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Tensor Distinction of Domains Resulting From Non-Ferroelastic Transitions to Subgroups of Index n > 2

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The method of determining the tensor distinction of domains resulting from non-ferroelastic phase transitions from a high symmetry phase of symmetry **G** to a low symmetry phase of symmetry **F** of index n = 2 in **G** (V. Janovec, L. Richterova, and D.B. Litvin, Ferroelectrics **40**, 95 (1993)) is extended to the general case of index n > 2. For all cases where n > 2, a tabulation is given of important physical property tensors which can distinguish between domains. This includes both physical property tensors associated with a primary order parameter which can distinguish between all domains, and those associated with secondary order parameters which can distinguish between some but not all domains.

1. INTRODUCTION

We consider crystalline domains which arise in a phase transition from a high symmetry phase of symmetry **G** to a low symmetry phase of symmetry **F**. We refer to the bulk structures of these domains in polydomain samples as *domain states* and denote these domain states by $S_1, S_2, \ldots, S_n$. Domains are most often distinguished by their bulk properties, i.e. according to their domain states. Consequently, the tensor distinction of domains by physical property tensors is equivalent to the tensor distinction of the corresponding domain states. For the purpose of determining the tensor distinction of any two domain states, the concept of a *domain pair* $\{S_i,S_j\}$ was introduced (Janovec, 1974). Domain pairs can be divided into two types: (1) A *non-ferroelastic* domain pair where the domain states S_i and S_j have the same (zero) spontaneous deformation, and (2) a *ferroelastic* domain pair where the domain states have different spontaneous deformations. Since the tensor of spontaneous deformation transforms in the same manner as the optical indicatrix, the domain states of a ferroelastic domain pair can be easily distinguished in a polarizing microscope. The domain states of a non-ferroelastic domain pair can not be distinguished in this manner. Thus, we consider here the tensor distinction of domains in non-ferroelastic transitions, i.e. where all domains have the same (zero) spontaneous deformation.

The tensor distinction of domains in non-ferroelastic transitions from a phase of symmetry **G** to a subgroup **F** of index n = 2 has been treated in detail (Janovec, Richterova, and Litvin (1993)). In this paper we complete the tensor distinction analysis of non-ferroelastic domains by extending it to the cases of n > 2. In Section 2 we briefly review the case of n = 2, and in Section 3 we extend the analysis to n > 2. Tables are also given of the tensor distinction by important physical property tensors in all cases of non-ferroelastic transitions with n > 2. As the tensor properties of domains are determined by point group considerations, we use here only point groups in the following group theoretical proceedures.

2. NON-FERROELASTIC TRANSITIONS TO A SUBGROUP OF INDEX n=2

In a non-ferroelastic phase transition from **G** to a subgroup **F** of index 2, $\mathbf{G} = \mathbf{F} + g\mathbf{F}$ and there are two domain states S_1 and S_2 where $S_2 = gS_1$, $S_1 = gS_2$. S_1 is invariant under $\mathbf{F}_1 = \mathbf{F}$ and S_2 under $\mathbf{F}_2 = g\mathbf{F}_1 g^{-1} = \mathbf{F}$. A domain pair $\{S_1,S_2\}$ with these properties is referred to as a completely transposable domain pair (Janovec, Litvin, and Fuksa (1995)). As **F** is a subgroup of index 2 one needs to consider the tensor distinction only of the domain pair $\{S_1,S_2\}$. A tensor *T* does not distinguish between the domains S_1 and S_2 if the form of the tensor *T* invariant under **F** is also invariant under g, and consequently under **G**. Only if the form of the tensor *T* invariant under **F** is not invariant under **G**, does the tensor distinguish between the two domains. A mathematical method has been given to determine if a tensor *T* distinguishes or not between the domains in this case where **F** is a subgroup of index 2 of **G**, and a tabulation of the tensor distinction due to a set of important material property tensors has been given for all 48 non-ferroelastic transitions from a group **G** to subgroups **F** of index 2 (Janovec, Richterova, and Litvin (1993)).

