Piezoelectric properties of domain engineered barium titanate single crystals with different volume fractions of domain walls

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A piezoelectric domain wall model has been developed to analyze the effective piezoelectric properties of domain engineered BaTiO₃ (BT) single crystals with different volume fractions of 90° domain walls. The model takes into account the nonuniform deformation in the domain wall region, which can create additional anisotropy to enhanced functional properties of multidomain single crystals. Our theoretical results indicate that a larger volume fraction of domain walls will produce larger effective piezoelectric coefficients. In addition, with the increase in domain wall volume fraction, [011]_c poled BT single crystals will have a much larger piezoelectric property enhancement than [111]_c poled BT single crystals. © 2009 American Institute of Physics.

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I. INTRODUCTION

Domain engineering is a newly developed technique, which could produce much superior piezoelectric properties in ferroelectric crystals, such as relaxor based (1-x)Pb(Mg_{1/3}Nb_{2/3})O₃-xPbTiO₃ (PMN-xPT) and (1-x)Pb(Zn_{1/3}Nb_{2/3})O₃-xPbTiO₃ (PZN-xPT) single crystals.¹⁻⁵ Very high piezoelectric constant ($d_{33} \sim 2500$ pC/N) and electromechanical coupling factor ($k_{33} \sim 94\%$) have been exhibited in [001]_c poled rhombohedral PZN-0.08PT single crystals.⁴ However, similar to Pb(Zr,Ti)O₃ ceramics, these piezoelectric materials contain lead, an environmentally unfriendly element.

In recent years, scientists have begun to apply a domain engineering principle to lead-free systems, hoping to improve their piezoelectric response.⁶⁻⁹ Several experimental works indicated that piezoelectric properties of tetragonal phase BaTiO₃ (BT) could be greatly enhanced if the crystal is poled along [111]_c of the cubic reference coordinates.^{6,7} An interesting phenomenon was observed in domain engineered BT crystals: The piezoelectric properties increase with the reduction in domain size. A two dimensional time dependent Ginzburg-Landau model has been used to simulate the piezoelectric response of domain engineered BT single crystals, and the theoretical model confirmed the enhancement phenomena due to domain size reduction.⁸ In engineered domain configurations of a BT single crystal, the effective macroscopic symmetry can be $mm2$ or $3m$ depending on whether the poling direction is along [011]_c or [111]_c.⁹ For this two types of structures, the effective properties of BT single crystals were estimated using the homogenization theory, but the effects of 90° domain walls were not considered so that the theoretical and the experimental results do not match very well.⁹

Usually, a 90° domain wall is much thicker than a 180° domain wall.¹⁰ Experimental observations also conformed

that a 180° domain wall has a negligible thickness while a 90° domain wall with noticeable energy has elastic strain and a finite width.¹¹⁻¹⁴ In a recent theoretical work, domain walls in the PMN-PT crystal have been treated as thin layer conductors,¹⁵ which means that the contribution from domain walls to the macroscopic piezoelectric properties was ignored. Moreover, the dielectric constants of the domain walls were assumed to be infinity in the conducting domain wall model, which is unphysical for an insulating crystal.

In this work, the 90° domain walls are defined as a piezoelectric medium with different material properties from those of adjacent domains. The dependence of effective piezoelectric properties on the domain wall volume fraction of multidomain BT single crystals has been systematically studied. The model provides a way to account for the contribution of 90° domain walls to the macroscopic properties of the multidomain system and may be used to guide the domain engineering technique for designing optimal domain configurations.

II. THEORETICAL MODEL

As shown in Fig. 1, the normal direction of the domain wall is always chosen as the y-axis in our calculations for the twin structure. For a ferroelectric system, the material properties satisfy the constitutive relations

$$S_{ij}^{(n)} = s_{ijkl}^{(n)} T_{kl}^{(n)} + d_{kij}^{(n)} E_k^{(n)}, \quad (1)$$

FIG. 1. A twin domain system with a domain wall in between.

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$$D_i^{(n)} = d_{ikl}^{(n)} T_{kl}^{(n)} + \varepsilon_{ik}^{(n)} E_k^{(n)} \quad (i, j, k, l = 1, 2, 3), \quad (2)$$

where S and T are the strain and stress; D and E are the electric displacement and electric field; s , d , and ε are short-circuit elastic compliance constant, piezoelectric coefficient, and stress-free dielectric constant, respectively; the superscript ($n=1, 2$ and w_{12}) is used to denote domain 1, domain 2, and the domain wall between domains 1 and 2, respectively.

