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On Tensor Distinction of Non-Ferroelastic Domains

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We show that for any two non-ferroelastic domains arising in a phase transition, it is always possible to find a coordinate system in which the two domains can be distinguished by the sign of a spontaneous component of a property-tensor. Application of these general results is illustrated by an example which shows possible optical distinction of non-ferroelastic domains.

Keywords Domains; tensor distinction; non-ferroelastic

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1. Introduction

Consider a phase transition between phases of symmetry **G** and **F**. The crystal splits into $n = |\mathbf{G}|/|\mathbf{F}|$ single domain states denoted by $S_1, S_2, \ldots, S_n$ and the symmetry group of each single domain state is denoted, respectively, as $\mathbf{F}_1 = \mathbf{F}, \mathbf{F}_2, \ldots, \mathbf{F}_n$. Writing the coset decomposition of **G** with respect to **F** as $\mathbf{G} = \mathbf{F} + g_2\mathbf{F} + \cdots + g_n\mathbf{F}$ we have for $i = 1, 2, \ldots, n$, $S_i = g_i S_1$ and $\mathbf{F}_i = g_i \mathbf{F} g_i^{-1}$. A domain pair (S_i, S_k) is called a non-ferroelastic domain pair if the two single domain states have the identical spontaneous strain. Strain is a physical property tensor of the type $[V^2]$. The form of this type of tensor for each of the 32 point groups depends only on the crystal family of the point group:

$$\underset{(a)}{\begin{pmatrix} A & D & E \\ D & B & F \\ E & F & C \end{pmatrix}} \quad \underset{(b)}{\begin{pmatrix} A & D & \\ D & B & \\ & & C \end{pmatrix}} \quad \underset{(c)}{\begin{pmatrix} A & & \\ & B & \\ & & C \end{pmatrix}} \quad \underset{(d)}{\begin{pmatrix} A & & \\ & A & \\ & & C \end{pmatrix}} \quad \underset{(e)}{\begin{pmatrix} A & & \\ & A & \\ & & A \end{pmatrix}}$$

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(a) Triclinic	1, $\boxed{\bar{1}}$
(b) Monoclinic	2, m, $\boxed{2/m}$
(c) Orthorhombic	222, mm2, $\boxed{mmm}$
(d) Tetragonal	4,$\bar{4}$,4/m, 422,4 mm, $\bar{4}$2 m, $\boxed{6/mmm}$
Hexagonal	3,$\bar{3}$,32,3 m,$\bar{3}$ m,6,$\bar{6}$,6/m, 622,6 mm, $\bar{6}$ m2, $\boxed{6/mmm}$
(e) Cubic	23, m$\bar{3}$,432,$\bar{4}$3 m, $\boxed{m\bar{3}\ m}$

We denote the crystal family of a point group **F** by Fam(**F**). Fam(**F**) is the boxed group in each of the rows given above.

The form of the [V^2] tensor invariant under **F** depends only on Fam(**F**). **F** is a normal subgroup of Fam(**F**). Let **F** $\subset$ Fam(**F**) and g_2 an element of Fam(**F**) not contained in **F**, then **F** + g_2**F** $\subseteq$ Fam(**F**).

For a non-ferroelastic domain pair [1, 2] (S_i, S_k), the symmetry group **F** of S_i is a subgroup of Fam(**F**). **F** is also the symmetry group of S_k. There exists an element g_{ik} of Fam(**F**) such that $g_{ik}S_i = S_k$ and $g_{ik}S_k = S_i$ and the domain pair is characterized by a *twin law* [3] $\mathbf{J}_{ik} = \mathbf{F} + g_{ik}\mathbf{F}$ where Fam($\mathbf{J}_{ik}$) = Fam(**F**). The form T(i) of a physical property tensor of type ***T*** in domain S_i is invariant under **F** and, in S_k, T(k) = g_{ik}T(i). The tensor distinction between the two domains is determined by the element g_{ik}.

The twin laws of all non-ferroelastic domain pairs are classified into 43 classes [4]:

