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Group theoretical analysis of the domain structure of SrBi₂Ta₂O₉ ferroelectric ceramic

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Abstract. The domain structure of the bismuth layered ferroelectric SrBi₂Ta₂O₉ (SBT) has been studied by group theoretical methods. It is shown that there should exist five types of domain pair independent of one another in SBT, namely: (1) translational domain pairs; (2) 180° (rotational) domain pairs; (3) translational–180° domain pairs; (4) 90° domain pairs; (5) translational–90° domain pairs. In addition, some experimental results are briefly discussed.

1. Introduction

Strontium bismuth tantalate (SBT), one of the Bi-layered ferroelectric compounds, has attracted much attention as the most promising candidate for non-volatile random-access-memory applications because of its high fatigue endurance and the possibility of it having a low polarization-switching voltage [1, 2], as well as its other useful properties [3–5]. The former two advantages have stimulated great interest in understanding the origins of the non-fatigue nature and switching mechanism in SBT, which are still not very clear as regards the microscopic structure aspect [6]. However, although the domain wall plays an important role in the processes of fatigue and switching in SBT, studies on the domain structure of SBT have been far less comprehensive. Some transmission electron microscopy (TEM) studies on both SBT single crystal [7] and thin films [8–15] have been performed, but little investigation of domain walls has been involved.

In this paper, space group analysis will be used to improve our understanding of the domain structure.

2. Space group decomposition

Coherent domain structure can be theoretically investigated in the case where it arises at a transition from a phase with space group G to a 'less symmetrical' phase with space group H , i.e., when H is a subgroup of G [16, 17]. G can be decomposed into left cosets with respect to H . It can be written as

$$G = H + p_2H + p_3H + \cdots + p_nH \quad (1)$$

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where n is the index of H in G , and p_i ($i = 2, 3, \dots, n$) are the symmetry operators of G which are lost during the course of the transition. However, the corresponding symmetry relationship between the domain states is bound to reappear after the transition. So the domain states are virtually determined by the series of operators p_i .

For SBT specifically, G is the space group for the paraelectric phase at high temperature, and H is that for the ferroelectric phase at room temperature. To carry out the analysis, both G and H must be known.

Rae described SBT at room temperature in the space group $A2_1am$ as a commensurate modulation of an idealized $Fmmm$ parent structure derived from an $I4/mmm$ structure [7]. So the space group of the prototype structure and the ferroelectric structure are $G = I4/mmm$ and $H = A2_1am$, respectively. For comparison between G and H , a common unit cell must be chosen for the two groups; this is always a common multiple of the Bravais cell of G and that of H [16]. For this reason, $F4/mmm$ has been chosen as the space group of G instead of $I4/mmm$.

Now we set out to decompose G into left cosets by means of the maximal non-isomorphic subgroup chain

$$F4/mmm \rightarrow Fmmm \rightarrow F2mm \rightarrow A2_1am$$

which is an imaginary process, but is beneficial in helping us to complete the decomposition. From $F4/mmm$ to $A2_1am$, as shown in table 1, step by step, the symmetry elements of $F4/mmm$ are removed in the following order: one fourfold axis, one twofold axis, and the $1/2$ translation along the diagonal line.

Table 1. The chain of maximal non-isomorphic subgroups for SBT.

Short symbol	Full symbol	Schoenflies symbol	No of space group
$F4/mmm$	$F \frac{4}{m} \frac{2}{m} \frac{2}{m}$	D_{4h}^{17} ↓ lost: $\{4^+ 0, 0, z\}$	No 139
$Fmmm$	$F \frac{2}{m} \frac{2}{m} \frac{2}{m}$	D_{2h}^{23} ↓ lost: $\{2^+ 0, 0, z\}$	No 69
$F2mm$	$F2mm$	C_{2v}^{18} ↓ lost: $\{t(1/2, 1/2, 0)\}$	No 42
$A2_1am$	$A2_1am$	C_{2v}^{12}	No 36

The decomposition can be formally expressed in the following way:

$$\begin{aligned}
 F4/mmm &= [\{1\} + \{4^+ 0, 0, z\}] && \underline{Fmmm} \\
 & && \downarrow \\
 &= [\{1\} + \{2^+ 0, 0, z\}] && \underline{F2mm} \\
 & && \downarrow \\
 &= [\{1\} + \{t(1/2, 1/2, 0)\}] && A2_1am(2).
 \end{aligned} \tag{2}$$

Hence

$$F4/mmm = [\{1\} + \{4^+ 0, 0, z\}][\{1\} + \{2^+ 0, 0, z\}][\{1\} + \{t(1/2, 1/2, 0)\}]A2_1am. \tag{3}$$

