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Latent Symmetry and Domain Average Engineered Ferroics

D. B. LITVIN,[1] V. K. WADHAWAN,[2] and D. M. HATCH[3]

[1]*Department of Physics, The Pennsylvania State University, Penn State Berks Campus, P.O. Box 7009, Reading PA 19610-6009, U.S.A.*
E-mail: u3c@psu.edu
[2]*Laser Materials Division, Centre for Advanced Technology, Indore 452 013, India*
E-mail: wadhawan@cat.ernet.in
[3]*Department of Physics & Astronomy, Brigham Young University, N-145 ESC Provo, UT 84602, U.S.A.*
E-mail: hatchd@byu.edu

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A domain average engineered sample of a multidomain ferroic consists of a very large number of crystalline domains, representing m domain states. m is less than the theoretically allowed maximum number n of domain states. The symmetry of such an engineered sample is shown to be the symmetry of a composite and consequently the concept of latent symmetry, which has explained unexpected symmetries of composites of geometrically shaped objects, can give rise to unexpected symmetries of domain average engineered ferroics. Two theorems of Vlachavas (Acta Cryst., A40 213–221 (1984)) on the symmetry of composites, by not considering the possibility of latent symmetry, are shown to be invalid.

Keywords: Latent symmetry; composites; domain engineering

INTRODUCTION

Static distributions of domains which lead to practical applications are the *domain average engineered* (DAE) multidomain ferroics [1]. Samples consists of a very large number of domains, representing m domain states where m is less than the theoretically allowed maximum number n of domain states. The response of a DAE sample to external fields is roughly described by tensorial properties averaged over all of the domain states involved. Fousek and Litvin [2] have introduced a classification of subsets of the domain states which arise in a ferroic phase transition from a parent phase of point group symmetry $\mathbf{G}$ to a ferroic phase of symmetry $\mathbf{F} \subset \mathbf{G}$, and have shown how to calculate the effective symmetry of DAE samples. Because of the piezoelectric properties of PZN-PT single crystals poled along one of the {001} directions [3–6], the phase transition from $\mathbf{m\bar{3}m}$ to $\mathbf{3m}$ was considered there, assuming that all m represented domains appear with equal probability among the large number of domains of the sample. A program to determine the point group symmetry of equal probability DAE samples has been developed by Shaparenko, Schlessman, and Litvin [7]. Fuksa and Janovec [8] have considered the general problem for point groups, i.e. without assuming the equal probability of represented domains. Hatch and Stokes have considered the formation of domains without restricting their considerations to point groups and have classified domains arising from structural changes in any space group [9]. They have also developed a program [10] to determine the symmetry of DAE ferroics in the general case (they do not assume equally probable domains) for any group-subgroup phase transition.

In this paper we shall show that the symmetry of a DAE sample of ferroics is the same as that of the symmetry of a composite. As a consequence, the concept of latent symmetry, which has been shown to explain unexpected symmetries in the point group symmetry of composites of geometrically shaped objects [11, 12], could also explain unexpected symmetries found in DAE samples of crystalline ferroics. Finally, two theorems by Vlachavas on the symmetry of composites are shown to be invalid.

COMPOSITES

A composite $S = \{A, g_2 A, \ldots, g_m A\}$ was defined by Litvin and Wadhawan [11] as an unordered set of objects constructed by applying a set $\{g_1, g_2, \ldots, g_m\}$, where $g_1 = 1$, of isometries to an object A of intrinsic symmetry $\mathbf{F}$. The objects are called the *components* of the composite. The symmetry of the composite is the symmetry of the superposition of the m components. The *latent symmetry* of the composite is any symmetry of the composite which is not a product of elements of the group $\mathbf{F}$ and the set of isometries $\{g_1, g_2, \ldots, g_m\}$. Cases of latent symmetry have been shown to be related to symmetries of subunits [12] of the object A and others to partial symmetries of components [11].

