Point Group Symmetries[*]

Daniel B. Litvin

Department of Physics, The Eberly College of Science, The Pennsylvania State University,
Penn State Berks Campus, P.O. Box 7009, Reading, PA 19610-6009, U.S.A.

ABSTRACT

The form of macroscopic physical property tensors of a crystalline structure can be determined from its magnetic or non-magnetic point group symmetry. In a ferroic crystal containing two or more equally stable domains of the same structure but of different spatial orientation, macroscopic tensorial physical properties that are different in domains, provide a *tensor distinction* of the domains. The use of point group symmetries in this tensor distinction is reviewed in this paper: Point group symmetry based classifications of domains have been defined to determine if specific macroscopic tensorial physical properties can provide a tensor distinction of all or some domains which arise in a phase transition. For pairs of domains, the tensor distinction is determined from a point group symmetry relationship, called a *twin law*. Recent work on *domain average engineering* in ferroics which focuses on the averaged point group symmetry and averaged physical properties of subsets of domains is also discussed.

Keywords: point groups, magnetic point groups, physical property tensors, tensor distinction, domains, ferroics

1. POINT GROUPS[1]

Traditionally, a crystalline medium is defined as a solid medium whose macroscopic physical properties can be characterized by associating with it a symmetry group which belongs to one of the 32 types of non-magnetic crystallographic point groups. If one considers only the purely geometrical characterization of a crystalline medium, the medium can also be considered trivially invariant under time inversion 1' . It follows that if a medium is invariant under an element R of a non-magnetic crystallographic point group **R** , it is then also invariant under the product R1' = R' . From a purely geometrical point of view, one might be tempted to then say that the medium and its physical properties are invariant under the group **R1',** the group consisting of all the elements R of **R** and the elements R of **R** multiplied by time inversion. Such a view was taken up by, for example, Zocher and Török[2]. However, such a view leads to erroneous predictions, as, for example, the prediction that the linear magnetoelectric effect is impossible in all crystalline media (see the book[3] by O'Dell for a history of the belief in the impossibility of this effect prior to its discovery in 1960).

Landau and Lifshitz[4] (1951) stressed that the absence of time inversion symmetry is a necessary condition for the existence of magnetically ordered crystalline material, as for example, ferromagnetic and antiferromagnetic media. For such materials, the medium and its physical properties are not invariant under a point group **R1'**. Dyaloshinski[5] (1959), using the magnetic crystallographic point group of antiferromagnetic Cr_2O_3, correctly predicted the existence of the magetoelectric effect in this material, an effect which was experimentally verified soon after[6,7].

Consequently, it is not just the 32 types of non-magnetic crystallographic point groups nor the 32 types of groups **R1'**, that one needs to consider when predicting the physical properties of crystalline media. It is the 122 types of magnetic crystallographic point groups which are to be used. Opechowski[8] has classified these groups into *magnetic superfamilies*: Let **R** denote one of the 32 types of non-magnetic crystallographic point groups. The magnetic superfamily of crystallographic groups of type **R** consists of :

a) Groups of the type **R**.

[*] Correspondence: Email: u3c@psu.edu Telephone: 610-396-6144 Fax: 610-396-6024

b) Groups of the type **R1'** where the time inversion group **1'** consists of the identity 1 and time inversion 1'.

c) Groups of the type **R**(**D**) = **D** + (**R**-**D**)1' where **D** is a subgroup of index two of **R**.

For example, the magnetic superfamily of **R** = **2/m** consists of :

a)	Groups of the type	**2/m**	= { 1, 2, $\bar{1}$, m }	=	**2/m**
b)	Groups of the type	**2/m1'**	= { 1, 2, $\bar{1}$, m, 1', 2', $\bar{1}$', m' }	=	**2/m1'**
c)	Groups of the type	**2/m(2)**	= { 1, 2, $\bar{1}$', m' }	=	**2/m'**
		2/m($\bar{1}$)	= { 1, 2', $\bar{1}$, m' }	=	**2'/m'**
		2/m(m)	= { 1, 2', $\bar{1}$', m }	=	**2'/m**

On the extreme right are the symbols of these types of groups where the **R**(**D**) notation has been replaced with a *primed* notation.

A complete listing of the 122 types of magnetic crystallographic point groups in groupings of magnetic superfamilies is given in Table 1. A computerized tabulation of group theoretical properties of the magnetic crystallographic point groups has recently been published by Schlessman and Litvin[9]. We shall use this *short international* notation of Table 1 throughout this paper. Note that we conform to the newest version of the International Tables for Crystallography[10] where symbols **m3** and **m3m** have been replaced by **m$\bar{3}$** and **m$\bar{3}$m** . Other notations exist, e.g. the group type denoted by **2/m(m)** = **2'/m** is denoted by $\mathbf{C_{2h}}$ ($\mathbf{C_s}$) in Schonflies notation and **2':m** in Shubnikov notation[11]. If one were to interpret 1' not as time inversion but the exchanging of two colors, this list becomes a list of the 120 types of two-color (black and white) point groups[12].

2. PHYSICAL PROPERTY TENSORS

The derivation and tabulation of physical property tensors invariant under the magnetic and non-magnetic crystallographic point groups have been considered by many authors (Jahn[13], Nye[14], Birss[15], Kopsky[16], Sands[17], Brandmuller & Winter[18], Bhagavatam[19], Bhagavatam and Pantulu[20], Tenenbaum[21], Grimmer[22] and references contained in these sources). Tables of a wide variety of physical property tensors invariant under non-magnetic crystallographic point groups have been given by Sirotin & Shaskolskaya[23] and Brandmuller, Bross, Bauer & Winter[24] and for both magnetic and non-magnetic point groups will appear in the forthcoming Volume D of the International Tables for Crystallography[25].