We assume nonslippery interfaces, and the corresponding continuity conditions for the mechanical and electrical properties are the three stress components $T_{22}^{(n)}$, $T_{23}^{(n)}$, and $T_{21}^{(n)}$, and the six strain components $S_{11}^{(n)}$, $S_{33}^{(n)}$, $S_{32}^{(n)}$, $S_{13}^{(n)}$, $S_{31}^{(n)}$, and $S_{12}^{(n)}$

are equal across the interfaces; the electric field components $E_1^{(n)}$, $E_2^{(n)}$, and $E_3^{(n)}$ are also continuous across the interface; due to the choice of the coordinates, the polarization component along the x -axis is zero, i.e., $P_1=0$, so that the electric displacement component D_1 is continuous across the interface, but D_2 and D_3 are not continuous.

Using the general constitutive equations (1) and (2), these boundary conditions can be expressed by the following matrix equation:^{15–17}

$$b^{(1)} \Gamma^{(1)} = b^{(2)} \Gamma^{(2)} = b^{(w_{12})} \Gamma^{(w_{12})}, \quad (3)$$

where

$$b^{(n)} = \begin{bmatrix} s_{11}^E & s_{12}^E & s_{13}^E & s_{14}^E & s_{14}^E & s_{15}^E & s_{16}^E & s_{16}^E & \frac{1}{2}d_{11} & \frac{1}{2}d_{11} & d_{21} & d_{31} \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ s_{13}^E & s_{23}^E & s_{33}^E & s_{34}^E & s_{34}^E & s_{35}^E & s_{36}^E & s_{36}^E & \frac{1}{2}d_{13} & \frac{1}{2}d_{13} & d_{23} & d_{33} \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ s_{14}^E & s_{24}^E & s_{34}^E & s_{44}^E & s_{44}^E & s_{45}^E & s_{46}^E & s_{46}^E & \frac{1}{2}d_{14} & \frac{1}{2}d_{14} & d_{24} & d_{34} \\ s_{15}^E & s_{25}^E & s_{35}^E & s_{45}^E & s_{45}^E & s_{55}^E & s_{56}^E & s_{56}^E & \frac{1}{2}d_{15} & \frac{1}{2}d_{15} & d_{25} & d_{35} \\ s_{16}^E & s_{26}^E & s_{36}^E & s_{46}^E & s_{46}^E & s_{56}^E & s_{66}^E & s_{66}^E & \frac{1}{2}d_{16} & \frac{1}{2}d_{16} & d_{26} & d_{36} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ \frac{1}{2}d_{11} & \frac{1}{2}d_{12} & \frac{1}{2}d_{13} & \frac{1}{2}d_{14} & \frac{1}{2}d_{14} & \frac{1}{2}d_{15} & \frac{1}{2}d_{16} & \frac{1}{2}d_{16} & \frac{1}{2}\varepsilon_{11}^T & \frac{1}{2}\varepsilon_{11}^T & \frac{1}{2}\varepsilon_{12}^T & \frac{1}{2}\varepsilon_{13}^T \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix} \quad (4)$$

and

$$[\Gamma^{(n)}]^t = [T_{11}, T_{22}, T_{33}, \frac{1}{2}T_{23}, \frac{1}{2}T_{32}, \frac{1}{2}(T_{13} + \frac{1}{2}T_{31}), \frac{1}{2}T_{12}, \frac{1}{2}T_{21}, E_1, E_1, E_2, E_3], \quad (5)$$

where the superscript t is used to denote a matrix transpose.

A matrix $M^{(n)}$, which is a function of $s_{ijkl}^{(n)}$, $d_{kij}^{(n)}$, and $\varepsilon_{ik}^{(n)}$, is defined below so that the matrix $[M^{(n)}\Gamma^{(n)}]$ has exactly the same form as Eq. (5), except that T and E have been replaced by S and D , respectively,