For example, in Fig. 1(a) we show a two-dimensional component A of symmetry $\mathbf{F} = \mathbf{m}_x$. In Fig. 1(b) we show the composite $S = \{A, m_y A\}$. The symmetry of the composite is $\mathbf{4_z m_x m_{xy}}$ and contains the latent symmetries $4_z, 4_z^{-1}, m_{xy}$, and $m_{\bar{x}y}$, i.e. symmetries which are not products of $\mathbf{F} = \mathbf{m}_x$ and the isometries $\{g_1, g_2\} = \{1, m_y\}$. In Fig. 2(a) we have a two-dimensional crystal of symmetry $\mathbf{F} = \mathbf{p2_z}$ with the translational subgroup $\mathbf{T} = \langle a\hat{i}, a\hat{j} \rangle$.

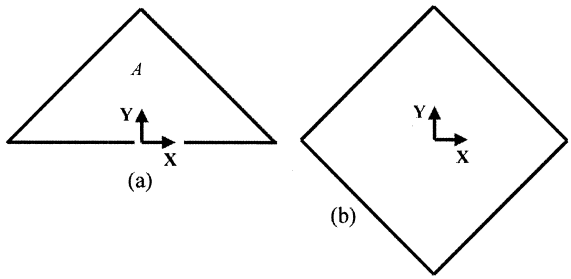

Figure 1. (a) Two dimensional components of A, (b) Composite $S = \{A, m_y A\}$.

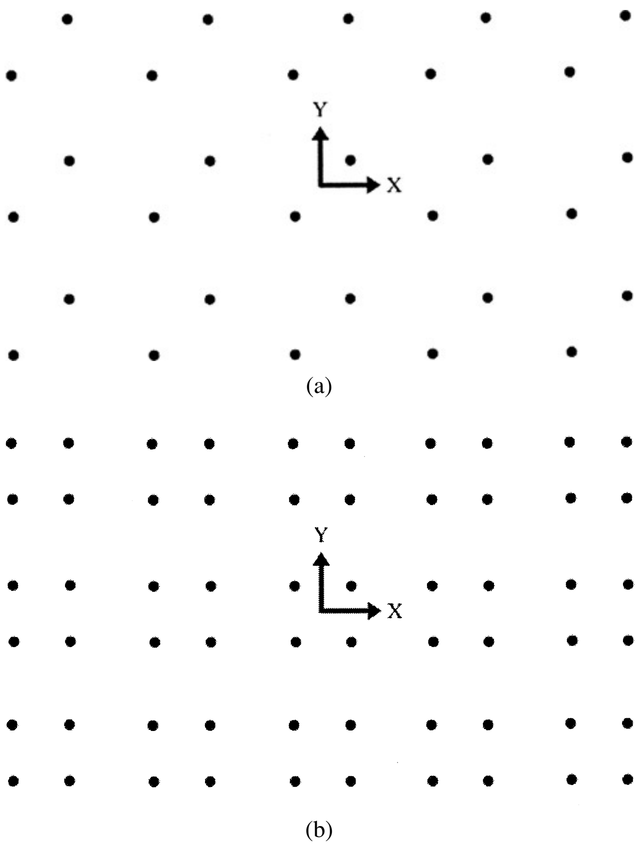

Figure 2. (a) Two dimensional crystal (b) Composite $\{A, g_2 A\}$ where A is the component of two dimensional crystal.

In Fig. 2(b) we have the composite $\{A, g_2 A\}$ where the component A is the two-dimensional crystal of Fig. 2(a) and $g_2 = m_y$. The symmetry of the composite is $\mathbf{p4_z m_x m_{xy}}$ with no change in the translational symmetry. The symmetry of the composite contains latent symmetries 4_z, 4_z^{-1}, m_{xy} , and $m_{\bar{x}y}$, symmetries which are not products of elements of $\mathbf{F} = \mathbf{p2_z}$ and the isometries $\{g_1, g_2\} = \{1, m_y\}$.

