

Classification of Domain Pairs and Tensor Distinction

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The symmetries of domain states of a domain pair (S_1, S_2) can be determined from the symmetry group F_1 of the first domain state and a twinning operation g_{12} which transforms this domain state into the second. A classification is introduced which classifies all possible domain pairs according to a classification of the pairs F_1 and g_{12} . One obtains 139 classes of which 43 correspond to non-ferroelastic domain pairs and 96 to ferroelastic domain pairs. The tensor distinction of domain states of a domain pair is determined by the group F_1 and g_{12} and all domain pairs belonging to the same class have the same tensor distinction. The 139 classes of pairs F_1 and g_{12} are tabulated along with their corresponding twinning group $K_{12} = \langle F_1, g_{12} \rangle$, the group generated by F_1 and g_{12} . The tensor distinction of domain states of domain pairs of each class is given for a variety of material property tensors.

Keywords: domains; tensors; symmetry

INTRODUCTION

Consider a ferroic phase transition of a crystalline structure from a phase of high symmetry G to a phase of low symmetry F . In the low symmetry phase arise domains, volumes of homogeneous crystalline structure differing only enantimorphically and/or in their orientation in space. We shall refer to the bulk structures of these domains in a polydomain sample as *domain states* and denote single domain states by S_1, S_2, \dots, S_n where n is the index of F in G . Domain states of a domain pair can exhibit different physical properties. We shall refer to this as *tensor distinction*, i.e. the distinction of domain states of

domain pairs by macroscopic tensorial physical property tensors. As these tensors depend only on the point group of the space group of the domain state, we shall interpret the symbols G and F to be the point groups of the high and low symmetry phases, respectively. We do not consider the disorientations of domains in ferroelastic samples, i.e. rotations of domains which arise as a result of the requirement that neighboring domains in polydomain samples must meet along a coherent boundary (see e.g. Janovec, Litvin, and Richterová¹). Consequently, all domain arising in a transition from G to F are related by elements of G .

Aizu² considered *global* tensor distinction, i.e. if a specific property tensor can distinguish among all, some or none of the domains which arise in a transition from G to F . Using a classification of transitions G to F , Litvin³ developed a method to determine such global tensor distinction and the global tensor distinction was given for all classes of transitions and property tensors of rank $n \leq 4$ (Litvin⁴).

We consider here the general case of the tensor distinction of domain pairs (S_i, S_j), two domains simultaneously observed by a single apparatus. The special case of non-ferroelastic phases have been considered elsewhere (Janovec, Richterová, and Litvin^{5,6}, Litvin and Janovec⁷).

TENSORIAL CLASSIFICATION OF DOMAIN PAIRS

In a phase transition from G to F , we write the coset expansion of the group G with respect to F : $G = F + g_2F + g_3F + \dots + g_nF$. Defining the domain state S_1 as the domain state invariant under F the remaining domain states are related to S_1 by the coset representatives $g_i, i=2,3,\dots,n$: $S_i = g_i S_1$. Any domain state S_i is related to any other domain state S_j by an element of G , i.e. $S_j = g_{ij} S_i$ where $g_{ij} = g_j g_i^{-1}$. The elements g_{ij} , like the coset representatives, are not unique, since any coset representative g_i can be replaced by any element of the coset $g_i F$. The domain state $S_i, i=2,3,\dots,n$ is invariant under the group $F_i = g_i F g_i^{-1}$. Let T denote a tensor type, and $T_i, i=1,2,\dots,n$ the sets of tensor components of the tensor type T in the domain states $S_i, i=1,2,\dots,n$. The two sets of tensor components T_i and T_j of the two domain states in a domain pair (S_i, S_j) can be determined as follows: T_i is the set of tensor components of the tensor type T invariant under the group F_i , the group under which S_i is invariant. T_j can be determined from $T_i, T_j = g_{ij} T_i$ where g_{ij} is an element of G which transforms the domain state S_i into the domain state S_j . ($T_j = g_{ij} T_i$ only represents the equation which relates the components of the tensors. The actual equation depends on

the transformational properties of the tensor type T and its rank (Nye⁸). Consequently, in a ferroic phase transition from G to F , the tensor distinction of a domain pair (S_i, S_j) is determined by the point group F_i and an element g_{ij} of G .