This can be further shortened, as follows:

$$G = \sum_{i=1}^8 p_i H \tag{4}$$

where

$$\begin{aligned}
 p_1 &= \{1\} & p_2 &= \{t(1/2, 1/2, 0)\} \\
 p_3 &= \{2\ 0, 0, z\} & p_4 &= \{2\ 0, 0, z\}\{t(1/2, 1/2, 0)\} \\
 p_5 &= \{4^+ 0, 0, z\} & p_6 &= \{4^+ 0, 0, z\}\{t(1/2, 1/2, 0)\} \\
 p_7 &= \{4^- 0, 0, z\} & p_8 &= \{4^- 0, 0, z\}\{t(1/2, 1/2, 0)\}.
 \end{aligned}$$

3. Discussion of the results

From the symmetry analysis performed, there follow some interesting physical conclusions.

Firstly, if H stands for one domain state, then $p_i H$ represents another domain state. The first domain state can be converted into the second one by p_i , which thus specifies the domain pair. Thus, it is clear that the number of domain states is 8. And obviously the number of domain pairs is at most 7 according to the theorem that *the number of types of domain pair is at most the number of domain state(s) minus one* [18]. Here, the domain pair associated with $p_1 H$ and $p_i H$ can be denoted by I_{1i} .

Furthermore, another theorem should be taken into account. The theorem is stated as follows:

Domain pairs I_{1i} and I_{1k} are crystallographically equivalent if, in the coset $p_i H$, there exists an operator q_i which is the inverse of some operator q_k belonging to the coset $p_k H$ [18].

On the basis of this, we can arrive at the conclusion that I_{15} and I_{17} are crystallographically equivalent owing to the fact that $p_5 = p_7^{-1}$. So are I_{16} and I_{18} .

Finally, the remaining five kinds of domain pair I_{12} , I_{13} , I_{14} , I_{15} , and I_{16} are not crystallographically equivalent and correspond to (1) translational domain pairs, (2) 180° (rotational) domain pairs, (3) 90° domain pairs, (4) translational–180° domain pairs; (5) translational–90° domain pairs, respectively. Each of them in the abstract sense represents a relationship of two domains that form one unique type of domain wall (boundary).

The five types of domain pair are illustrated in figure 1. In each illustration, there are two domain states that have the diagonal as the line of demarcation. The upper one is taken as the original domain state; accordingly, the lower one is the domain state obtained through the operation of p . The arrows, which indicate the inclination of the polarization vectors, are parallel to the $[1, 1, 0]$ direction. The plane of the paper is chosen as that of the a – b plane, for convenience. And to make the shift clear, two different arrow heads, of the same size and shape, are utilized.

4. Experiments

Some experimental work has already been done in our laboratory [19]. TEM observation has provided two types of pattern. Because the patterns of the initial domain state and its variants obtained through the operation of p_2 , p_3 , and p_4 do not differ, we could hardly distinguish between the TEM patterns for translational, 180°, and translational–180° transformations. Likewise, 90° and translational–90° transformations cannot be distinguished from each other by means of the TEM patterns. This seems to explain why we have only observed two types of pattern.

Fortunately, the image of the antiphase boundary, which is related to the translational domain pairs, can be clearly observed as a curve in dark-field electron micrographs because of its unique characteristic of superlattice reflection, which results from the relative translation