$$M^{(n)} = \begin{bmatrix} s_{11}^E & s_{12}^E & s_{13}^E & s_{14}^E & s_{14}^E & s_{15}^E & s_{16}^E & s_{16}^E & \frac{1}{2}d_{11} & \frac{1}{2}d_{11} & d_{21} & d_{31} \\ s_{12}^E & s_{22}^E & s_{23}^E & s_{24}^E & s_{24}^E & s_{25}^E & s_{26}^E & s_{26}^E & \frac{1}{2}d_{12} & \frac{1}{2}d_{12} & d_{22} & d_{32} \\ s_{13}^E & s_{23}^E & s_{33}^E & s_{34}^E & s_{34}^E & s_{35}^E & s_{36}^E & s_{36}^E & \frac{1}{2}d_{13} & \frac{1}{2}d_{13} & d_{23} & d_{33} \\ s_{14}^E & s_{24}^E & s_{34}^E & s_{44}^E & s_{44}^E & s_{45}^E & s_{46}^E & s_{46}^E & \frac{1}{2}d_{14} & \frac{1}{2}d_{14} & d_{24} & d_{34} \\ s_{14}^E & s_{24}^E & s_{34}^E & s_{44}^E & s_{44}^E & s_{45}^E & s_{46}^E & s_{46}^E & \frac{1}{2}d_{14} & \frac{1}{2}d_{14} & d_{24} & d_{34} \\ s_{15}^E & s_{25}^E & s_{35}^E & s_{45}^E & s_{45}^E & s_{55}^E & s_{56}^E & s_{56}^E & \frac{1}{2}d_{15} & \frac{1}{2}d_{15} & d_{25} & d_{35} \\ s_{16}^E & s_{26}^E & s_{36}^E & s_{46}^E & s_{46}^E & s_{56}^E & s_{66}^E & s_{66}^E & \frac{1}{2}d_{16} & \frac{1}{2}d_{16} & d_{26} & d_{36} \\ s_{16}^E & s_{26}^E & s_{36}^E & s_{46}^E & s_{46}^E & s_{56}^E & s_{66}^E & s_{66}^E & \frac{1}{2}d_{16} & \frac{1}{2}d_{16} & d_{26} & d_{36} \\ \frac{1}{2}d_{11} & \frac{1}{2}d_{12} & \frac{1}{2}d_{13} & \frac{1}{2}d_{14} & \frac{1}{2}d_{14} & \frac{1}{2}d_{15} & \frac{1}{2}d_{16} & \frac{1}{2}d_{16} & \frac{1}{2}\varepsilon_{11}^T & \frac{1}{2}\varepsilon_{11}^T & \frac{1}{2}\varepsilon_{12}^T & \frac{1}{2}\varepsilon_{13}^T \\ \frac{1}{2}d_{11} & \frac{1}{2}d_{12} & \frac{1}{2}d_{13} & \frac{1}{2}d_{14} & \frac{1}{2}d_{14} & \frac{1}{2}d_{15} & \frac{1}{2}d_{16} & \frac{1}{2}d_{16} & \frac{1}{2}\varepsilon_{11}^T & \frac{1}{2}\varepsilon_{11}^T & \frac{1}{2}\varepsilon_{12}^T & \frac{1}{2}\varepsilon_{13}^T \\ d_{21} & d_{22} & d_{23} & d_{24} & d_{24} & d_{25} & d_{26} & d_{26} & \frac{1}{2}\varepsilon_{12}^T & \frac{1}{2}\varepsilon_{12}^T & \varepsilon_{22}^T & \varepsilon_{23}^T \\ d_{31} & d_{32} & d_{33} & d_{34} & d_{34} & d_{35} & d_{36} & d_{36} & \frac{1}{2}\varepsilon_{13}^T & \frac{1}{2}\varepsilon_{13}^T & \varepsilon_{23}^T & \varepsilon_{33}^T \end{bmatrix}. \quad (6)$$

TABLE I. Elastic compliance constants s_{ij}^E (10^{-12} m²/N), piezoelectric constants d_{ij} (10^{-12} C/N), and dielectric constants ϵ_{ij}^T (ϵ_0) of the BT crystal in the single-domain state (Ref. 9).

Elastic constants: s_{ij}^E (10^{-12} m ² /N)					
s_{11}^E	s_{12}^E	s_{13}^E	s_{33}^E	s_{44}^E	s_{66}^E
7.38	-1.39	-4.41	13.1	16.4	7.46
Piezoelectric constants: d_{ij} (10^{-12} C/N)			Dielectric constants: ϵ_{ij}^T (ϵ_0)		
d_{31}	d_{33}	d_{15}	ϵ_{11}^T	ϵ_{33}^T	
-33.72	93.95	560.7	4366	132	

For the twin structure shown in Fig. 1, we can write out the averages of $\bar{\Gamma}$ and $\bar{M}\bar{\Gamma}$ as a weighted sum of individual contributions,¹⁵⁻¹⁷

$$\bar{\Gamma} = \sum_{n=1,2,w_{12}} v^{(n)} \Gamma^{(n)}, \quad (7)$$

$$\bar{M}\bar{\Gamma} = \sum_{n=1,2,w_{12}} v^{(n)} M^{(n)} \Gamma^{(n)}, \quad (8)$$

where $v^{(1)}$, $v^{(2)}$, and $v^{(w_{12})}$ are volume fractions of the domain 1, domain 2, and the domain wall between domains 1 and 2, respectively, with $v^{(1)} + v^{(2)} + v^{(w_{12})} = 1$.

