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TENSOR DISTINCTION OF FERROELASTIC DOMAIN STATES IN COMPLETELY TRANSPOSABLE DOMAIN PAIRS

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We present tensor distinction of ferroelastic domains for a large class of ferroelastic domain states that form so called completely transposable domain pairs. We give the 15 possible relations (twin laws) between these ferroelastic domain states. For each twin law we list the numbers of components of important material property tensors that are different and that are equal in the two single domain states of the domain pair. We demonstrate how these twin laws and tensor distinction can be influenced by disorientations, i.e. rotations of single domain states needed to achieve coherent junction of two ferroelastic domain states along a planar domain wall.

1. INTRODUCTION

Domain structures consist of domains. Bulk structures $S_i, S_k, \ldots$ of domains, called *domain states*, have the same low symmetry structure and in the continuum description differ only in spatial orientation. When observed from one laboratory coordinate system they may exhibit different tensor properties. This tensor distinction is important, e.g., for finding and applying appropriate methods for observing domains, for determining average tensor properties of polydomain samples and for discussing the behavior of domain structures in external fields.

Recently, we have examined tensor distinction in non-ferroelastic phases.[1] In this contribution we demonstrate specific features of relations between bulk structures of ferroelastic domains and present tensor distinction for a class of ferroelastic domain states that form so called completely transposable pairs.

2. FERROELASTIC DOMAIN PAIRS AND DISORENTATIONS

When examining tensor distinction of two domains D_i and D_k we are comparing tensor properties of their domain states S_i and S_k. Instead of describing S_i and S_k by their orientations we shall characterize the relation between S_i and S_k by a suitable point group which will allow us to determine tensor distinction by group-theoretical procedures.

Two domain states S_i, S_k considered irrespectively of their coexistence form a *domain pair* $\{S_i, S_k\}$. Domain pair can be treated algebraically as an unordered set $\{S_i, S_k\} = \{S_k, S_i\}$ or, geometrically, as a superposition of domain states S_i and S_k. Symmetrically, the domain pair is specified by the symmetry group F_i of S_i which consists of the operations of the symmetry group G of the high-symmetry (parent) phase that leave S_i invariant,

$$F_i = \{g \in G \mid gS_i = S_i\}, \tag{1}$$

and by an operation $j'_{ik} \in G$ that transforms S_i into S_k, $j'_{ik}S_i = S_k$. If, further, j'_{ik} transforms also S_k into S_i , i.e. if $j'_{ik}S_i = S_k$, and $j'_{ik}S_k = S_i$, then the domain pair is referred to as a *transposable (ambivalent*[1]*) domain pair.* The operation j'_{ik} exchanging the domain states can be considered a symmetry operation of $\{S_i, S_k\}$. If, moreover, the domain states S_i and S_k have the same symmetry group, $F_i = F_k$, then the pair is called a *completely transposable domain pair.* The symmetry group of such a pair can be expressed in the form of a dichromatic group

$$J_{ik} = F_i + j'_{ik}F_i, \tag{2}$$

where the unprimed operations of F_i leave invariant both S_i and S_k whereas primed operations of the left coset $j'_{ik}F_i$ exchange S_i and S_k. The group J_{ik} fully specifies the domain pair $\{S_i, S_k\}$ and we say that J_{ik} in Eq. (3) expresses the *twin law* of a completely transposable domain pair $\{S_i, S_k\}$.

Depending on the spontaneous deformations $e^{(i)}$ and $e^{(k)}$ of S_i and S_k, resp., we can distinguish between *non-ferroelastic domain pairs* for which $e^{(i)} = e^{(k)}$ and *ferroelastic domain pairs* for which $e^{(i)} \neq e^{(k)}$. For completely transposable domain pairs a simple criterion holds: $\{S_i, S_k\}$ is ferroelastic if and only if Fam$F_i \subset$ FamJ_{ik}, where the symbol Fam denotes the crystal family of a group.[1]

There are 15 dichromatic groups of the form (2) that satisfy conditions Fam$F_i \subset$ FamJ_{ik} and $F_i = F_k$. These twin laws are listed in the first three columns of Table I. Before discussing the tensor distinction in these domain pairs we recall some specific features of ferroelastic domain structures.