3. NON -FERROELASTIC TRANSITIONS TO A SUBGROUP OF INDEX n > 2

In addition to the 48 non-ferroelastic transitions from a group **G** to subgroups **F** of index 2, there are 11 to subgroups of index n > 2. Ten such transitions are to a subgroup of index n = 4 and one to a subgroup of index n = 8, see Table 1 and subgroup diagrams, Figures 1-3. The coset decomposition of **G** with respect to **F** is written as:

$$\mathbf{G} = \mathbf{F} + g_2\mathbf{F} + g_3\mathbf{F} + \dots + g_n\mathbf{F}$$

There are n domains $S_i = g_iS_1$, $i = 1,2,\dots,n$ and n^2 domain pair $\{S_i,S_j\}$, $i,j = 1,2,\dots,n$. Domain pairs can be classified into classes of domain pairs (Janovec,

(1972) and Litvin and Wike (1989)) where all domain pairs of a single class are distinguished by the same set of tensors. A common property in all non-ferroelastic transitions is that **F** is an invariant subgroup of **G**. Consequently, the number of classes of domain pairs is exactly n. A set of domain pair, one from each class, can be chosen as the set $\{S_1,S_i\}$, i = 1,2,...,n. We then must determine the tensor distinction of each of the n-1 domain pair $\{S_1,S_i = g_iS_1\}$, i = 2,...,n.

A second common property in all non-ferroelastic transitions is that each **F** + g_i**F**, i = 2,...,n , constitutes a subgroup $\mathbf{H}_i$ of **G**. Consequently, to each of the n-1 domain pair $\{S_1,S_i = g_iS_1\}$, i = 2,...,n , we associate two groups, the groups **F** and $\mathbf{H}_i$, where **F** is a subgroup of index 2 of $\mathbf{H}_i$. A tensor *T* does not distinguish between the domains S_1 and $S_i = g_iS_1$ if the form of the tensor *T* invariant under **F** is also invariant under g_i, and consequently under $\mathbf{H}_i$. Only if the form of the tensor *T* invariant under **F** is not invariant under $\mathbf{H}_i$, does the tensor distinguish between the two domains. Since **F** is a subgroup of index n = 2 of $\mathbf{H}_i$, one can directly use the results (see Section 2 above) of the analysis of tensor distinction in non-ferroelastic transitions to a subgroup of index 2 to the tensor distinction here in transitions to a subgroup of index n > 2.

For example, consider the non-ferroelastic phase transition from **G** = 6/mmm to **F** = 3m1, a subgroup of index 4. The coset decomposition of G with respect to F can be written as

$$\mathbf{G} = \mathbf{F} + g_2\mathbf{F} + g_3\mathbf{F} + g_4\mathbf{F}$$

with $g_2 = 6_z$, $g_3 = 2_x$, and $g_4 = 2_1$. The groups $\mathbf{H}_i = \mathbf{F} + g_i\mathbf{F}$, i = 2,3,4 are $\mathbf{H}_2$ = 6mm, $\mathbf{H}_3$ = $\bar{3}$m1, and $\mathbf{H}_4$ = $\bar{6}$m2, the three groups in Figure 3 which contain **F** = 3m1 as a subgroup of index 2. The n^2 = 16 domain pairs in this case are classified into n = 4 classes of domain pairs, and we determine the tensor distinction of the n-1 = 3 domain pair $\{S_1,S_i=g_iS_1\}$, i = 2,3,4. The tensor distinction of each domain pair $\{S_1,S_i\}$ can be found in existing tables (Janovec, Richterova, and Litvin (1993)) under the tensor distinction of domain pairs in the case of the non-ferroelastic phase transition between $\mathbf{H}_i$ and its subgroup **F** of index 2. That is, for the tensor distinction analysis of domain pairs in the non-ferroelastic phase transition from **G** = 6/mmm to **F** = 3m1, a subgroup of index n = 4, we must consider the tensor distinction in the n-1 = 3 non-ferroelastic phase transitions from $\mathbf{H}_2$ = 6mm, $\mathbf{H}_3$ = $\bar{3}$m1, and $\mathbf{H}_4$ = $\bar{6}$m2 to **F** = 3m1. The results of such an analysis is given in Table 1.