The form of the physical property tensors invariant under magnetic crystallographic points can be derived from the existing tables of physical property tensors invariant under non-magnetic crystallographic point groups: Let V denote a polar vector tensor and $V^n = V \times V \times \ldots \times V$ the nth ranked product of V, and let *e* and *a* denote zero-rank tensors that change sign under spatial inversion $\bar{1}$ and time inversion 1' , respectively. It has been shown by Litvin[26] that the form of a physical property tensor transforming as a tensor aV^n, eV^n, or aeV^n invariant under a magnetic point group **M** is the same as the form of a physical property tensor transforming as a tensor V^n or eV^n invariant under a related non-magnetic point group **R**. Tables are given listing the groups **R** corresponding to all magnetic point groups **M** for tensor types[26].

From the Taylor expansion of the density of stored free enthalpy, the polarization P, magnetization M, and mechanical deformation s_{ij} can be written in a third order expansion in terms of the electric field E , magnetic Field H, and stress tensor T as[27]:

$$P_i = \kappa_i^o + \kappa_{ij} E_j + (1/2)\,\kappa_{ijk} E_j E_k + \alpha_{ij} H_j + \alpha_{ijk} H_j E_k + (1/2)\,\beta_{ijk} H_j H_k + d_{ijk} T_{jk}$$

$$M_i = \chi_i^o + \chi_{ij} H_j + (1/2)\,\chi_{ijk} H_j H_k + \alpha_{ij} E_j + \beta_{ijk} E_j H_k + (1/2)\,\alpha_{ijk} E_j E_k + g_{ijk} T_{jk}$$

$$s_{ij} = s^{o}_{ij} + d_{ijk}E_k + g_{ijk}H_k$$

In Table 2, the name of each coefficient, corresponding phenomena, and tensor type are given. A survey of these and higher order magnetoelectric effects has recently been given at this conference[28].

For the magnetoelectric effect, the magnetoelectric susceptibility α_{ij} transforms as a tensor of the type aeV^2. From the tables of reference 22, the form of the magnetoelectric effect tensor invariant under the magnetic point group $\mathbf{\bar{4}'2'm}$ is the same as the form of a tensor of the type eV^2 invariant under the non-magnetic point group **4mm**. The latter, for the point group $\mathbf{4_z m_x m_{xy}}$ is given by Sirotin & Shaskolskaya[23] as

$$\begin{bmatrix} 0 & A & 0 \\ -A & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

which agrees with the form of the magnetoelectric physical property tensor invariant under $\mathbf{\bar{4}_z'2_x'm_{xy}}$ given by Birss[15].

3. TENSOR DISTINCTION OF DOMAINS IN FERROIC CRYSTALS

A ferroic crystal contains two or more equally stable *domains*, volumes of the same homogeneous crystalline structure in different spatial orientations. These domains can coexist in a crystal and may be distinguished by the values of components of certain macroscopic tensorial physical properties of the domains. Crystals in which the domains may be distinguished by spontaneous polarization, magnetization, or strain are called primary ferroic crystals. Crystals who domains are characterized by differences in the piezoelectric tensor is an example of a secondary ferroic crystal[29,30]. Ferroic crystals have been discussed by Newnham[31] and Wadhawan[32] and secondary ferroic crystals in particular by Aizu[29], Newnham and Cross[33,34] and Newnham and Skinner[35].

Consider a ferroic phase transition, a phase transition of a crystalline structure from a phase of higher point group symmetry **G** to a phase of lower point group symmetry **F**. In the lower symmetry phase there are $n = |\mathbf{G}|/|\mathbf{F}|$ *single domain states* $S_1,S_2,...,S_n$, where $|\mathbf{G}|$ and $|\mathbf{F}|$ denote the number of elements in **G** and **F**, respectively. Single domain states have the same crystalline structure and differ only in their orientation in space. *Domain states* will refer to the bulk structures, with their specific orientations in space, of domains in a polydomain sample. Several disconnected domains can have the same domain state. Domain states represent then the structures that appear in a polydomain sample, irrespective of in which domain.

In *non-ferroelastic* polydomain phases, the orientation of each domain state coincides with the orientation of a single domain state. The number of domain states is therefore the same as the number of single domain states. In *ferroelastic* polydomain phases, because of disorientations, i.e. rotations of domains that arise as a result of the requirement that neighboring domains in the polydomain sample must meet along a coherent boundary, domain states in general differ in their orientation from single domain states, and the number of domain states is in general greater than the number of single domain states. In distinction with domains in non-ferroelastic polydomain phases, the orientations are then, in general, not related by the rotational parts of the elements of **G**. We shall consider here ferroelastic polydomain phases in the *parent-clamping approximation* (Zigmund[36]; Janovec et al[37]) which disregards the disorientations. We disregard the disorientations, the number and orientation of domain states in a ferroelastic polydomain sample then also coincide with the number and orientations of single domain states, as in non-ferroelastic polydomain samples.

The domain states, denoted also by $S_1,S_2,...,S_n$, are related by elements of **G** not in **F**: We write the group **G** in a left coset decomposition with respect to **F**

$$\mathbf{G} = \mathbf{F} + g_2\mathbf{F} + g_3\mathbf{F} + ... + g_n\mathbf{F} \tag{1}$$

where the elements g_i, i = 1,2,...,n , g_1=1, are called the *coset representatives* of the coset decomposition of **G** with respect to **F**. The choice of coset representatives is not unique, the coset representative g_i can be replaced by $g_i f$, where f is an element of **F**. Defining the domain state S_1 as the domain invariant under **F**, the orientations of the remaining domain states are related to S_1 by the coset representatives of Eq. (1), i.e. $S_i = g_i S_1$, i = 2,3,...,n. In addition, each domain state S_i , i = 1,2,...,n , is invariant under the group $\mathbf{F}_i \equiv g_i \mathbf{F} g_i^{-1}$.