In non-ferroelastic phases the number and orientations of possible domain states are not influenced by coexistence of domain states and do not depend on the form of the domain structure. Domain states in the polydomain sample are identical with *single domain states*, i.e. with bulk structures of single domains. All possible domain pairs in non-ferroelastic phases are completely transposable.[1]

The basic difference, and the main source of complications for ferroelastic phases lies in the fact that the number and orientation of ferroelastic domain states in polydomain samples differ from that of single domain states and depend on the specific form of the domain structure. In each case, however, domain states can be related in a unique way to single domain states which thus form a reliable reference system of domain states.

To illustrate this let us consider possible coexistence of two ferroelastic domain states that appear in the ferroelastic phase of the phase transition with $G = 4/mmm$ and $F = m_x m_y m_z$. In Figure 1 the tetragonal parent phase is represented by dotted square P

TABLE I Twin laws, axes, permissible walls and tensor distinction of ferroelastic domain states in completely transposable domain pairs

$F_i = F_k$...symmetry of domain states S_i and S_k, j'_{ik}...operation exchanging domain states S_i and S_k, J_{ik}...dichromatic point group expressing the twin law, D_a...alternating representation of J_{ik} subducing the identity representation in F_i
tensor designation: ϵ...enantiomorphism, V...polarization, $[V^2]$...deformation, permittivity, $\epsilon[V^2]$...optical activity, $V[V^2]$...piezoelectricity, electrooptics, $\epsilon V[V^2]$...electrogyration, $[[V^2]^2]$...elasticity, $[V^2]^2$...piezooptics, electrostriction

completely transposable ferroelastic domain pair							opposite (equal) tensor components							
$F_i = F_k$	j'_{ik}	J_{ik}	D_a	axis	permis. walls		ϵ	V	$[V^2]$	$\epsilon[V^2]$	$V[V^2]$	$\epsilon V[V^2]$	$[[V^2]^2]$	$[V^2]^2$
1	$2'$	$2'$	B	$[k\bar{h}0]$	(001)	$(hk0)_e$	0(1)	2(1)	2(4)	2(4)	10(8)	10(8)	8(13)	16(20)
1	m'	m'	A''	$[k\bar{h}0]$	$(001)_e$	$(hk0)$	1(0)	1(2)	2(4)	4(2)	8(10)	10(8)	8(13)	16(20)
$\bar{1}$	m'	$2'/m'$	B_g	$[k\bar{h}0]$	(001)	$(hk0)$	0(0)	0(0)	2(4)	0(0)	0(0)	10(8)	8(13)	16(20)
2_z	$2'_x$	$2'2'2$	B_1	$[001]$	(100)	(010)	0(1)	1(0)	1(3)	1(3)	5(3)	5(3)	4(9)	8(12)
2_z	m'_x	$m'm'2$	A_2	$[001]$	(100)	(010)	1(0)	0(1)	1(3)	3(1)	3(5)	5(3)	4(9)	8(12)
m_z	m'_x	$m'2'm$	B_2	$[010]$	$(100)_e$	(010)	0(0)	1(1)	1(3)	1(1)	5(5)	5(3)	4(9)	8(12)
$2_z/m$	m'_x	$m'm'm$	B_{1g}	$[001]$	(100)	(010)	0(0)	0(0)	1(3)	0(0)	0(0)	5(3)	4(9)	8(12)
2	$4'$	$4'$	B	$[001]$	$(hk0)$	$(k\bar{h}0)$	0(1)	0(1)	2(2)	2(2)	4(4)	4(4)	6(7)	10(10)
2	$\bar{4}'$	$\bar{4}'$	B	$[001]$	$(hk0)$	$(k\bar{h}0)$	1(0)	1(0)	2(2)	2(2)	4(4)	4(4)	6(7)	10(10)
$2_z/m$	$4'$	$4'/m$	B_g	$[001]$	$(hk0)$	$(k\bar{h}0)$	0(0)	0(0)	2(2)	0(0)	0(0)	4(4)	6(7)	10(10)
2_x22	$2'_{xy}$	$4'22'$	B_1	$[001]$	(110)	$(1\bar{1}0)$	0(1)	0(0)	1(2)	1(2)	2(1)	2(1)	3(6)	5(7)
m_xm2	m'_{xy}	$4'mm'$	B_1	$[001]$	(110)	$(1\bar{1}0)$	0(0)	0(1)	1(2)	1(0)	2(3)	2(1)	3(6)	5(7)
m_xm2	$2'_{xy}$	$\bar{4}'m2'$	B_2	$[001]$	(100)	(010)	0(0)	1(0)	1(2)	0(1)	3(2)	2(1)	3(6)	5(7)
2_x22	m'_{xy}	$\bar{4}'2m'$	B_1	$[001]$	(110)	$(1\bar{1}0)$	1(0)	0(0)	1(2)	2(1)	1(2)	2(1)	3(6)	5(7)
m_xmm	m'_{xy}	$4'/mmm'$	B_{2g}	$[001]$	(110)	$(1\bar{1}0)$	0(0)	0(0)	1(2)	0(0)	0(0)	2(1)	3(6)	5(7)