We classify all possible domain pairs (S_i, S_j) into classes where all domain pairs in a single class are distinguished by components of tensors of the same set of tensor types. Two domain pairs, (S_i, S_j) whose tensor distinction is determined by the point group F_i and element g_{ij} , and (S_r, S_s) whose tensor distinction is determined by F_r and g_{rs} are said to belong to the same class of domain pairs if there exists an element r of the full rotation group R such that

$$rF_i r^{-1} = F_r \quad \text{and} \quad r g_{ij} r^{-1} = g_{rs} f_r \quad (1)$$

where f_r is an element of F_r . The appearance of the element f_r is due to the non-uniqueness of the choice of g_{ij} . This second condition can be replaced with a condition on cosets:

$$r g_{ij} F_i r^{-1} = g_{rs} F_r \quad (2)$$

This classification is simultaneously a classification of all pairs F_i and g_{ij} . Two domain pairs, which have corresponding F_i and g_{ij} belonging to the same class of pairs F_i and g_{ij} , belong to the same class of domain pairs. It can be shown that if two domain pairs belong to the same class, then if tensors of a given tensor type can (can not) distinguish between the domains of the first domain pair, then they can (can not) distinguish between the domains of the second domain pair. We shall call this classification the *tensorial classification of domain pairs*.

This classification of domain pairs is similar to the *crystallographic double coset classification* of domain pairs (Janovec⁹; Litvin & Wike¹⁰): For domain pairs arising in a transition from G to F , two domain pairs (S_i, S_j) and (S_r, S_s) are said to belong to the same double coset classification of domain pairs if there is an element g of G such that $(gS_i, gS_j) = (S_r, S_s)$. Consequently, there exists an element r of G which satisfies equations (1) and (2), and therefore two domain pairs in the same double coset class are also in the same tensorial class of domain pairs. However, two domain pairs belonging to *different* double coset classes may belong to the *same* tensorial class. (On a different classification of domain pairs, see Fuksa and Janovec¹¹.)

The tensorial classification of domain pairs, denoted now by (S_i, S_j) , classifies all domain pairs according to their corresponding F_i and g_{ij} . There are 139 classes. In Table I we list the F_i and g_{ij} of one domain pair from each of the 139 classes. In the first column we give a sequential numbering. An asterisk following the sequential numbering denotes the 43 classes of non-ferroelastic

domain pairs, domain pairs with the same (zero) spontaneous deformation (This number of classes differs from the 48 classes of non-ferroelastic domain pairs given in Janovec, Richterová, and Litvin⁶ because of the tensorial classification scheme used here.) The remaining 96 classes are of ferroelastic domain pairs. F_1 and g_{12} are given in the next two columns. In the fourth column we give the twinning group $K_{12} = \langle F_1, g_{12} \rangle$, the group generated by F_1 and g_{12} . (See Janovec, Litvin, and Fuksa¹²) for use of the twinning group in the tensor distinction of domain pairs.)

TENSOR DISTINCTION

We give the tensor distinction of domains in domain pairs for all 139 classes of domain pairs for seven tensor types: (1) ϵ enantiomorphism (2) V spontaneous polarization (3) $\epsilon[V^2]$ optical activity (4) $V[V^2]$ piezoelectricity, electrooptics (5) $\epsilon V[V^2]$ electrogyration (6) $[[V^2]^2]$ linear elasticity (7) $[V^2]^2$ piezoptics, electrostriction. In the fifth column of Table 1, for each class, is given a string of seven letters. Each letter denotes the tensor distinction of the domains of domain pairs in that class for the seven tensor types given in the above table. The sequential order of the letters corresponds to the sequential numbers of the tensor types. "Y" denotes that a physical property represented by a tensor of that tensor type can distinguish between the domains of domain pairs of that class. "N" denotes that the tensor can not distinguish between the domains. "Z" denotes that the tensor is identically zero in both domains.