For example, if $\mathbf{G} = \mathbf{4_z/m_z m_x' m_{xy}'}$ and $\mathbf{F} = \mathbf{2_{xy}'/m_{xy}'}$, then

$\mathbf{F}$ = { 1	$\bar{1}$	$2_{xy}'$	m_{xy}' }	$g_1 = 1$		$\mathbf{F}_1 \equiv g_1 \mathbf{F} g_1^{-1} = \mathbf{2_{xy}'/m_{xy}'}$
$g_2\mathbf{F}$ = { 2_z	m_z	$2_{\bar{x}y}'$	$m_{\bar{x}y}'$ }	$g_2 = 2_z$	$S_2 = 2_z S_1$	$\mathbf{F}_2 \equiv g_2 \mathbf{F} g_2^{-1} = \mathbf{2_{xy}'/m_{xy}'}$
$g_3\mathbf{F}$ = { $2_y'$	4_z	$\bar{4}_z$	m_y' }	$g_3 = 2_y'$	$S_3 = 2_y' S_1$	$\mathbf{F}_3 \equiv g_3 \mathbf{F} g_3^{-1} = \mathbf{2_{\bar{x}y}'/m_{\bar{x}y}'}$
$g_4\mathbf{F}$ = { $2_x'$	4_z^3	m_x'	$\bar{4}_z^3$ }	$g_4 = 2_x'$	$S_4 = 2_x' S_1$	$\mathbf{F}_4 \equiv g_4 \mathbf{F} g_4^{-1} = \mathbf{2_{\bar{x}y}'/m_{\bar{x}y}'}$

We shall be interested here in what is referred to as *tensor distinction*, i.e. the distinction of the domains in a polydomain phase of a ferroic phase transition by macroscopic tensorial physical properties of tensor types ***T*** . As the set of domain states represent the structure of all domains in a polydomain phase, we consider the tensor distinction of the domain states.

We denote by T_i, i = 1,2,...,n , the form of the tensors of a tensor type ***T*** in the set of domain states $S_1,S_2,...,S_n$ of a polydomain sample. The tensors T_i, i=1,2,...,n are all given in a single coordinate system, e.g. the coordinate system of the parent phase structure or of one of the domain states. A tensor type ***T*** is said to be able to distinguish between two domain states, with corresponding tensors T_i and T_j of the type ***T***, if $T_i \neq T_j$. In particular, we consider two types of tensor distinction problems:

a) *Global Tensor Distinction*: We consider whether or not a tensor type ***T*** can distinguish among all domain states.

b) *Domain Pair Tensor Distinction*: For each pair of domain states, we consider whether or not a tensor type ***T*** can distinguish between the domain states of the domain pair.

Global Tensor Distinction: Consider a ferroic phase transition of a crystalline structure from a phase of higher symmetry **G** to a phase of lower symmetry **F**. Let $S_1,S_2,...,S_n$ denote the domain states of the lower symmetry phase, ***T*** a tensor type, and tensors T_i, i=1,2,...,n the form of the tensor type ***T*** in the domain states $S_1,S_2,...,S_n$. Following the terminology of Aizu[38], if the set of tensors T_i, i = 1,2,...,n , are all distinct, then we shall say that the tensor ***T*** provides a *full* distinction of the domain states S_i , i = 1,2,...,n , and the transition is a *full* ferroic phase transition with respect to tensor type ***T***. Each domain state is then characterized by a distinct form of tensor type ***T***, and macroscopic physical properties of this tensor type can distinguish all domain states. If the set of tensors T_i, i = 1,2,...,n, are not all distinct, but not all identical, then we shall say that the tensor ***T*** provides a *partial* distinction of the domain states, and the transition is a *partial* ferroic phase transition with respect to tensor type ***T***. A tensor of type ***T*** can then distinguish among some but not all of the domain states. If the set of tensors T_i, i = 1,2,...,n , are all identical, then the tensor type ***T*** provides no distinction, we shall say a *null* distinction, of the domain states. The transition is referred to as a *null* ferroic phase transition with respect to the tensor type ***T.***

Litvin[39] has subdivided the "null" case into two: The case where the set of tensors T_i, i = 1,2,...,n , are all identically zero, is referred to as *zero* distinction, and only in the case where the set of tensors are all identical and *non-zero* is it referred to as null distinction.

Concomitant with the classification of ferroic phase transitions into full, partial, null, and zero classes with respect to a specific tensor type $\boldsymbol{T}$, is the classification of ferroic phase transitions with respect to the higher and lower symmetry phase groups **G** and **F**. Using a classification introduced by Aizu[40] , Litvin[39] derived 247 classes of non-magnetic ferroic phase transitions and a general method for determining the global tensor distinction for classes of ferroic phase transitions A tabulation of the global tensor distinction of all 247 classes of non-magnetic ferroic phase transitions for all non magnetic tensor types $\boldsymbol{T}$ of rank $n \leq 4$ has been given by Litvin[41]. There has not been an analogous listing of the classes of magnetic ferroic phase transitions.

Domain Pair Tensor Distinction: Consider a ferroic phase transition of a crystalline structure from a phase of higher symmetry **G** to a phase of lower symmetry **F**. Let $S_1,S_2,...,S_n$ denote the domain states of the lower symmetry phase, $\boldsymbol{T}$ a tensor type, and tensors T_i, i=1,2,...,n the form of tensor type $\boldsymbol{T}$ in the domain states $S_1,S_2,...,S_n$. We now consider all *ordered domain pairs* $\{S_i,S_j\}$, $i,j = 1,2,...,n$, $i \neq j$. The tensors T_i and T_j of the two domain states in the domain pair $\{S_i,S_j\}$ can be determined as follows: if T_i is the form of tensor type $\boldsymbol{T}$ that is invariant under the point group $\mathbf{F}_i$, the point group of the domain state S_i. T_j can be determined from T_i, $T_j = g_{ij}T_i$, where g_{ij} is an element of **G** that transforms domain state S_i into domain state S_j, i.e. $S_j = g_{ij}S_i$. ($T_j = g_{ij}T_i$ only represents the equation that relates the components of the tensors. The actual equation depends on the transformational properties of the tensor type $\boldsymbol{T}$ and its rank (Nye[14]). The element g_{ij} is not unique, as any element of the coset $g_{ij}\mathbf{F}_i$ can be used. Consequently, in a ferroic phase transition from **G** to **F**, the tensor distinction of a domain pair $\{S_i,S_j\}$ can be determined by the point group $\mathbf{F}_i$ and the element g_{ij} of **G**.