and the two orthorhombic single domain states $S_i = 1$ and $S_k = 2$ by dashed rectangles 1 and 2 with symmetry $F_1 = F_2 = m_x m_y m_z$. A geometrical representation of the *single domain pair* {1,2} is given on the left side of Figure 2. An operation $j'_{12} = m'_{\bar{x}y}$ exchanges 1 and 2, hence the domain pair {1,2} is completely transposable. The symmetry group of this pair is $J_{12} = m_x m_y m_z + m'_{\bar{x}y}\{m_x m_y m_z\} = 4'/m_z m_x m'_{xy}$.

It has been shown[2,3,4] that for a ferroelastic domain pair there exist two mutually perpendicular planes, called *permissible walls*, along which two domain states can meet in a compatible way, i.e. without dislocations or other singular defects. To achieve such a connection the single domain states must be rotated by a *disorientation angle* φ and $-\varphi$ about the intersecton of permissible domain walls called an *axis of the domain pair.* The rotated structures will be called *disoriented domain states* and domain pairs in which two disoriented domain states have a common plane (permissible wall) will be called *compatible domain pairs.*

In our example permissible domain walls are denoted W^I and W^{II} and the axes of the domain pair passes through the origin O. From Figures 1 and 2 it follows that disoriented domain states 1^+ and 2^- form a compatible domain pair $\{1^+, 2^-\}$ with a common plane W^{II} whereas 1^- and 2^+ in the compatible pair $\{1^-, 2^+\}$ share the plane W^I. Domain states in both compatible domain pairs have a common symmetry group in G which is, according to Eq. (1), $F_{1^-} = F_{1^+} = F_{2^-} = F_{2^+} = 2_z/m_z$. Domain states in both compatible domain pairs are exchanged by the operation $j'_{1^+2^-} = m'_{\bar{x}y}$, both compatible domain pairs are, therefore, completely transposable and have the same symmetry group $J_{1^+2^-} = J_{1^-2^+} = \{2_z/m_z\} + m'_{\bar{x}y}\{2_z/m_z\} = m'_{xy}m'_{\bar{x}y}m_z$. Thus disorientation reduces symmetry of domain states and of domain pairs as well.

In Table I we list for each of the 15 twin laws the orientation of the axis of the domain pair and of two perpendicular permissible walls. It can be easily shown that for the first 7 twin laws (given in the upper box) neither the symmetry of the domain states nor that of domain pairs are influenced by disorientations. For the remaining 8 twin laws the symmetry (twin law) $\hat{J}_{ik}$ of the compatible domain pairs is lower than the symmetry (twin law) J_{ik} of the corresponding single domain pair (see Table II). In the first three cases of Table II (middle box of Table I) the symmetry of domain states is not influenced by disorientations, therefore $\hat{J}_{ik} = F_i$ and the compatible pairs are no more transposable. In remaining five cases of Table II (lower box of Table I) not only J_{ik} but also the symmetry of domain states $F_i = F_k$ is lowered by disorientations and the compatible domain pairs with reduced symmetry $\hat{J}_{ik}$ remain completely transposable (see our example).

