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NON-FERROELASTIC TWIN LAWS AND DISTINCTION OF DOMAINS IN NON-FERROELASTIC PHASES

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We show that within continuum description there exist 48 possible relations (twin laws) between structures of two non-ferroelastic domains. All these twin laws can be expressed by dichromatic point groups. For each twin law we give the number of components of important material property tensors that have opposite sign in the two domains under consideration.

INTRODUCTION

Domains in non-ferroelastic phases cannot be simply observed in a polarizing microscope. There exist, however, other properties (expressible by appropriate material property tensors) that allow to distinguish such domains. Distinction of ferroelectric non-ferroelastic domains has been discussed recently in Ref. 1. Here we shall present an extension of this work to all non-ferroelastic domain structures that can appear in non-ferroelastic phases. Since we shall be interested in tensor distinction of domains we shall use continuum description and point groups only.

DOMAIN STATES IN NON-FERROELASTIC PHASES

We consider a ferroic transition from a prototype (parent) phase with symmetry G to a ferroic (distorted) phase with symmetry F, where $F < G$. The ferroic phase is degenerate: it can appear in n_o homogeneous single domain orientational states

$S_1, S_2, ..., S_n$ which have the same structure and differ only in spatial orientation.[2] We call these states *single domain states (SDS's)*. The number n_o of SDS's equals

$$n_o = | G | : | F | , \tag{1}$$

where $| G |$ and $| F |$ denotes the number of symmetry operations in G and F, resp. Symmetry groups of SDS's $S_1, S_2, ..., S_n$ are $F_1, F_2, ..., F_n$, resp. Further, we introduce a more general concept of *domain states (DS's)* which denote bulk structures (or their orientations) of domains in polydomain samples. Several disconnected domains can possess the same DS. DS's of a polydomain sample thus represent structures that appear in the sample, irrespectively in which domain.

According to Aizu[2] a ferroic phase is *non-ferroelastic* if all of the SDS's have the same (zero) spontaneous deformation. A simple criterion can be formulated in terms of crystal families[§] : A ferroic phase is non-ferroelastic if and only if

$$F < G, \quad \mathrm{Fam}(F) = \mathrm{Fam}(G); \tag{2}$$

if $\mathrm{Fam}(F) < \mathrm{Fam}(G)$ the ferroic phase is full or partial ferroelastic one.[2]

Domain states of non-ferroelastic phases have the following specific properties:

(i) DS's have a common lattice and their orientation is not affected by the coexistence, number and shape of domains in a domain structure. (DS's in ferroelastic phases depend on these factors). DS's coincide with SDS's (in contrast to polydomain ferroelastic phases where SD's differ from SDS's due to disorientations[4]) and the number of possible DS's equals the number of SDS's n_o given by Eq. (1).

(ii) All DS's have the same symmetry group, $F_1 = F_2 = ... = F_n = F$. (This groups may be different for ferroelastic SDS's and DS's.)

NON-FERROELASTIC DOMAIN PAIRS AND THEIR TWIN LAWS

Macroscopic properties that are different in two chosen domains are determined by the relation between their DS's. Two DS's S_i and S_k form a *domain pair* (DP)[5] $\{S_i, S_k\} = \{S_k, S_i\}$. An DP $\{S_i, S_k\}$ is *ambivalent* if there exists $g'_{ik} \in G$ such that

$$g'_{ik}S_i = S_k \quad \text{and} \quad g'_{ik}S_k = S_i. \tag{3}$$

Symmetry group J_{ik} of an ambivalent DP $\{S_i, S_k\}$ can be expressed as[6]

$$J_{ik} = F_{(ik)} + g'_{ik}F_{(ik)} \, , \tag{4}$$

where $F_{ik} = F_i \cap F_k$ and g'_{ik} fulfils (3). Group J_{ik} has the structure of a dichromatic group in which unprimed operations $F_{(ik)}$ represent trivial symmetry operations and primed operations $g'_{ik}F_{(ik)}$ non-trivial operations of the DP $\{S_i, S_k\}$. The group J_{ik} specifies in a convenient way the relation between S_i and S_k. We shall call it the *twin law of the ambivalent domain pair* $\{S_i, S_k\}$.

[§] *Crystal family* of a point group P = crystal system of P, with exception of trigonal groups which belong to the hexagonal family.[3] We shall represent crystal family of P by the holohedral point group of P, $\mathrm{Fam}(P)$ = holohedral group of P, where we put Fam(trigonal group) = $6/mmm$.