We will classify all possible domain pair $\{S_i,S_j\}$ into classes where all domain pair in a single class are distinguished by the same set of tensor types. To this end we introduce the following tensor classification of domain pair:

Two domain pairs, $\{S_i,S_j\}$ whose tensor distinction is determined by the point group $\mathbf{F}_i$ and element g_{ij} and $\{S_{i'},S_{j'}\}$ whose tensor distinction is determined by the point group $\mathbf{F}_{i'}$ and element $g_{i'j'}$, are said to be in the same class of domain pair if there exists an element r of the full rotation group $\mathscr{R}$ such that:

$$r\mathbf{F}_i r^{-1} = \mathbf{F}_{i'} \tag{2a}$$

and

$$r g_{ij} r^{-1} = g_{i'j'} f_{i'} \tag{2b}$$

where $f_{i'}$ is an element of $\mathbf{F}_{i'}$. The appearance of the element $f_{i'}$ in Equation (2b) is due to the non-uniqueness of the choice of the coset representative $g_{i'j'}$. To remove any non-uniqueness in the Equations (2a,b), we can replace Equation (2b) with the condition:

$$r g_{ij}\mathbf{F}_{\mathbf{i}} r^{-1} = g_{i'j'}\mathbf{F}_{\mathbf{i'}} \tag{2c}$$

All elements of the coset $g_{ij}\mathbf{F}_{\mathbf{i}}$, i.e. all elements of **G** that transform the domain state S_i into the domain state S_j , are taken by Equation (2c) into all the elements of **G** that transform the domain state $S_{i'}$ into the domain state $S_{j'}$. If two domain pairs belong to the same class of domain pair, then if a tensor type can (can not) distinguish between the first pair of domains, then it can (cannot) distinguish between the second pair of domains[42]. We shall refer to these classes of domain pair as *equivalence tensor classes of domain pair*, or simply as *tensor classes of domain pair*.

This tensor classification of domain pairs is equivalent to the following classification (Janovec[43]) of ordered domain pairs: Two domain pairs, $\{S_i,S_j\}$ and $\{S_{i'},S_{j'}\}$ are said to be in the same class of domain pair if there exists an element r of the full rotation group $\mathscr{R}$ such that $\{rS_i,rS_j\} = \{S_{i'},S_{j'}\}$. This is a classification of *ordered* domain pairs. That is, the *unordered* pair of domain pairs $\{S_i,S_j\}$ and $\{S_j,S_i\}$ are not automatically placed in the same tensor class. While if a tensor of type T can or cannot distinguish between domain state S_i and S_j it is trivial to conclude it can or cannot distinguish between the domain states S_j and S_i, we do not use a classification of unordered domain pairs.

There is a second classification of domain pair[43]. Because of its relationship to the *double coset decomposition* of **G** with respect to **F**, we shall refer to it as the classification of domain pair into *double coset classes of domain pair*. The double coset decomposition of **G** with respect to **F** is written as

$$\mathbf{G} = \mathbf{F}g_1^{dc}\mathbf{F} + \mathbf{F}g_2^{dc}\mathbf{F} + \mathbf{F}g_3^{dc}\mathbf{F} + \ldots + \mathbf{F}g_m^{dc}\mathbf{F} \qquad (3)$$

where g_i^{dc}, i = 1,2, …, m are the double coset representatives. A symbol $\mathbf{F}g_i^{dc}\mathbf{F}$ means the set of distinct elements $f g_i^{dc} \hat{f}$, where f and $\hat{f}$ are elements of **F.** Sets of cosets constitute a single double coset. For example, if $\mathbf{G} = \mathbf{4_z/m_zm_x'm_{xy}'}$ and $\mathbf{F} = \mathbf{2_{xy}'/m_{xy}'}$, then

$$\begin{array}{llllllll}
\mathbf{F}g_1^{dc}\mathbf{F} = \{ & 1 & \bar{1} & 2_{xy}' & m_{xy}' & \} & & g_1^{dc} = 1 \\
\mathbf{F}g_2^{dc}\mathbf{F} = \{ & 2_z & m_z & 2_{\bar{x}y}' & m_{\bar{x}y}' & \} & & g_2^{dc} = 2_z \\
\mathbf{F}g_3^{dc}\mathbf{F} = \{ & 2_y' & 4_z & \bar{4}_z & m_y' & & & \\
 & 2_x' & 4_z^3 & m_x' & \bar{4}_z^3 & \} & & g_3^{dc} = 2_y'
\end{array}$$

where there are three double cosets, the third consisting of a set of two cosets.

Two domain pairs $\{S_i,S_j\}$ and $\{S_{i'},S_{j'}\}$ belong to the same double coset class of domain pair if there exists an element g of **G** such that $\{gS_i,gS_j\} = \{S_{i'},S_{j'}\}$. All domain pairs belonging to the same double coset class also belong to the same tensor class of domain pair. However, domain pairs that belong to *different* double coset classes may also belong to the same tensor class of domain pair. For example, in a phase transition between $\mathbf{G} = 2_x2_y2_z$ and $\mathbf{F} = 1$, where $S_2=2_xS_1$, $S_3=2_yS_1$, and $S_4=2_zS_1$, the two domain pairs $\{S_1,S_2\}$ and $\{S_1,S_3\}$ belong to two different double coset classes of domain pair. In this case, in Equations (2) we have $F_i = F_{i'} = 1$, $g_{ij} = 2_x$, and $g_{i'j'} = 2_y$. With $r = 2_{xy}$, Equations (2) are satisfied and these two domain pairs belong to the same tensor class of domain pair.