TABLE II Symmetry reduction of tetragonal twin laws by disorientation

J_{ik}	$4'_z$	$\bar{4}'_z$	$4'_z/m_z$	$4'_z 2_x 2'_{xy}$	$4'_z m_x m'_{xy}$	$\bar{4}'_z m_x 2'_{xy}$	$\bar{4}'_z 2_x m'_{xy}$	$4'_z/m_z m_x m'_{xy}$
$\hat{J}_{ik}$	2_z	2_z	$2_z/m_z$	$2'_{xy}2'_{\bar{x}y}2_z$	$m'_{xy}m'_{\bar{x}y}2_z$	$2'_{xy}2'_{\bar{x}y}2_z$	$m'_{xy}m'_{\bar{x}y}2_z$	$m'_{xy}m'_{\bar{x}y}m_z$

3. TENSOR DISTINCTION OF FERROELASTIC DOMAIN STATES

Discussion of tensor distinction in completely transposable ferroelastic domain pairs is similar to that in non-ferroelastic domain pairs.[1] Let us consider a material property tensor $\mathbf{T}$ and a specific twin law J_{ik}. Components of $\mathbf{T}$ transform as a set of basis functins of a (generally reducible) representation $D^{\mathbf{T}}$ of J_{ik}. Distinct components of $\mathbf{T}$ transform as basis functions of an alternating representation D_a of J_{ik} which subduces the identity representation in F (this representation D_a is given in the fourth column of Table); equal non-zero components of $\mathbf{T}$ transform as basis function of the identity representation D_1

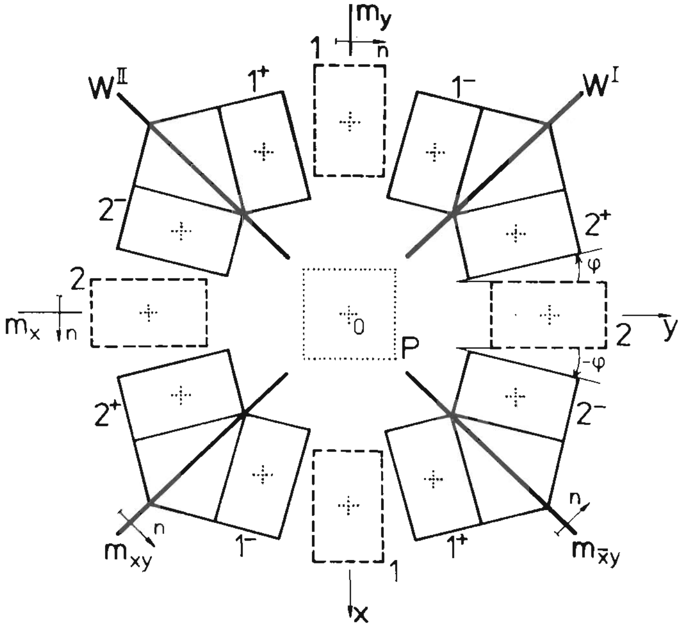

FIGURE 1 Exploded view of the single domain states 1, 2 and disoriented domain states $1^+, 1^-, 2^+, 2^-$. W^I and W^{II} are permissible walls, the axis of the ferroelastic domain pair {1,2} is perpendicular to the plane of the Figure and passes through the origin O. Rectangles representing domain states should be shifted so that their centers (dotted crosses) are at the axis.