A *domain pair* $\{S_i, S_k\}$ is *non-ferroelastic* if S_i and S_k possess the same (zero) spontaneous deformation. A necessary and sufficient condition for an ambivalent DP to be non-ferroelastic is

$$\mathrm{Fam}(F_{(ik)}) = \mathrm{Fam}(J_{ik}). \tag{5}$$

It can be shown that *all* $\frac{1}{2}n_o(n_o - 1)$ *DP's that can be formed from* n_o *DS's of a non-ferroelastic phase are ambivalent, non-ferroelastic and their twin law has the form*

$$J_{ik} = F + g'_{ik}F, \tag{6}$$

where F is the common symmetry group of the DS's S_i and S_k.

TABLE I Symmetry reductions $G \to F$ generating twin law J_{ik}

G	F	J_{ik}
$\bar{1}$, $2/m$ (mmm, $4/m$, $4/mmm$, $\bar{3}$, $\bar{3}1m$, $\bar{3}m1$ $6/m$, $6/mmm$, $m\bar{3}$, $m\bar{3}m$)	1	$\bar{1}'$
$2/m$ (mmm, $4/m$, $4/mmm$, $\bar{3}1m$, $\bar{3}m1$, $6/m$, $6/mmm$, $m\bar{3}$, $m\bar{3}m$)	2	$2/m'$
$2/m$ (mmm, $4/m$, $4/mmm$, $\bar{3}1m$, $\bar{3}m1$, $6/m$, $6/mmm$, $m\bar{3}$, $m\bar{3}m$)	m	$2'/m$
mmm ($4/mmm$, $6/mmm$, $m\bar{3}$, $m\bar{3}m$)	222	$m'm'm'$
mmm ($4/mmm$, $6/mmm$, $m\bar{3}$, $m\bar{3}m$)	$mm2$	mmm'
$4/m$, $4/mmm$ ($m\bar{3}m$)	4	$4/m'$
$4/m$, $4/mmm$ ($m\bar{3}m$)	$\bar{4}$	$4'/m'$
422 $4/mmm$, 432 ($m\bar{3}m$)	4	$42'2'$
$4mm$ $4/mmm$ ($m\bar{3}m$)	4	$4m'm'$
$\bar{4}2m$, $4/mmm$, $\bar{4}3m$ ($m\bar{3}m$)	$\bar{4}$	$\bar{4}2'm'$
$\bar{4}m2$, $4/mmm$, $\bar{4}3m$ ($m\bar{3}m$)	$\bar{4}$	$\bar{4}m'2'$
$4/mmm$ ($m\bar{3}m$)	$4/m$	$4/mm'm'$
$4/mmm$ ($m\bar{3}m$)	422	$4/m'm'm'$
$4/mmm$ ($m\bar{3}m$)	$4mm$	$4/m'mm$
$4/mmm$ ($m\bar{3}m$)	$\bar{4}2m$	$4'/m'm'm$
$\bar{3}$, $\bar{3}m1$, $\bar{3}1m$, $6/m$, $6/mmm$ ($m\bar{3}$, $m\bar{3}m$)	3	$\bar{3}'$
321, $\bar{3}m1$, 622, $\bar{6}2m$, $6/mmm$ (432, $m\bar{3}m$)	3	$32'1$
312, $\bar{3}1m$, 622, $\bar{6}m2$, $6/mmm$ (432, $m\bar{3}m$)	3	$312'$
$3m1$, $\bar{3}m1$, $6mm$, $\bar{6}m2$, $6/mmm$ ($\bar{4}3m$ $m\bar{3}m$)	3	$3m'1$
$31m$, $\bar{3}1m$, $6mm$, $\bar{6}2m$, $6/mmm$ ($\bar{4}3m$ $m\bar{3}m$)	3	$31m'$
$\bar{3}m1$, $6/mmm$ ($m\bar{3}m$)	$\bar{3}$	$\bar{3}m'1$
$\bar{3}1m$, $6/mmm$ ($m\bar{3}m$)	$\bar{3}$	$\bar{3}1m'$
$\bar{3}m$, $6/mmm$ ($m\bar{3}m$)	32	$\bar{3}'m'$
$\bar{3}m$, $6/mmm$ ($m\bar{3}m$)	$3m$	$\bar{3}'m$
6, $6/m$, 622 $6mm$, $6/mmm$	3	$6'$
$\bar{6}$, $6/m$ $\bar{6}2m$ $\bar{6}m2$, $6/mmm$	3	$\bar{6}'$