In the first two columns of Table 1 are listed the groups **G** and **F** of the 11 non-ferroelastic transitions to a subgroup of index n > 2. For each such transition, the following three columns list the domain pair $\{S_1,S_i\}$, g_i, and $\mathbf{H}_i$ for i = 2,3,...,n . In the i-th row in the remaining seven columns is listed whether or not the physical property tensor listed at the top of the column can distinguish between the domains of the domain pair $\{S_1,S_i\}$. [e.g. ϵ denotes enantiomorphism, V spontaneous polarization, $\epsilon[V^2]$ optical activity, $V[V^2]$ piezoelectricity, electrooptics, $\epsilon V[V^2]$ electrogyration, $[[V^2]^2]$ linear elasticity, and

$[V^2]^2$ piezooptics, electrostriction.] An "x" denotes that the physical property tensor can distinguish between the domains, a blank entry denotes that it can not.

Figures 1-3 show diagramatically the groups H_i, $i = 2,...,n$ used in the tensor distinction of domains for all non-ferroelastic transitions between G and subgroups F of index $n > 2$. In all non-ferroelastic transitions the groups G and F belong to the same family of point groups. Consequently we give separately in the three figures chains of subgroups of index 2 corresponding to the tetragonal, cubic, and hexagonal/trigonal families of point groups. The holohedral point group of each family is given at the top of the each diagram. In each row below the holohedral point group are listed the subgroups of index 2 of the point groups of the row above, the subgroups of specific point groups denoted by a line between the groups. For phase transitions between G and and a subgroup F of index $n > 2$, the groups H_i, $i = 2,...,n$ are those supergroups of index 2 of F which are subgroups of G (i.e. which are connected by lines between G and F). For example, for G = 6/m and F = 3, the groups H_i, $i = 2,3,4$, are $H_1 = \bar{3}$, $H_2 = 6$, and $H_3 = \bar{6}$.

From Table 1, for each phase transition, one can also determine which of the listed physical property tensors are associated with primary order parameters and can distinguish between all domains, are associated with secondary order parameters which can distinguish between some but not all domains, or can not distinguish between any of the domains. For a phase transition between specific groups G and F, and a specific physical property tensor, if the column in Table 1 under the physical property tensor contains an "x" in all rows corresponding to the listed domain pairs, then the physical property tensor is associated with a primary order parameter. If there is an "x" in only some but not all rows, then the physical property tensor is associated with a secondary order parameter. If the column is empty, then the physical property tensor can not distinguish between any of the domains.

For example, consider the phase transition between G = 6/mmm and F = 6 . A physical property tensor of the type $V[V^2]$ is associated with a primary order parameter. The remaining physical property tensors listed in Table 1, except of the type $[[V^2]^2]$, are associated with secondary order parameters. A physical property tensor of the type $[[V^2]^2]$ can not distinguish between any of the domains resulting from this phase transition.

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Table 1: Tensor Distinction in Non-Ferroelastic Transitions to a subgroup of index n > 2.