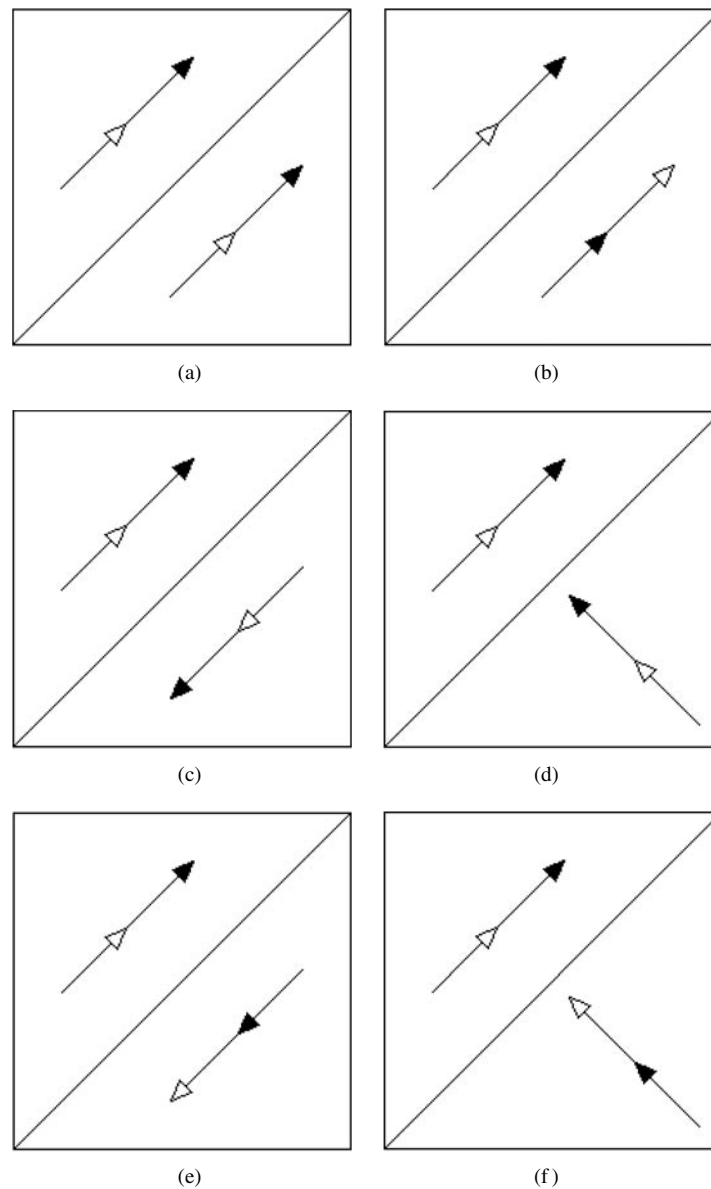


Figure 1. Typical domain configurations of SBT: (a) original; (b) the translational domain pair; (c) the 180° (rotational) domain pair; (d) the 90° domain pair; (e) the translational- 180° domain pair; (f) the translational- 90° domain pair.

of the two domains. And the contrast of a 180° domain wall (related to 180° domain pairs) has been identified thanks to the failure of Friedel's law. Consequently, the translational- 90° domain wall (related to translational- 90° domain pairs) has also been identified. Moreover, without any difficulty, the 90° domain wall (related to 90° domain pairs) was already confirmed earlier.

However, further observations, especially involving the translational- 180° domain wall (related to translational- 180° domain pairs), are still needed.

5. Conclusions

In conclusion, the domain structure of SBT has been investigated by space group analysis. Through the space group analysis, five types of domain pair in SBT have been predicted, namely: (1) translational; (2) 180° (rotational); (3) translational–180°; (4) 90°; (5) translational–90°. Four of them have been confirmed experimentally.

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References

- [1] Paz de Araujo C A *et al* 1995 *Nature* **374** 627
- [2] Noguchi T, Hase T and Miyasaka Y 1996 *Japan. J. Appl. Phys.* **35** 4900
- [3] Robertson J *et al* 1996 *Appl. Phys. Lett.* **69** 1704
- [4] Zhang Z G *et al* 1998 *Appl. Phys. Lett.* **73** 788
- [5] Zhang Z G *et al* 1998 *Appl. Phys. Lett.* **73** 3674
- [6] Dimos D *et al* 1996 *J. Appl. Phys.* **80** 1682
- [7] Rae A D 1992 *Acta Crystallogr. B* **48** 418
- [8] Yang H M, Luo J S and Lin W T 1997 *J. Mater. Res.* **12** 1145
- [9] Scott J F *et al* 1996 *MRS Bull.* **21** (July) 33
- [10] Ami T *et al* 1996 *Mater. Res. Soc. Symp. Proc.* **415** 195
- [11] Gutleben C D *et al* 1996 *Mater. Res. Soc. Symp. Proc.* **415** 201
- [12] Zafar S *et al* 1997 *J. Appl. Phys.* **82** 4469
- [13] Ito Y *et al* 1996 *Japan. J. Appl. Phys.* **35** 4925
- [14] Koiwa I *et al* 1996 *Japan. J. Appl. Phys.* **35** 4946
- [15] Chu P Y *et al* 1996 *J. Mater. Res.* **11** 1065
- [16] Guymont M 1978 *Phys. Rev. B* **18** 5385
- [17] Janovec V *et al* 1989 *Ferroelectrics* **98** 171
- [18] Wang R H and Guo K X 1990 *Symmetry Groups in Crystallography* (Beijing: Scientific Press) ch 10 (in Chinese)
- [19] Ding Y, Liu J S and Wang Y N 2000 *Appl. Phys. Lett.* **76** 103