Finally, by combining Eqs. (3), (7), and (8), we can represent the matrix form of the effective properties of the twin structure in terms of the properties of the two domains and the domain wall,

$$\bar{M} = \left[\sum_{n=1,2,w_{12}} v^{(n)} M^{(n)} [b^{(n)}]^{-1} \right] \cdot \left[\sum_{n=1,2,w_{12}} v^{(n)} [b^{(n)}]^{-1} \right]^{-1}. \quad (9)$$

III. RESULTS AND DISCUSSION

A. Domain engineered BT single crystal

The crystallographic symmetry of BT single crystals is tetragonal $P4mm$ at room temperature. For a BT crystal poled along $[011]_c$, the two variants $[010]_c$ and $[001]_c$ have equal volume fractions, i.e., $v^{(1)} = v^{(2)}$, so that the macroscopic symmetry becomes $mm2$.⁹ The properties of the two domains can be described by the single-domain data, as listed in Table I. The dependence of the effective piezoelectric properties on the volume fraction of 90° domain walls can be described by Eq. (9). For $[011]_c$ poled crystals, the global coordinates are defined with respect to the cubic coordinates in the following fashion: $x \leftrightarrow [100]_c$, $y \leftrightarrow [01\bar{1}]_c$, and $z \leftrightarrow [011]_c$.

When a BT single crystal is poled along $[111]_c$, the three variants $[100]_c$, $[010]_c$, and $[001]_c$ coexist and have the same volume fraction, i.e., $v^{(1)} = v^{(2)} = v^{(3)}$, leading to a macroscopic $3m$ symmetry. If we assume $v^{(w_{12})} = v^{(w_{13})} = v^{(w_{23})}$, then Eq. (9) can be used to describe the effective properties of any two of these three variants with a domain wall in between. Hence, by repeatedly applying Eq. (9), the dependence of the effective piezoelectric properties on the domain wall volume fraction can be obtained for a $[111]_c$ poled BT single crystal.

It should be mentioned that when calculating the properties of each pair, a local coordinate system is assumed with the y-axis always perpendicular to the domain wall. After each calculation, the effective properties of each pair will be rotated to the global coordinates: $x \leftrightarrow [1\bar{1}0]_c$, $y \leftrightarrow [11\bar{2}]_c$, $z \leftrightarrow [111]_c$.

B. 90° domain wall properties

We use different weighting factors for different properties of 90° domain walls in order to match the experimental results. These weighting factors can be obtained by fitting the theoretical values to the corresponding experimental values. The fitting procedure is as follows: First, we use the average properties of the two domains in the twin structure as initial approximations of the domain wall properties; then, the weighting factors a_{ij} , b_{ij} , and c_{ij} for elastic compliance, piezoelectric, and dielectric coefficients of a 90° domain wall are adjusted so that the resulting theoretical elastic compliance, piezoelectric, and dielectric constants will have the best fit to the corresponding experimental values. For example, the elastic compliance constants of the domain wall are expressed as

$$s_{ij}^w = a_{ij} \bar{s}_{ij} \quad (i, j = 1, 2, 3, 4, 5, 6), \quad (10)$$

where s_{ij}^w refers to the elastic compliance constants of the domain wall and $\bar{s}_{ij}$ refers to the initial averaging value of the elastic compliance constants of the two adjacent domains. In the same way, the piezoelectric and dielectric properties of the 90° domain wall can be described.

Since one should not choose these factors arbitrarily, the following rules are defined when determining these weighting factors: (a) the number of different values of a_{ij} , b_{ij} , and c_{ij} should be as less as possible; (b) the macroscopic symmetry of the multidomain BT single crystal should not be changed by the choice of these factors; (c) calculated effective material constants should be in reasonable agreement with the corresponding experimental values. Following these rules, we have determined a set of factors:

$$a_{ij} = \begin{cases} 0.8, & i = 1, j = 2, 3 \text{ or } i = 2, j = 1, 3 \text{ or } i = 3, j = 1, 2 \\ 1.2, & i = j = 4 \\ 1, & \text{else,} \end{cases} \quad (11)$$

TABLE II. Dependence of effective piezoelectric properties on the volume fraction of 90° domain walls for a domain engineered BT single crystal with a $mm2$ macroscopic symmetry. Piezoelectric constants d_{ij} are in the units of (10^{-12} C/N), and $v^{(w12)}$ is the domain wall volume fraction.