G	F	$\{S_1,S_i\}$	g_i	H_i	ϵ	V	$\epsilon[V^2]$	$V[V^2]$	$\epsilon V[V^2]$	$[[V^2]^2]$	$[V^2]^2$
6/mmm	6	$\{S_1,S_2\}$	2_x	622		x		x	x		x
		$\{S_1,S_3\}$	$\bar{1}$	6/m	x	x	x	x			
		$\{S_1,S_4\}$	m_x	6mm	x		x	x	x		x
6/mmm	$\bar{3}$	$\{S_1,S_2\}$	6_z	6/m					x	x	x
		$\{S_1,S_3\}$	2_x	$\bar{3}$m1					x	x	x
		$\{S_1,S_4\}$	2_1	$\bar{3}$1m					x	x	x
6/mmm	321	$\{S_1,S_2\}$	6_z	622				x	x	x	x
		$\{S_1,S_3\}$	$\bar{1}$	$\bar{3}$m1	x		x	x			
		$\{S_1,S_4\}$	$\bar{6}_z$	$\bar{6}$2m	x		x	x	x	x	x
6/mmm	312	$\{S_1,S_2\}$	6_z	622				x	x	x	x
		$\{S_1,S_3\}$	$\bar{1}$	$\bar{3}$1m	x		x	x			
		$\{S_1,S_4\}$	$\bar{6}_z$	$\bar{6}$m2	x		x	x	x	x	x
6/mmm	3m1	$\{S_1,S_2\}$	6_z	6mm				x	x	x	x
		$\{S_1,S_3\}$	2_x	$\bar{3}$m1		x		x			
		$\{S_1,S_4\}$	2_1	$\bar{6}$m2		x		x	x	x	x
6/mmm	31m	$\{S_1,S_2\}$	6_z	6mm				x	x	x	x
		$\{S_1,S_3\}$	2_1	$\bar{3}$1m		x		x			
		$\{S_1,S_4\}$	2_x	$\bar{6}$2m		x		x	x	x	x
6/mmm	$\bar{6}$	$\{S_1,S_2\}$	6_z	6/m				x			
		$\{S_1,S_3\}$	2_x	$\bar{6}$2m				x	x		x
		$\{S_1,S_4\}$	2_1	$\bar{6}$m2				x	x		x
6/mmm	3	$\{S_1,S_2\}$	6_z	6				x	x	x	x
		$\{S_1,S_3\}$	2_x	321		x		x	x	x	x
		$\{S_1,S_4\}$	2_1	312		x		x	x	x	x
		$\{S_1,S_5\}$	$\bar{1}$	$\bar{3}$	x	x	x	x			
		$\{S_1,S_6\}$	$\bar{6}_z$	$\bar{6}$	x	x	x	x	x	x	x
		$\{S_1,S_7\}$	m_x	3m1	x		x	x	x	x	x
		$\{S_1,S_8\}$	m_1	31m	x		x	x	x	x	x
4/mmm	$\bar{4}$	$\{S_1,S_2\}$	2_x	$\bar{4}$2m			x	x	x	x	x
		$\{S_1,S_3\}$	$2_{\bar{x}y}$	$\bar{4}$m2			x	x	x	x	x
		$\{S_1,S_4\}$	4_z	4/m			x	x			
4/mmm	4	$\{S_1,S_2\}$	2_x	422		x		x	x	x	x
		$\{S_1,S_3\}$	$\bar{1}$	4/m	x	x	x	x			
		$\{S_1,S_4\}$	m_x	4mm	x		x	x	x	x	x
m$\bar{3}$m	23	$\{S_1,S_2\}$	$2_{\bar{x}y}$	432				x	x		x
		$\{S_1,S_3\}$	$\bar{1}$	m$\bar{3}$	x		x	x			
		$\{S_1,S_4\}$	$m_{\bar{x}y}$	$\bar{4}$3m	x		x		x		x

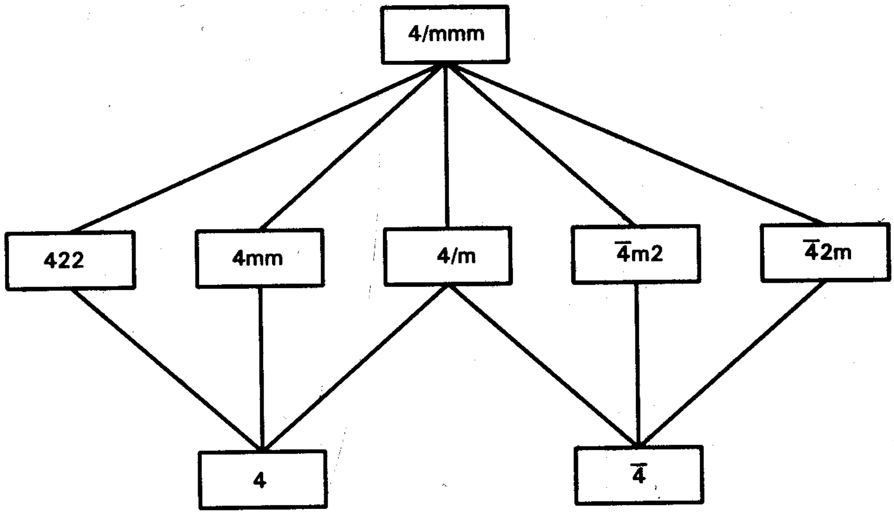

Figure 1: Subgroup chains of index 2 for the tetragonal family of point groups.