TABLE I, *cont.*

G	F	J_{ik}
$6/m$, $6/mmm$	$\bar{3}$	$6'/m'$
$6/m$, $6/mmm$	6	$6/m'$
$6/m$, $6/mmm$	$\bar{6}$	$6'/m$
622, $6/mmm$	32	$6'22'$
622, $6/mmm$	6	$62'2'$
$6mm$, $6/mmm$	$3m$	$6'mm'$
$6mm$, $6/mmm$	6	$6m'm'$
$\bar{6}2m$, $6/mmm$	32	$\bar{6}'2m'$
$\bar{6}2m$, $6/mmm$	$\bar{6}$	$\bar{6}2'm'$
$\bar{6}m2$, $6/mmm$	$3m$	$\bar{6}'m2'$
$\bar{6}m2$, $6/mmm$	$\bar{6}$	$\bar{6}m'2'$
$6/mmm$	$\bar{3}m$	$6'/m'mm'$
$6/mmm$	$6/m$	$6/mm'm'$
$6/mmm$	622	$6/m'm'm'$
$6/mmm$	$6mm$	$6/m'mm$
$6/mmm$	$\bar{6}2m$	$6'/mm'm$
$m\bar{3}$, $m\bar{3}m$	23	$m'\bar{3}$
432, $m\bar{3}m$	23	$4'32'$
$\bar{4}3m$, $m\bar{3}m$	23	$\bar{4}'3m'$
$m\bar{3}m$	$m\bar{3}$	$m\bar{3}m'$
$m\bar{3}m$	432	$m'\bar{3}m'$
$m\bar{3}m$	$\bar{4}3m$	$m'\bar{3}m$

There are 48 crystallographically different dichromatic point groups that fulfil condition (5). These groups represent all possible twin laws of non-ferroelastic DP's and are displayed in the third column of Table I, together with symmetry groups F (second column). This list is identical with 48 dichromatic point groups used by Curien and Le Corre to designate twins by merohedry and reticular merohedry (except cubic reticular merohedry).[7]

Groups G that fulfil for given F and J_{ik} the relation

$$F < J_{ik} \leq G \qquad (7)$$

represent symmetries of possible prototype phases for which the phase transition $G \to F$ leads to the appearance of the twin law J_{ik} in the non-ferroelastic phase (for G's in the first column without brackets) or in the partial ferroelastic phase (G's within the brackets).

TENSOR DISTINCTION OF NON-FERROELASTIC DOMAINS

Let us consider a material property tensor $\mathbf{T}$ and a specific twin law (6) of a DP $\{S_i, S_k\}$. If $m_J^{\mathbf{T}}$ denotes the number of components of $\mathbf{T}$ in J_{ik} and $m_F^{\mathbf{T}}$ that in F then the difference $m^{\mathbf{T}} = m_F^{\mathbf{T}} - m_J^{\mathbf{T}}$ gives the number of components that are different in DS's S_i and S_k. Numbers $m_F^{\mathbf{T}}$ and $m_J^{\mathbf{T}}$ can be found e.g. in Ref. 8. Numbers $m^{\mathbf{T}}$ for all non-ferroelastic twin laws J_{ik} and important material property tensors $\mathbf{T}$ are given in Table II.

There is an alternative and more elegant method for determining $m^{\mathbf{T}}$: Distinct components of $\mathbf{T}$ transform as basis functions of an alternating representation $D_a^{\mathbf{T}}$ of J_{ik} which subduces the identity representation in F (the representation $D_a^{\mathbf{T}}$ is given in the fourth column of Table II). The components of the tensor $\mathbf{T}$ transform as a set of basis functions of a representation $D^{\mathbf{T}}$. The number $m^{\mathbf{T}}$ equals the multiplicity of $D_a^{\mathbf{T}}$ in $D^{\mathbf{T}}$.

The results can be applied also to twins by merohedry[7] (twin-lattice symmetry[9]).

TABLE II Non-ferroelastic twin laws and numbers of distinct tensor components. F...symmetry of both domain (twin) components S_i and S_k, J_{ik}...dichromatic point group expressing the twin law, fe: n = non-ferroelectric domain pair, e = ferroelectric domain pair (see Ref. 1), D_a^{T} ... alternating irreducible representation of J_{ik} that subduces the identity representation in F, ϵ...enantiomorphism, V...spontaneous polarization, $\epsilon[V^2]$...optical activity, $V[V^2]$...piezoelectricity, electrooptics, $\epsilon V[V^2]$...electrogyration, $[[V^2]^2]$...linear elasticity, $[V^2]^2$...piezooptics, electrostriction.