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68)	$m_y m_x 2_x$	2_{yz}	$m_x 3_{xyz} m_y$	ZY.YYY.YYY	104)*	3_x	m_x	$\bar{6}_x$	Y.Y.Y.Y.Y.Y.Y
69)	$m_y m_x 2_{xy}$	m_{xz}	$m_x 3_{xyz} m_y$	ZYY.YYY.Y	105)	3_{xyz}	m_y	$m_x 3_{xyz}$	Y.Y.Y.Y.Y.Y.Y
70)	$m_y m_x 2_{xy}$	2_{yz}	$m_x 3_{xyz} m_y$	ZYY.YYY.Y	106)	3_{xyz}	m_x	$2_3 3_{xyz}$	Y.Y.Y.Y.Y.Y.Y
71)	$m_x m_x 2_x$	2_1	$6/m_x 2_1$	Z.Y.Y.Y.Y.Y	107)	3_{xyz}	m_x	$4_3 3_{xyz} m_y$	Y.Y.Y.Y.Y.Y.Y
72)	$m_x m_x 2_x$	m_1	$6/m_x m_1$	Z.Y.Y.Y.Y.Y	108)	3_{xyz}	2_{yz}	$4_3 3_{xyz} 2_{xy}$	N.Y.Y.Y.Y.Y.Y
73)	$m_x m_x 2_x$	2_1	$6/m_x m_1$	Z.N.Y.Y.Y.Y	109)*	3_x	2_x	$6/m_x 2_x$	Z.Z.Z.Z.Y.Y.Y
74)	$m_x m_x 2_x$	2_1	$6/m_x m_1 m_y$	Z.Y.Y.Y.Y.Y	110)*	3_x	2_x	$3/m_x$	Z.Z.Z.Z.Y.Y.Y
75)	$m_x m_x m_x$	2_{yz}	$4/m_x m_x m_y$	Z.Z.Z.Z.Y.Y	111)	3_{xyz}	2_x	$m_x 3_{xyz} m_y$	Z.Z.Z.Z.Y.Y.Y
76)	$m_x m_x m_x$	2_{yz}	$m_x 3_{xyz} m_y$	Z.Z.Z.Z.Y.Y	112)	3_{xyz}	2_x	$3/m_x$	Z.Z.Z.Z.Y.Y.Y
77)	$m_y m_x m_x$	2_1	$6/m_x m_x m_1$	Z.Z.Z.Z.Y.Y	113)*	3_2	1	$3/m_x$	Z.Z.Z.Z.Y.Y.Y
78)	$m_x m_x m_x$	2_1	$4/m_x$	Z.Z.Z.Z.Y.Y	114)*	3_2	2_x	$6, m_x 2_1$	Y.Z.Y.Y.N.N.N
79)*	4_x	2_x	$4, 2, 2_{xy}$	Y.Y.Y.Y.N.N.N	115)*	3_2	m_x	$4, 3, 2_{xyz}$	Z.Z.Z.Z.Y.Y.Y
80)*	4_x	m_x	$4, m_x 2_{xy}$	N.Y.N.Y.Y.Y	116)	$3_{xyz} 2_{xy}$	2_x	$m_x 3_{xyz} m_y$	N.Z.Y.Y.Y.Y.Y
81)*	4_x	2_{xz}	$4, 2, 2_{xy}$	Y.N.Y.Y.Y.Y	117)	$3_{xyz} 2_{xy}$	m_x	$3/m_x$	Y.Z.Y.Y.Y.Y.Y
82)	4_x	2_{xz}	$m_x 3_{xyz} m_y$	Y.Y.Y.Y.Y.Y	118)*	3_{xyz}	2_x	$6, m_x m_1$	Z.N.Z.Y.Y.Y.Y
83)	4_x	1	$4/m_x$	Z.Z.Y.Y.N.N.N	120)*	3_{xyz}	2_x	$6, m_x 2_1$	Z.Y.Z.Y.Y.Y.Y
84)*	4_x	2_x	$4, 2, m_{xy}$	Z.Z.Y.Y.Y.Y	121)	$3_{xyz} m_y$	2_x	$4_3 3_{xyz} m_y$	Z.Y.Z.Y.Y.Y.Y
85)*	4_x	2_{yz}	$m_x 3_{xyz} m_y$	Z.Z.Y.Y.Y.Y	122)	$3_{xyz} m_y$	2_x	$m_x 3_{xyz} m_y$	Z.Y.Z.Y.Y.Y.Y