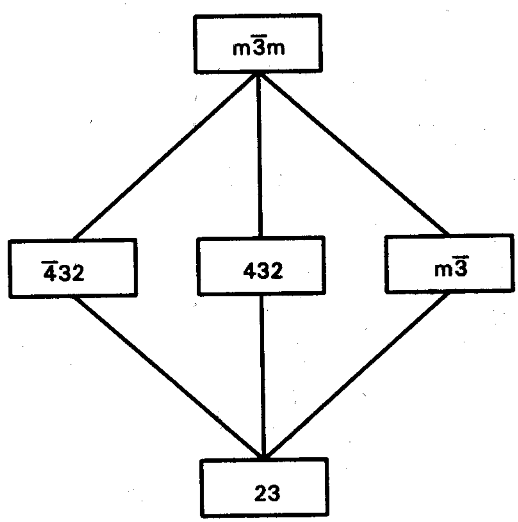

Figure 2: Subgroup chains of index 2 of cubic family of point groups

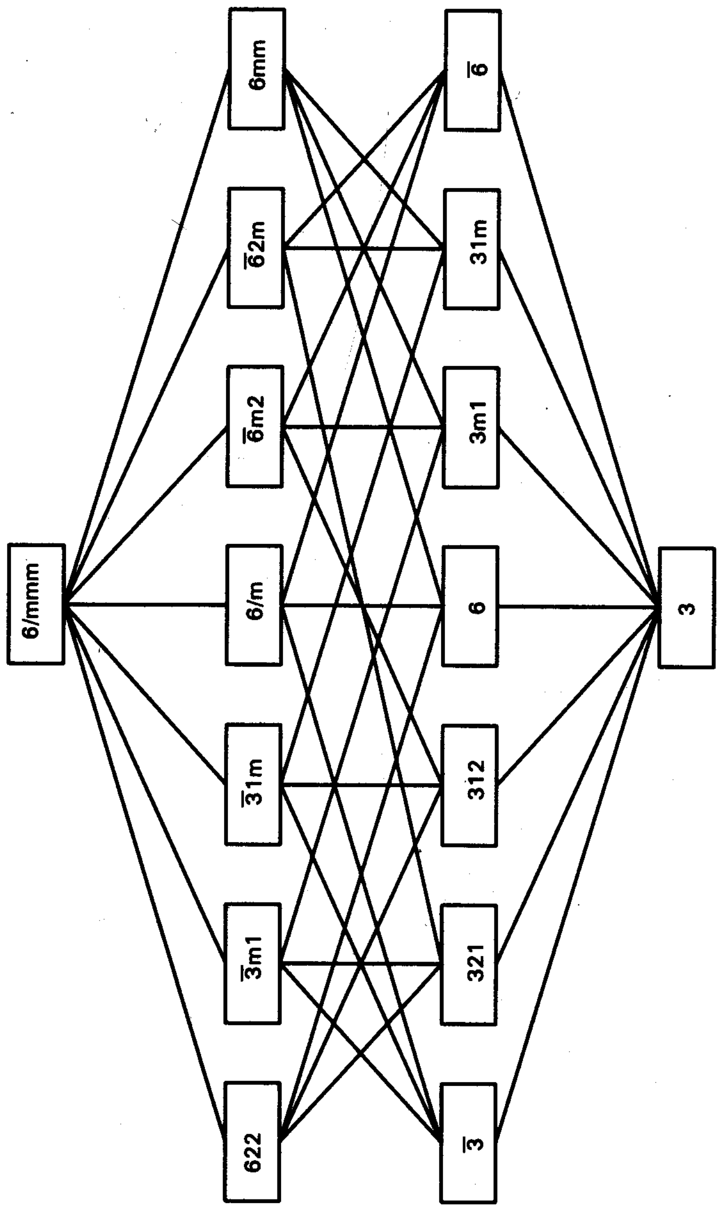

Figure 3: Subgroup chains of index 2 for the hexagonal/trigonal family of point groups.