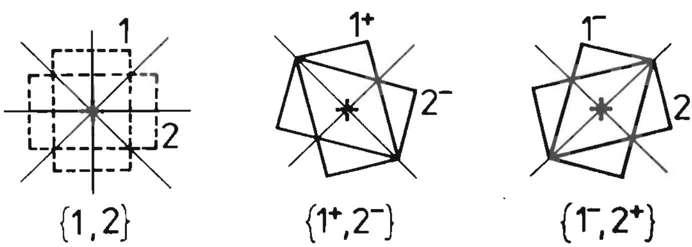

FIGURE 2 Single domain pair {1,2} and compatible domain pairs $\{1^+, 2^-\}$, $\{1^-, 2^+\}$. Diagonal solid lines passing through the center represent mirror planes and two-fold axes which exchange domain states. Vertical and horizontal lines represent mirror planes and two-fold axes which leave domain states 1 and 2 invariant.

of J_{ik}. Number $m_a^{\mathbf{T}}$ of distinct components and number $m_J^{\mathbf{T}}$ of equal componets of $\mathbf{T}$ in domain states of a domain pair are equal to the multiplicity of D_a and D_1 in $D^{\mathbf{T}}$, resp. In Table I numbers $m_a^{\mathbf{T}}$ and $m_J^{\mathbf{T}}$ (given in the parenthesis) are presented for all 15 ferroelastic completely transposable twin laws J_{ik} and for 8 important material property tensors $\mathbf{T}$. Since D_a is one dimensional then in properly chosen (canonical) coordinate system $\hat{x}, \hat{y}, \hat{z}$ the distinct tensor components in S_i and in S_k differ only in sign.

In our example we find in the Table I for the single domain pair {1,2} with $J_{12} = 4'/mm_x m'_{xy}$ and for, e.g., the second rank tensor $[V^2]$ the numbers $m_a^{[V^2]} = 1$, i.e. one component of $[V^2]$ has opposite sign in 1 and 2, and $m_J^{[V^2]} = 2$, i.e. two non-zero independent components are equal in 1 and 2. The tensor $[V^2]$ has in the canonical coordinate system $\hat{x} \parallel [110], \hat{y} \parallel [\bar{1}10], \hat{z} = z$ the form of the first matrix given below, where the components A and C are equal in domain states 1 and 2 whereas the component D has opposite sign in domain states 1 and 2 :

$$\begin{pmatrix} A & \pm D & 0 \\ \pm D & A & 0 \\ 0 & 0 & C \end{pmatrix}, \begin{pmatrix} \hat{A} & \pm\hat{D} & 0 \\ \pm\hat{D} & \hat{B} & 0 \\ 0 & 0 & \hat{C} \end{pmatrix} = \begin{pmatrix} A + D\sin 2\varphi & \pm D\cos 2\varphi & 0 \\ \pm D\cos 2\varphi & A - D\sin 2\varphi & 0 \\ 0 & 0 & C \end{pmatrix}$$

For the compatible pair $\{1^+, 2^-\}$ with $J_{1^+2^-} = m'_{xy} m'_{\bar{x}y} m_z$ we find in the seventh line of the Table I for $[V^2]$ the numbers $m_a^{[V^2]} = 1$, i.e. again one independent component which has opposite sign in 1^+ and 2^-, and $m_J^{[V^2]} = 3$ independent components that are equal in 1^+ and 2^-. The second and third matrices given above display corresponding matrix form of $[V^2]$ in the canonical coordinate system $\hat{x}, \hat{y}, \hat{z}$. One independent component $\hat{D}$ changes sign in 1^+ and 2^- and three independent components $\hat{A}, \hat{B}, \hat{C}$ are equal in 1^+ and 2^-. As the last matrix shows all these four components are functions of A, C, D from the first matrix and the angle of disorientation φ.

In general, for 7 twin laws in the upper box of Table I the numbers $m_a^{\mathbf{T}}$ and $m_J^{\mathbf{T}}$ of opposite and equal tensor components are not influenced by disorientatins, i.e. the numbers given in the upper box of Table I hold both for single domain pairs and for compatible domain pairs. For 5 twin laws in the lower box of Table I the numbers $m_a^{\mathbf{T}}$ and $m_J^{\mathbf{T}}$ are smaller for single domain pairs than for compatible domain pairs and both can be determined from Tables I and II, similarly as in our example. For 3 remaining cases in the middle box one can use Table I but for single domain pairs only. Discussion of corresponding compatible domain pairs, which are no more completely transposable, falls outside the scope of this paper.

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