Computer software exists to calculate the double coset classification of domain pairs for both non-magnetic[44] and magnetic[9] point groups. These tabulations also provide indexing and point group symmetry of the domain states, permutations of the domain states under the elements of G, and domain pair characterizing groups, as well as the double coset classification of the domains. The number of double coset classes of domain pairs $\{S_i,S_j\}$ is equal to the number of double cosets in the double coset decomposition of **G** with respect to **F**. A list of one representative double coset from each class of double cosets is $\{S_1, g_i^{dc}S_1\}$, i = 1, 2, … , m , where m is the number of double cosets in equation (3). For example, if $\mathbf{G} = \mathbf{4_z/m_zm_x'm_{xy}'}$ and $\mathbf{F} = \mathbf{2_{xy}'/m_{xy}'}$, then there are three classes whose representative domain pairs are $\{S_1,S_1\}$, $\{S_1,S_2\}$, and $\{S_1,S_3\}$.

Pairs of domains $\{S_i,S_j\}$ are characterized by two groups, the *symmetry group* and *twinning group* of the domain pair. The symmetry group $\mathbf{J}_{ij}$ of the domain pair $\{S_i,S_j\}$ is defined by

$$\mathbf{J}_{ij} = \mathbf{F}_{ij} + g_{ij}^* \, \mathbf{F}_{ij} \qquad (4)$$

where $\mathbf{F}_{ij} = \mathbf{F}_i \bigcap \mathbf{F}_j$ consists of all elements that simultaneously leave both domain states invariant and g_{ij}^* which interexchanges the two domain states, i.e. $g_{ij}^*S_i = S_j$ and $g_{ij}^*S_j = S_i$. The twinning group[45] $\mathbf{K}_{ij}$ of a domain pair $\{S_i,S_j\}$ is defined by

$$\mathbf{K}_{ij} = < \mathbf{F}_i \, , g_{ij} > \qquad (5)$$

where $\mathbf{F}_i$ is the point group of S_i and $g_{ij}S_i = S_j$, and is the group generated by g_{ij} and the elements of the group $\mathbf{F}_i$.

For every magnetic point group **G**, subgroup **F** and representative domain pair $\{S_1, g_i^{dc}S_1\}$, i = 2, 3, … , m there exist tabulations of the domain pair's symmetry group and twinning group[9,44]. The case i = 1 is not considered as the corresponding domain pair $\{S_i,S_j\}$ consists of identical domain states. We consider only one domain pair from each class because the relative spatial orientations is the same for the two domain states in each domain pair of a single class[46]. For example, for $\mathbf{G} = \mathbf{4_z/m_zm_x'm_{xy}'}$ and $\mathbf{F} = \mathbf{2_{xy}'/m_{xy}'}$, for the domain pairs $\{S_1,S_2\}$, and $\{S_1,S_3\}$ one has[44]:

	$\{S_1, g_i^{dc}S_1\}$	$\mathbf{J}_{ij} = \mathbf{F}_{ij} + g_{ij}{}^* \mathbf{F}_{ij}$	$\mathbf{K}_{ij} = < \mathbf{F}_i , g_{ij} >$
i = 2	$\{S_1,S_2\}$	$\mathbf{m_z m_{xy}' m_{\bar{x}y}}' = \mathbf{2_{xy}'/m_{xy}'} + 2_z\mathbf{2_{xy}'/m_{xy}'}$	$\mathbf{m_z m_{xy}' m_{\bar{x}y}}' = <\mathbf{2_{xy}'/m_{xy}'}, 2_z>$
i = 3	$\{S_1,S_3\}$	$\mathbf{2_y/m_y} = \bar{\mathbf{1}} + 2_y' \bar{\mathbf{1}}$	$\mathbf{m_z m_{xy}' m_{\bar{x}y}}' = <\mathbf{2_{xy}'/m_{xy}'}, 2_z>$

Note that the tensor distinction of a domain pair $\{S_i,S_j\}$ is determined by the domain pair's twinning group. The form T_i of a tensor of type **T** in the first domain S_i is that form of **T** invariant under $\mathbf{F_i}$, the symmetry group of the first domain. In the second domain S_j , the form T_j of the tensor **T** is given by $T_j = g_{ij}T_i$. If the element g_{ij} leaves T_i invariant, then the tensor can not distinguish between the two domains of the domain pair. If the element g_{ij} does not leave T_i invariant, then the tensor can distinguish between the two domains of the domain pair. Another way of interpreting this condition for the distinction of two domains is: If the form of a tensor of type **T** invariant under $\mathbf{F}_i$ is (is not) also invariant under $\mathbf{K}_{ij}$ then the tensor of type **T** can not (can) distinguish between the domains of a domain pair $\{S_i,S_j\}$.

To tabulate all tensor classes of domain pair $\{S_i,S_j\}$ one tabulates the group $\mathbf{F}_i$ and element g_{ij} of one domain pair from each tensor class of domain pairs. This has been done for non-magnetic point groups where one finds 139 tensor classes of non-magnetic domain pair $\{S_i,S_j\}$[47] . In Table 3 we list the twenty-two tensor classes of domain pair where $\mathbf{F_i}$ is a point group of the type **222** or **mm2**. 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 reference 48 because of the tensor classification scheme used here.) Those without an asterisk are tensor classes of ferroelastic domain pairs. Also listed is the twinning group $\mathbf{K_{ij}}$ and for each of these classes, what is the tensor distinction for seven types of physical property tensors: e enantiomorphism; V spontaneous polarization; $e[V^2]$ optical activity; $V[V^2]$ piezoelectricity; $eV[V^2]$ electrogyration; $[[V^2]^2]$ linear elasticity; and $[V^2]^2$ piezoptics . "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, and "Z" denotes that the tensor is identically zero in both domains.