86)	4_x	2_x	$4, 2, m_{xy}$	Z.Z.Y.Y.Y.Y	123)	$3_{xyz} m_y$	2_x	$m_x 3_{xyz} m_y$	Z.Z.Z.Z.Y.Y.Y
87)	4_x	2_x	$m_x 3_{xyz} m_y$	Z.Z.Z.Z.Y.Y	124)*	$3_{xyz} m_x$	2_x	$6/m_x m_x m_1$	Z.Z.Z.Z.Y.Y.Y
88)*	$4/m_x$	1	$4/m_x m_x m_y$	Y.Z.Y.Y.N.N.N	125)*	6_x	2_x	$6/m_x$	Y.Y.Y.Y.N.N.N
89)	$4/m_x$	2_{xz}	$m_x 3_{xyz} m_y$	N.Z.Y.Y.Y.Y	127)*	6_x	m_x	$6, m_x m_1$	Y.N.Y.Y.Y.N.Y
90)*	$4, 2, 2_{xy}$	2_{xz}	$4/m_x m_x m_y$	Z.Y.Z.Y.Y.Y	128)*	6_x	1	$6/m_x$	Z.Z.Z.Y.Y.N.Y
91)	$4, 2, 2_{xy}$	2_{xz}	$4/m_x m_x m_y$	Z.Y.Z.Y.Y.Y	129)*	6_x	2_1	$6/m_x 2_1$	Z.Z.Z.Y.Y.N.Y
92)	$4, 2, 2_{xy}$	2_{xz}	$m_x 3_{xyz} m_y$	Z.Y.Z.Y.Y.Y	130)*	$6/m_x$	2_x	$6/m_x m_x m_1$	Z.Z.Z.Z.Y.N.Y
93)*	$4, m_x m_y$	2_{xz}	$m_x 3_{xyz} m_y$	Z.Y.Z.Y.Y.Y	131)*	$6, 2, 2_1$	1	$6/m_x m_x m_1$	Y.Z.Y.Y.N.N.N
94)	$4, m_x m_y$	2_{xz}	$m_x 3_{xyz} m_y$	Z.Z.Y.Y.Y.Y	132)*	$6, m_x m_1$	1	$6/m_x m_x m_1$	Z.Z.Y.Y.N.N.N
95)	$4, 2_{xy} m_x$	2_{xz}	$m_x 3_{xyz} m_y$	Z.Z.Y.Y.Y.Y	133)*	$6, m_x 2_1$	1	$6/m_x m_x m_1$	Z.Z.Z.Y.N.N.N
96)	$4, 2, m_{xy}$	2_1	$4/m_x m_x m_y$	Z.Z.Y.Y.Y.Y	134)*	$2, 3_{xyz}$	1	$m_x 3_{xyz}$	Z.Z.Z.Y.N.N.N
97)	$4, 2, m_{xy}$	2_1	$4/m_x m_x m_y$	Z.Z.Y.Y.Y.Y	135)*	$2, 3_{xyz}$	2_{yz}	$4, 3, 2_{xy}$	Z.Z.Z.Y.N.N.N
98)*	$4, 2, m_{xy}$	2_x	$m_x 3_{xyz} m_y$	Z.Z.Z.Z.Y.Y	136)*	$2, 3_{xyz}$	2_{yz}	$4, 3, 2_{xy}$	N.Z.N.Y.Y.N.Y
99)	$4/m_x m_x m_y$	2_x	$m_x 3_{xyz} m_y$	Z.Z.Z.Z.Y.Y	137)*	$2, 3_{xyz}$	m_1	$4, 3, 2_{xy} m_y$	Y.Z.Y.Y.Y.N.Y
100)*	3_x	2_x	$3, 2_x$	N.Y.N.Y.Y.Y	138)*	$4, 3_{xyz} 2_{xy}$	1	$m_x 3_{xyz} m_y$	Z.Z.Z.Z.N.N.N
101)*	3_x	m_x	$3, 2_x$	Y.N.Y.Y.Y.Y	139)*	$m_x 3_{xyz}$	1	$m_x 3_{xyz} m_y$	Y.Z.Y.Z.N.N.N
102)*	3_x	1	3_x	Y.Y.Y.Y.N.N.N			2_{yz}	$m_x 3_{xyz} m_y$	Z.Z.Z.Z.Y.N.Y
103)*	3_x	2_x	6_x	N.N.N.Y.Y.Y			2_{yz}	$m_x 3_{xyz} m_y$	Z.Z.Z.Z.Y.N.Y

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