DOMAIN AVERAGE ENGINEERED FERROICS

Consider a ferroic phase transition from a parent phase of symmetry $\mathbf{G}$ to a ferroic phase of symmetry $\mathbf{F} \subset \mathbf{G}$. From the coset decomposition $\mathbf{G} = \mathbf{F} + g_2\mathbf{F} + \cdots + g_n\mathbf{F}$, where $g_1 = 1$, the ferroic phase consists of n types of domains $D_i = g_i D_1$, $i = 1, 2, \ldots, n$ where the symmetry of the domain of type D_1 is $\mathbf{F}$.

In a DAE sample, the sample consists of a very large number of domains, representing $m < n$ of the n possible types of domain states. Assuming the equal representation of the m types of domain states, the symmetry of the sample is the symmetry of the superposition of the set of m domain states $\{D_1, D_2, \ldots, D_m\} = \{D_1, g_2 D_1, \ldots, g_m D_1\}$. Consequently, the symmetry of a DAE ferroic sample is the symmetry of the composite $\{D_1, g_2 D_1, \ldots, g_m D_1\}$ made up of the component D_1 and components generated from D_1 by the set of isometries $\{g_1, g_2, \ldots, g_m\}$. [In the more general case where subsets of the m domain states are not equally represented in the engineered sample, the symmetry of the sample is that of the set of composites $\{D_1, ., g_a D_1\}\{g_b D_1, ., g_c D_1\} \ldots \{g_k D_1, ., g_m D_1\}$, each composite containing equally represented domains.] It follows, e.g. Fig. 2(b), that the symmetry of DAE samples may contain latent symmetries, i.e. symmetries which are not products of the elements of the group $\mathbf{F}$ and the set of isometries $\{g_1, g_2, \ldots, g_m\}$.

VLACHAVAS' THEOREMS ON COMPOSITES

Vlachavas [13] has given the following two theorems: (1) *Given a two component composite $\{A, gA\}$ where the component A is of point group symmetry* $\boldsymbol{F}$*, the order of the point group symmetry of the composite is 2/k the order of the group* $\boldsymbol{F}$ *where "k" is a positive integer* and the corollary (2) *The lowest order of the composite point group symmetry is 2 and the highest is two times the order of the group* $\boldsymbol{F}$. The composites in Fig. 1 is a counterexample to this theorem [14], as also is the example in Fig. 2.

In Fig. 1(a), the order of the point group symmetry $\mathbf{F} = \mathbf{m}_y$ of the component A is 2. The theorem predicts the order of the point group symmetry of the composite, shown in Fig. 1(b), to be either $(2/1) \times 2 = 4$ or $(2/2) \times 2 = 2$ while the order of the actual point group symmetry $\mathbf{4}_z\mathbf{m}_x\mathbf{m}_{xy}$ of the composite is 8. For the second example, the point group symmetry of Fig. 2(a) is $\mathbf{F} = \mathbf{2}_z$. The theorem predicts that the point group symmetry of the composite in Fig. 2(b) is of order 2 or 4. The actual point group symmetry of Fig. 2(b) is $\mathbf{4}_z\mathbf{m}_x\mathbf{m}_{xy}$, of order 8. It follows that the tables concerning the listings of all possible symmetries of composites made up of two components are not complete, i.e. Table 3 of reference [13] and Table 1 of the work by Ponds and Vlachavas on bicrystallography [15].

While these two tables are invalid for composites they are valid for bicrystals. This is a consequence of the construction of a bicrystal from a two-component composite, i.e. after the introduction of a boundary into the two-component composite, one component is deleted from one side of the boundary and the second component from the other side. Any symmetry of the bicrystal must either leave each of the components simultaneously individually invariant, or the symmetry must completely exchange the two components. This is not the case for composites where a symmetry may also transform part of a component into the same component and another part of the component into a different component, as the symmetry 4_z in Fig. 1(b).

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