The purpose of the above classification of domain pairs into tensor classes is to provide a classification in which one can determine whether or not a tensor of a specific tensor type can or cannot distinguish between the domains of the domain pair. If a tensor of a specific type can distinguish between the domains, then subsequently one would wish to know which components are the same and which are different in the two domains. This additional problem we shall refer to as *tensor component distinction*. While we do not intend to focus on this problem here, the above classification of domain pairs into tensor classes has been chosen to take the tensor component distinction problem into account. For two pairs of domain pairs belonging to the same tensor class of domain pair there exist coordinate systems for each pair where the tensor component distinction is the same. That is, if a specific component is the same (different) within the domains of the first domain pair, the identical component is the same (different) within the domains of the second pair. It is for this reason that a tensor classification has been defined where domain pairs belonging to classes #69 and #70 are in distinct classes even though the identical groups $\mathbf{F}_i$ and $\mathbf{K}_{ij}$ are associated with them (And consequently the tensor distinction of domain pairs belonging to both these classes is identical.) The tensor *component* distinction of domain pairs of these two classes is different:

Consider the polarization tensor ***P*** and two domain pairs, a domain pair of tensor class #69 with

$\mathbf{F}_i = \mathbf{m_{\bar{x}y} m_z 2_{xy}}$, $g_{ij} = m_{\bar{x}z}$ and $\mathbf{K}_{ij} = \mathbf{m_z \bar{3}_{xyz} m_{xy}}$ $\qquad P_i = (P,P,0) \quad P_j = (0,P,P)$

and a domain pair of tensor class #70 with

$\mathbf{F}_i = \mathbf{m_{\bar{x}y} m_z 2_{xy}}$, $g_{ij} = 2_{\bar{y}z}$ and $\mathbf{K}_{ij} = \mathbf{m_z \bar{3}_{xyz} m_{xy}}$ $\qquad P_i = (P,P,0) \quad P_j = (-P,0,-P)$.

While polarization does distinguish between the domains in both domain pairs, since both have the same $\mathbf{F_i}$ and $\mathbf{K_{ij}}$, the tensor component distinction is distinct. Comparing the polarization tensors in the domains of the domain pair of tensor class #69 one finds that one component remains the same while the remaining two interexchange, while in the domains of the domain pair of tensor class #70 all three components change.

While a complete list of the 139 tensor classes of non-magnetic domain pairs has been derived, given in terms of 139 non-magnetic twinning laws, there is no complete list in the case of magnetic domain pairs. Only special cases have been considered. One such case is when the twinning group consists of two coset,

$$\mathbf{K}_{ij} = < \mathbf{F}_i , g_{ij} > = \mathbf{F}_i + g_{ij} \mathbf{F}_i \qquad (6)$$

where the element g_{ij} not only transforms S_i into S_j of the domain pair $\{S_i,S_j\}$ but also transforms S_j into S_i (this element interexchanges the two domains of the domain pair and consequently could be denoted as in the symmetry group, equation (4), as g_{ij}*). Such twinning groups are called *completely transposable* twinning groups or twinning laws[49] (Previously, this was referred to as an ambivalent twin law[50].) The point groups of the two domains S_i and S_j of a domain pair $\{S_i,S_j\}$ having a completely transposable twinning group are the same, i.e. :

$$\mathbf{F_j} \equiv g_{ij}\mathbf{F_i}g_{ij}^{-1} = \mathbf{F_i}$$

The completely transposable twinning group is uniquely characterized by the group $\mathbf{K_{ij}}$ and the group $\mathbf{F_i}$, *a subgroup of index two* of $\mathbf{K_{ij}}$.

Completely transposable non-magnetic twin laws have been used in determining macroscopic tensorial physical properties that distinguish domains of a domain pair in the cases of non-ferroelastic and ferroelectric non-ferroelastic domains[48,49]. Because $\mathbf{F_i}$ is a subgroup of index two of $\mathbf{K_{ij}}$, the mathematical structure of non-magnetic completely transposable twinning groups is the same as that of black and white (dichromatic, anti-symmetry) groups and magnetic groups[8,12]. For example, consider the non-magnetic completely transposable twinning group

$$\mathbf{4_z2_x2_{xy}} = \mathbf{4_z} + 2_x \mathbf{4_z}$$

where the elements of $\mathbf{F_i} = \mathbf{4_z} = \{ 1,\ 4_z,\ 2_z,\ 4_z^{-1} \}$ leave invariant both of the domains of the domain pair $\{S_i,S_j\}$, and the elements of the second coset $g_{ij}\mathbf{F_i} = 2_x\, \mathbf{4_z} = \{ 2_x,\ 2_y,\ 2_{xy},\ 2_{\bar{x}y} \}$ interexchange the two domains. This non-magnetic completely transposable twinning group has been given the symbol $\mathbf{4_z2_x'2_{xy}'}$, where an unprimed symbol as $\mathbf{4_z}$ denotes that the element 4_z leaves both domains invariant, and a primed symbol as $\mathbf{2_x'}$ denotes that the element 2_x interexchanges the two domains of the domain pair[48]. With the possibility of confusing this type of symbol with that of a magnetic point group, we do not use it. Instead one could replace the prime with an asterisk, e.g. $\mathbf{4_z2_x{*}2_{xy}{*}}$, where the asterisk now denotes that the symbol denotes an element which interexchanges the two domains.