Model $v^{(w12)}$ (%)	Conducting domain wall			Piezoelectric domain wall		
	d_{31}	d_{32}	d_{33}	d_{31}	d_{32}	d_{33}
8	-13.86	-170.43	194.32	-17.68	-200.03	221.48
4	-14.21	-178.08	202.53	-16.12	-192.91	216.09
1	-14.46	-183.83	208.67	-14.93	-187.54	212.06

$$b_{ij} = \begin{cases} 2, & i = 1, j = 5 \text{ or } i = 2, j = 4 \text{ or } i = 3, j = 1, 2 \\ 1.6, & \text{else,} \end{cases} \quad (12)$$

$$c_{ij} = \begin{cases} 2, & i = j = 2 \text{ or } i = j = 3 \\ 0.9, & \text{else.} \end{cases} \quad (13)$$

C. Effective macroscopic piezoelectric properties

The effective piezoelectric properties of BT single crystals with different volume fractions of domain walls are listed in Tables II and III for the case of the $mm2$ symmetry and for the case of the $3m$ symmetry, respectively. The theoretical results based on the conducting domain wall model of Ref. 15 are also listed for comparison. It can be noticed from Tables II and III that the piezoelectric coefficients calculated based on the piezoelectric domain wall model increase with the increase in the 90° domain wall volume fraction. Since the domain wall thickness does not depend on the domain size, a larger domain wall volume fraction means a smaller domain size. Our model, therefore, can predict the domain size dependence of the effective properties of multi-domain structures. The trend predicted by our model is consistent with the experimental results of Wada and Tsurumi.⁶ and Wada *et al.*⁷ However, the calculated results using the conducting domain wall model show the opposite trend. So, the contribution from the 90° domain wall to macroscopic piezoelectric properties must be taken into consideration.

In addition, the calculated values based on the piezoelectric domain wall model have a much better agreement with the experimental values than the calculations in Ref. 9, which ignored the 90° domain wall contribution. It further demonstrates that 90° domain wall contributions should not be ignored, especially when the domains become very small.

Interestingly, our piezoelectric domain wall model predicts a much larger property enhancement in $[011]_c$ poled samples (Table II) than in $[111]_c$ poled samples (Table III) when the domain size is getting smaller. This enhancement may be used in practical applications.

There are still some inconsistencies between our theoretical results and experimental observations, which may not be totally due to the imperfection of the theoretical model. As pointed out by Wada and Tsurumi⁶ and Wada *et al.*,⁷ a multiphase may coexist in the BT single crystals used in the experiments, which often generates higher piezoelectric coefficients. The model treats the twin structure as three uniform regions, which also introduce some errors. In reality, the domain wall is an inhomogeneous transition region between the twin domains. As the domain size becomes smaller, the polarization vectors within the domains also become tilted and continue to vary instead of a constant value within the domain wall.^{8,18}

IV. SUMMARY AND CONCLUSIONS

Based on the quasistatic assumption, a piezoelectric domain wall model was presented to describe the dependence of the effective properties of the domain engineered BT single crystals on the domain wall volume fraction. In a twin structure with a 90° domain wall in between, the domain wall is treated as a separate region with material properties different from those of the adjacent domains. Our theoretical results show the same trend as what had been observed experimentally; i.e., a higher domain wall volume fraction produces a stronger piezoelectric effect. Our model also predicts that $[011]_c$ poled BT single crystals should exhibit a much larger piezoelectric property enhancement with an increase of 90° domain wall volume fraction than $[111]_c$ poled BT single crystals.

TABLE III. Dependence of effective piezoelectric properties on the volume fraction of 90° domain walls for a domain engineered BT single crystal with a $3m$ macroscopic symmetry. Piezoelectric constants d_{ij} are in the units of (10^{-12} C/N), and $v^{(w)}$ is the total volume fraction of domain walls.

Experiment value (Ref. 6)			Conducting domain wall			Piezoelectric domain wall		
Domain size (μm)	d_{31}	d_{33}	$v^{(w)}$ (%)	d_{31}	d_{33}	$v^{(w)}$ (%)	d_{31}	d_{33}
6.5	-180.1	...	8	-80.92	170.05	8	-101.18	205.46
13.3	-134.7	...	4	-82.89	174.14	4	-93.59	192.96
>40	-97.8	...	2	-83.87	176.19	2	-89.40	185.94

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