$\mathbf{J}_{ik}$	**F**	g_{ik}	$\mathbf{J}_{ik}$	**F**	g_{ik}
1) $\bar{1}$	$\mathbf{1}$	$\bar{1}$	23) $\mathbf{6_z2_x2_1}$	$\mathbf{3_z2_x}$	2_z
2) $\mathbf{2_z/m_z}$	$\mathbf{2_z}$	$\bar{1}$	24) $\mathbf{\bar{6}_z\ m_12_x}$	$\mathbf{3_z2_x}$	m_z
3) $\mathbf{2_z/m_z}$	$\mathbf{m_z}$	$\bar{1}$	25) $\mathbf{\bar{3}_z\ m_x}$	$\mathbf{3_zm_x}$	$\bar{1}$
4) $\mathbf{m_xm_ym_z}$	$\mathbf{2_x2_y2_z}$	$\bar{1}$	26) $\mathbf{6_zm_xm_1}$	$\mathbf{3_zm_x}$	2_z
5) $\mathbf{m_xm_ym_z}$	$\mathbf{m_xm_y2_z}$	$\bar{1}$	27) $\mathbf{\bar{6}_z\ m_x2_1}$	$\mathbf{3_zm_x}$	m_z
6) $\mathbf{4_z/m_z}$	$\mathbf{4_z}$	$\bar{1}$	28) $\mathbf{6_z/m_zm_xm_1}$	$\mathbf{\bar{3}_z\ m_x}$	2_z
7) $\mathbf{4_z2_x2_{xy}}$	$\mathbf{4_z}$	2_x	29) $\mathbf{6_z/m_z}$	$\mathbf{6_z}$	$\bar{1}$
8) $\mathbf{4_zm_xm_{xy}}$	$\mathbf{4_z}$	m_x	30) $\mathbf{6_z2_x2_1}$	$\mathbf{6_z}$	2_x
9) $\mathbf{4_z/m_z}$	$\mathbf{\bar{4}_z}$	$\bar{1}$	31) $\mathbf{6_zm_xm_1}$	$\mathbf{6_z}$	m_x
10) $\mathbf{\bar{4}_z\ 2_xm_{xy}}$	$\mathbf{\bar{4}_z}$	2_x	32) $\mathbf{6_z/m_z}$	$\mathbf{\bar{6}_z}$	$\bar{1}$
11) $\mathbf{4_z/m_zm_xm_{xy}}$	$\mathbf{4_z/m_z}$	2_x	33) $\mathbf{\bar{6}_z\ m_x2_1}$	$\mathbf{\bar{6}_z}$	m_x
12) $\mathbf{4_z/m_zm_xm_{xy}}$	$\mathbf{4_z2_x2_{xy}}$	$\bar{1}$	34) $\mathbf{6_z/m_zm_xm_1}$	$\mathbf{6_z/m_z}$	2_x
13) $\mathbf{4_z/m_zm_xm_{xy}}$	$\mathbf{4_zm_xm_{xy}}$	2_x	35) $\mathbf{6_z/m_zm_xm_1}$	$\mathbf{6_z2_x2_1}$	$\bar{1}$
14) $\mathbf{4_z/m_zm_xm_{xy}}$	$\mathbf{\bar{4}_z\ 2_xm_{xy}}$	$\bar{1}$	36) $\mathbf{6_z/m_zm_xm_1}$	$\mathbf{6_zm_xm_1}$	$\bar{1}$
15) $\mathbf{3_z2_x}$	$\mathbf{3_z}$	2_x	37) $\mathbf{6_z/m_zm_xm_1}$	$\mathbf{\bar{6}_z\ m_x2_1}$	$\bar{1}$
16) $\mathbf{3_zm_x}$	$\mathbf{3_z}$	m_x	38) $\mathbf{m_z\bar{3}_{xyz}}$	$\mathbf{2_z3_{xyz}}$	$\bar{1}$
17) $\mathbf{\bar{3}_Z}$	$\mathbf{3_z}$	$\bar{1}$	39) $\mathbf{4_z3_{xyz}2_{xy}}$	$\mathbf{2_z3_{xyz}}$	2_{xy}
18) $\mathbf{6_z}$	$\mathbf{3_z}$	2_z	40) $\mathbf{\bar{4}_Z\ 3_{xyz}m_{xy}}$	$\mathbf{2_z3_{xyz}}$	m_{xy}
19) $\mathbf{\bar{6}_Z}$	$\mathbf{3_z}$	m_z	41) $\mathbf{m_z\bar{3}_{xyz}\ m_{xy}}$	$\mathbf{\bar{4}_Z\ 3_{xyz}m_{xy}}$	$\bar{1}$
20) $\mathbf{6_z/m_z}$	$\mathbf{\bar{3}_Z}$	2_z	42) $\mathbf{m_z\bar{3}_{xyz}\ m_{xy}}$	$\mathbf{4_z3_{xyz}2_{xy}}$	$\bar{1}$
21) $\mathbf{\bar{3}_Z\ m_x}$	$\mathbf{\bar{3}_Z}$	2_x	43) $\mathbf{m_z\bar{3}_{xyz}\ m_{xy}}$	$\mathbf{m_z\bar{3}_{xyz}}$	2_{xy}
22) $\mathbf{\bar{3}_Z\ m_x}$	$\mathbf{3_z2_x}$	$\bar{1}$			

2. Tensor Distinction

Consider a non-ferroelastic domain pair (S_i, S_k). The matrix form of the relationship between the forms of the tensor $\boldsymbol{T}$ in the two domains is

$$T(k)_a = D(g_{ik})_{a,b} T(i)_b \tag{1}$$

where $T(i)_b$ are the components of the form of the tensor $\boldsymbol{T}$ in S_i and $T(k)_a$ in S_k. We shall show: *For any two non-ferroelastic domains there exists a coordinate system in which the two domains can be distinguished by the sign of a component of a physical property tensor.*