We use a double group notation $\mathbf{K_{ij}}$ [$\mathbf{F_i}$] for completely transposable twinning groups and have tabulated the 380 classes of magnetic completely transposable twinning groups[51]. Let **Q** denote one of the 32 types of non-magnetic point groups, there are six types of magnetic completely transposable twinning groups

1:	**Q**[**H**]	2:	**Q**1'[**Q**]	3:	**Q**1'[**H**1'] = **Q**[**H**]**1'**
4:	**Q**1'[**Q**(**H**)] = **Q**(**H**)**1'***	5:	**Q**(**H**)[**H**]	6:	**Q**(**H**)[**K**(**N**)]

(7)

where **H** and **K** are subgroups of index 2 of **Q**, and **N** is a subgroup of index **2** of **K,** a prime denotes time inversion and an asterisk denotes that an element interexchanges the two domains.. Representative twinning groups of classes belonging to the family of **Q** = **222** are

6.1	1	$\mathbf{2_x2_y2_z}[\mathbf{2_z}]$	$\mathbf{2_x{*}2_y{*}2_z}$	$\mathbf{2_x2_y2_z\{2_z\}}$
6.2	2	$\mathbf{2_x2_y2_z1'}[\mathbf{2_x2_y2_z}]$	$\mathbf{2_x2_y2_z1'{*}}$	$\mathbf{2_x2_y2_z1'{*}}$
6.3	3	$\mathbf{2_x2_y2_z1'}[\mathbf{2_z1'}]$	$\mathbf{2_x{*}2_y{*}2_z\ 1'}$	$\mathbf{2_x2_y2_z\{2_z\}1'}$

(8)

6.4	4	$\mathbf{2_x2_y2_z1'}[\,2_x'2_y'2_z]$	$\mathbf{2_x'2_y'2_z1'*}$	$\mathbf{2_x2_y2_z(2_z)1'*}$
6.5	5	$\mathbf{2_x'2_y'2_z[2_z]}$	$\mathbf{2_x'*2_y'*2_z}$	$\mathbf{2_x2_y2_z(2_z)\{2_z\}}$
6.6	6	$\mathbf{2_x'2_y'2_z[2_x']}$	$\mathbf{2_x'2_y'*2_z*}$	$\mathbf{2_x2_y2_z(2_z)\{2_x(1)\}}$

The first column gives a sequential numbering.
The second column gives the type of the twinning group with the numbering given in equation (7).
The third column gives the double group notation $\mathbf{K_{ij}}$ $[\mathbf{F_i}]$.
The fourth column gives a single group notation $\mathbf{K_{ij}}$ where a prime denotes time inversion and an asterisk denotes that the element interexchanges the two domains.

The mathematical structure of magnetic completely transposable twinning groups is the same as that of the so-called double anti-symmetry groups introduced by Zamorzaev & Sokolov[52-54], where the prime and asterisk here are the analogous double anti-symmetries. Double anti-symmetry point groups are defined in the following context: All points of a finite object are assigned two signs, each of which can take one of two values usually interpreted as a plus or minus sign. In addition to the point group transformations of the unsigned finite object, one defines transformations of the signs, a transformation 1' which reverses the value of the first sign and 1* which reverses the value of the second sign. A double anti-symmetry point group is an invariance group of such a signed finite object, i.e. the group of those point group transformations and point group transformations coupled with 1', 1* , or 1'* which leave the signed finite object invariant. By interpreting time inversion 1' and interexchanging of domains 1* as sign reversing transformations, a magnetic completely transposable twinning group becomes a double anti-symmetry group. In the fifth column in (8) we list the standard double anti-symmetry notation for the groups. The format of this notation is $\mathbf{A}(\mathbf{B})\{\mathbf{C}\}$ where $\mathbf{B}$ is the subgroup of index 2 of $\mathbf{A}$ of elements which are not primed, and $\mathbf{C}$ is the subgroup of index 2 of $\mathbf{A}$ of elements which do not have an asterisk.

Of the 380 magnetic completely transposable twinning groups, 141 are non-ferroelastic magnetoelectric twinning groups[55]. That is, twinning groups of domain pairs where the two domains have the same (zero) spontaneous deformation tensor (they are non-ferroelastic) and have distinct magnetoelectric tensors. For a domain pair with the non-ferroelastic magnetoelectric twinning group $K_{ij}[F_i]$ = $\mathbf{4_z2_x'2_{xy}'[4_z]}$, in Table 4, we give the form of eight tensor types in the two domains . Note that the spontaneous deformation tensor $[V^2]$ is the same in both domains and the magnetoelectric tensor aeV^2 is distinct.

4. DOMAIN TENSORS AND TENSOR COVARIANTS

In describing the physical properties of crystals by tensors, the components of the tensors are usually given in a cartesian coordinate system[14]. However, in relating these components to parameters that drive phase transitions, it is more appropriate and revealing to relate these cartesian components first to what are called *tensorial covariants*[56]. Tensorial covariants are linear combinations of the cartesian components of tensors which transform as sets of basis functions of irreducible representations of the point group **G** in a phase a phase transition from a high symmetry phase with point group **G** to a lower symmetry phase of point group **F**[57]. These have been calculated[57,58]. Extensive tables have been given by Kopsky[59] which enable one to calculate the cartesian components of physical property tensors in domains, which arise in a phase transition from **G** to **F**, in terms of tensor covariants.

