase transformation from the $ca_1$ phase to the $a_1$ phase. The anisotropic strain factor has opposite effect on the figure of merit and the pyroelectric coefficient, respectively. The out-of-plane pyroelectric coefficient can be effectively improved, but the figure of merit decreases, by decreasing the magnitude of the anisotropic strain factor. Moreover, we have also studied the effect of biaxial isotropic strain on the in-plane dielectric permittivity and the dielectric tunability in order to compare with the experimental results. When the biaxial isotropic strain $u_{m1}=0.0016$, our theoretical results are well consistent with the experimental results. On the whole, the theoretical insight into the impact of in-plane anisotropic strains on the dielectric and pyroelectric properties of BST thin films will undoubtedly provide an instructive clue for the experimental researchers on how to enhance the dielectric tunability and pyroelectric response of the BST thin films.

ACKNOWLEDGMENTS

This work was supported by the Research Grant of the Hong Kong Polytechnic University under Grant No. G-U032, the National Natural Science Foundation of China under Grant Nos. 10574129, 10174049, and 10474069, and the National Science Foundation of JiangSu Education Committee of China under the Grant No. 04KJB140118.