We show the validity of this theorem using Eq. (1) and the above list of twin laws of non-ferroelastic domain pairs. We find that for every non-ferroelastic domain pair (S_i, S_k) there exists a coordinate system in which the matrix $D(g_{ik})_{a,b}$ is diagonal with all entries along the diagonal either $+1$ or -1. The theorem then follows from Eq. (1):

We choose a cartesian coordinate system x, y, z. In such a coordinate system each component of T_a can be indexed by a product $a = a_1 a_2 \ldots a_n$ where each a_j is x, y, or z. The matrix D_{ab} is then the product

$$D(g)_{ab} = \delta(g) V(g)_{a_1 b_1} \otimes V(g)_{a_2 b_2} \otimes \cdots \otimes V(g)_{a_n b_n} \tag{2}$$

where V is the three-dimensional vector representation and $\delta(g) = \det V(g)$. If $V(g_{ik})$ is diagonal, then $D(g_{ik})$ is diagonal. In the above list, only when $g_{ik} = 2_{xy}$ and m_{xy} is $V(g_{ik})$ not diagonal. In these cases, classes 39, 40 and 43, one can rotate the coordinate system 45° about the z-axis where g_{ik} can now be taken as 2_x and m_x, respectively. Consequently, in all cases there exists a coordinate system in which the matrix $D(g_{ik})_{a,b}$ is diagonal. Since the diagonal entries on matrices V are either $+1$ or -1, then, from equation (2), the entries on the diagonal matrix $D(g)_{ab}$ are either $+1$ or -1. If $D(g_{ik})_{aa} = 1$ then the ath component of T can not distinguish between the domains. If $D(g_{ik})_{aa} = -1$, and $T(i)_{aa} \neq 0$, then the ath component does distinguish between the domains.

One can determine which components distinguish between two non-ferroelastic domains as follows: We define n_x, n_y, and n_z as the number of x, y, and z's , respectively, in the index $a = a_1 a_2 \ldots a_{\mathbf{n}}$. From Eq. (2), we have:

$$D(g_{ik})_{aa} = \delta(g_{ik}) [V(g_{ik})_{xx}]^{n_x} [V(g_{ik})_{yy}]^{n_y} [V(g_{ik})_{zz}]^{n_z} \tag{3}$$

3. Tensor Distinction Example

Consider the twin law $\mathbf{\bar{4}_z 3_{xyz} m_{xy}} = \mathbf{2_z 3_{xyz}} + m_{xy}\ \mathbf{2_z 3_{xyz}}$ of a non-ferroelastic domain pair (S_i, S_k) and the quadratic susceptibility tensor, a physical property tensor of the type $\boldsymbol{T} = V^3$. In a new coordinate system $(x', y', z) = (x + y, x - y, z)$, the twin law becomes $\mathbf{\bar{4}_z 3_{x'y'z} m_{xy}} = \mathbf{2_z 3_{x'y'z}} + m_{x'}\ \mathbf{2_z 3_{x'y'z}}$. Using standard tables [5] one finds the form T(i) of the tensor V^3 in domain S_i , invariant under $\mathbf{2_z 3_{xyz}}$, to be

$$T(i)_{x'm'n'} = \begin{pmatrix} 0 & 0 & M \\ 0 & 0 & N \\ M & -N & 0 \end{pmatrix}; \quad T(i)_{y'm'n'} = \begin{pmatrix} 0 & 0 & -N \\ 0 & 0 & -M \\ N & -M & 0 \end{pmatrix};$$

$$T(i)_{zm'n'} = \begin{pmatrix} M & N & 0 \\ -N & -M & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

where $m', n' = x', y', z$. Using Eq. (3), the matrix $D(m_{x'})$ is of the form:

$$D(m_{x'})_{x'm'n',x'm'n'} = \begin{pmatrix} 1 & -1 & -1 \\ -1 & 1 & 1 \\ -1 & 1 & 1 \end{pmatrix}_{m'n'} \quad D(m_{x'})_{y'm'n',y'm'n'} = \begin{pmatrix} -1 & 1 & 1 \\ 1 & -1 & -1 \\ 1 & -1 & -1 \end{pmatrix}_{m'n'}$$

$$D(m_{x'})_{zm'n',zm'n'} = \begin{pmatrix} -1 & 1 & 1 \\ 1 & -1 & -1 \\ 1 & -1 & -1 \end{pmatrix}_{m'n'}$$

Using Eq. (1), the form of the quadratic susceptibility tensor $T(k) = D(m_{x'})T(i)$ is then, using Eq. (1),

$$T(k)_{x'm'n'} = \begin{pmatrix} 0 & 0 & -M \\ 0 & 0 & N \\ -M & -N & 0 \end{pmatrix}; \quad T(k)_{y'm'n'} = \begin{pmatrix} 0 & 0 & -N \\ 0 & 0 & M \\ N & M & 0 \end{pmatrix};$$

$$T(k)_{zm'n'} = \begin{pmatrix} -M & N & 0 \\ -N & M & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

and we have the forms of the tensor in the domain pair in a coordinate system where the components are either the same or of opposite sign in the domains.

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