F	J_{ik}	fe	D_a^{T}	ϵ	V	$\epsilon[V^2]$	$V[V^2]$	$\epsilon V[V^2]$	$[[V^2]^2]$	$[V^2]^2$
1	$\bar{1}'$	e	A_u	1	3	6	18	0	0	0
2	$2/m'$	e	A_u	1	1	4	8	0	0	0
m	$2'/m$	e	B_u	0	2	2	10	0	0	0
222	$m'm'm'$	n	A_u	1	0	3	3	0	0	0
$mm2$	mmm'	e	B_{1u}	0	1	1	5	0	0	0
4	$4/m'$	e	A_u	1	1	2	4	0	0	0
$\bar{4}$	$4'/m'$	n	B_u	0	0	2	4	0	0	0
4	$42'2'$	e	A_2	0	1	0	3	3	1	3
4	$4m'm'$	n	A_2	1	0	2	1	3	1	3
$\bar{4}$	$\bar{4}2'm'$	n	A_2	0	0	1	2	3	1	3
$\bar{4}$	$\bar{4}m'2'$	n	A_2	0	0	1	2	3	1	3
$4/m$	$4/mm'm'$	n	A_{2g}	0	0	0	0	3	1	3
422	$4/m'm'm'$	n	A_{1u}	1	0	2	1	0	0	0
$4mm$	$4/m'mm$	e	A_{2u}	0	1	0	3	0	0	0
$\bar{4}2m$	$4'/m'm'm$	n	B_{1u}	0	0	1	2	0	0	0
3	$\bar{3}'$	e	A_u	1	1	2	6	0	0	0
3	$32'1$	e	A_2	0	1	0	4	4	1	4
3	$312'$	e	A_2	0	1	0	4	4	1	4
3	$3m'1$	n	A_2	1	0	2	2	4	1	4
3	$31m'$	n	A_2	1	0	2	2	4	1	4
$\bar{3}$	$\bar{3}m'1$	n	A_{2g}	0	0	0	0	4	1	4
$\bar{3}$	$\bar{3}1m'$	n	A_{2g}	0	0	0	0	4	1	4
32	$\bar{3}'m'$	n	A_{1u}	1	0	2	2	0	0	0
$3m$	$\bar{3}'m$	e	A_{2u}	0	1	0	4	0	0	0
3	$6'$	n	B	0	0	0	2	2	2	4
3	$\bar{6}'$	e	A''	1	1	2	4	2	2	4
$\bar{3}$	$6'/m'$	n	B_g	0	0	0	0	2	2	4
6	$6/m'$	e	A_u	1	1	2	4	0	0	0
$\bar{6}$	$6'/m$	n	B_u	0	0	0	2	0	0	0
32	$6'22'$	n	B_1	0	0	0	1	1	1	2
6	$62'2'$	e	A_2	0	1	0	3	3	0	2

TABLE II, *cont.*

F	J_{ik}	fe	D_a^{T}	ϵ	V	$\epsilon[V^2]$	$V[V^2]$	$\epsilon V[V^2]$	$[[V^2]^2]$	$[V^2]^2$
$3m$	$6'mm'$	n	B_2	0	0	0	1	1	1	2
6	$6m'm'$	n	A_2	1	0	2	1	3	0	2
32	$\bar{6}'2m'$	n	A_1''	1	0	2	1	1	1	2
$\bar{6}$	$\bar{6}2'm'$	n	A_2'	0	0	0	1	3	0	2
$3m$	$\bar{6}'m2'$	e	A_2''	0	1	0	3	1	1	2
$\bar{6}$	$\bar{6}m'2'$	n	A_2'	0	0	0	1	3	0	2
$\bar{3}m$	$6'/m'mm'$	n	B_{1g}	0	0	0	0	1	1	2
$6/m$	$6/mm'm'$	n	A_{2g}	0	0	0	0	3	0	2
622	$6/m'm'm'$	n	A_{1u}	1	0	2	1	0	0	0
$6mm$	$6/m'mm$	e	A_{2u}	0	1	0	3	0	0	0
$\bar{6}2m$	$6'/mm'm$	n	B_{2u}	0	0	0	1	0	0	0
23	$m'\bar{3}$	n	A_u	1	0	1	1	0	0	0
23	$4'32'$	n	A_2	0	0	0	1	1	0	1
23	$\bar{4}'3m'$	n	A_2	1	0	1	0	1	0	1
$m\bar{3}$	$m\bar{3}m'$	n	A_{2g}	0	0	0	0	1	0	1
432	$m'\bar{3}m'$	n	A_{1u}	1	0	1	0	0	0	0
$\bar{4}3m$	$m'\bar{3}m$	n	A_{2u}	0	0	0	1	0	0	0

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