For example, in the phase transition from $\mathbf{G} = \mathbf{m_z\,\bar{3}_{xyz}\,m_{xy}}$ to $\mathbf{F} = \mathbf{m_xm_ym_z}$, which corresponds to phase transitions in lead zirconate[60] and cesium lead chloride[61] , the cartesian components of the spontaneous deformation tensor, "u" in the notation of Kopsky[57], in terms of its tensorial covariants in the domain invariant under $\mathbf{F} = \mathbf{m_xm_ym_z}$ are given by:

$$u_{xx} = u^+_1/3-u^+_{3x}/3 +u^+_{3y}/\sqrt{3} \qquad u_{xy} = u_{yx} = 0$$
$$u_{yy} = u^+_1/3-u^+_{3x}/3 -u^+_{3y}/\sqrt{3} \qquad u_{xz} = u_{zx} = 0$$
$$u_{zz} = u^+_1/3+u^+_{3x}/3 \qquad u_{yz} = u_{zy} = 0$$

where u^+_1 is invariant under $\mathbf{G} = \mathbf{m_z}\,\bar{\mathbf{3}}_{\mathbf{xyz}}\,\mathbf{m_{xy}}$, transforms as a basis function of the identity representation of **G**, and { u^+_{3x} , u^+_{3y} } transform as a set of basis functions for the Γ_3^+ irreducible representation of **G**. Knowing how the tensorial covariants transform under elements of $\mathbf{m_z}\,\bar{\mathbf{3}}_{\mathbf{xyz}}\,\mathbf{m_{xy}}$ allows one to calculate the components of this tensor in each of the six domains which arise in this phase transition. The non-zero components are:

	u_{xx}	u_{yy}	u_{zz}
S_1	$u^+_1/3-u^+_{3x}/3+u^+_{3y}/\sqrt{3}$	$u^+_1/3-u^+_{3x}/3-u^+_{3y}/\sqrt{3}$	$u^+_1/3+u^+_{3x}/3$
S_2	$u^+_1/3+u^+_{3x}/3$	$u^+_1/3-u^+_{3x}/3+u^+_{3y}/\sqrt{3}$	$u^+_1/3-u^+_{3x}/3-u^+_{3y}/\sqrt{3}$
S_3	$u^+_1/3-u^+_{3x}/3-u^+_{3y}/\sqrt{3}$	$u^+_1/3+u^+_{3x}/3$	$u^+_1/3-u^+_{3x}/3+u^+_{3y}/\sqrt{3}$
S_4	$u^+_1/3-u^+_{3x}/3-u^+_{3y}/\sqrt{3}$	$u^+_1/3-u^+_{3x}/3+u^+_{3y}/\sqrt{3}$	$u^+_1/3+u^+_{3x}/3$
S_5	$u^+_1/3+u^+_{3x}/3$	$u^+_1/3-u^+_{3x}/3-u^+_{3y}/\sqrt{3}$	$u^+_1/3-u^+_{3x}/3+u^+_{3y}/\sqrt{3}$
S_6	$u^+_1/3-u^+_{3x}/3+u^+_{3y}/\sqrt{3}$	$u^+_1/3+u^+_{3x}/3$	$u^+_1/3-u^+_{3x}/3-u^+_{3y}/\sqrt{3}$

In general[59] it can be shown that in this phase transition only a tensor, as a tensor of the type u, with tensorial covariants which transform as a set of basis functions for the Γ_3^+ can distinguish between all six domains. That is, only these tensors are fully ferroic in Aizu's classification[38]. One can also find general relationships among the cartesian components from such tables, e.g. from the above,

$$u_{xx}(S_1) = u_{yy}(S_2) = u_{zz}(S_3) = u_{yy}(S_4) = u_{zz}(S_5) = u_{xx}(S_6)$$
$$u_{yy}(S_1) = u_{zz}(S_2) = u_{xx}(S_3) = u_{xx}(S_4) = u_{yy}(S_5) = u_{zz}(S_6)$$
$$u_{zz}(S_1) = u_{xx}(S_2) = u_{yy}(S_3) = u_{zz}(S_4) = u_{xx}(S_5) = u_{yy}(S_6)$$

If the phase transition is driven by a parameter which does not transform as or couple with a basis function of Γ_3^+ then in the lower symmetry phase $u^+_{3x} = u^+_{3y} = 0$ and $u_{11}(S_i) = u_{22}(S_i) = u_{33}(S_i)$ for i = 1, 2, … , 6.

5. DOMAIN AVERAGE ENGINEERING OF FERROICS

Multidomain samples of ferroics (ferroelectrics, ferroelastics and related materials) can give rise to new macroscopic properties. In *domain-average-engineered* samples of ferroic crystals the specimen is subdivided into a very large number of domains, representing μ domain states where μ is smaller than the theoretically allowed maximum number n, see Equation (1), and forming a regular or irregular pattern. Its response to external fields is roughly described by tensorial properties averaged over all involved domain states. An example of domain average engineering is the piezoelectric properties of PZN-PT single crystals poled along one of the {001} directions[62-64]. Assuming that the material went through the phase transition from $\mathbf{G} = \mathbf{m}\bar{\mathbf{3}}\mathbf{m}$ to $\mathbf{F} = \mathbf{3m}$, poling along [100] supports the coexistence of four domain states with spontaneous polarization along the directions [111], $[1\bar{1}1]$, $[11\bar{1}]$ and $[1\bar{1}\bar{1}]$, with equal probability. The effective symmetry of a domain-average-engineered system is given by a point group.

The classification of subsets of domains and the determination of the effective symmetry point group of a domain-average-engineered sample has been given by Fousek, Litvin, & Cross[65] : We consider a phase transition from a phase of higher point group symmetry **G** to a phase of lower point group symmetry **F**. Two subsets of domains $\{S_1, S_2, ..., S_\mu\}$ and $\{S'_1, S'_2, ..., S'_\mu\}$ are said to belong to the same class of subsets of domains if there exists and element g of **G** such that $g\{S_1, S_2, ..., S_\mu\} = \{gS_1, gS_2, ..., gS_\mu\}= \{S'_1, S'_2, ..., S'_\mu\}$. The symmetry group **H** of a subset of domains $\{S_1, S_2, ..., S_\mu\}$ is defined as the group of all elements g of **G** which leave the set invariant, i.e. $g\{S_1, S_2, ..., S_\mu\}$ =

$\{S_1, S_2, ..., S_\mu\}$. The group **H** represents the effective symmetry of the domain–average–engineered system consisting of the subset of domains $\{S_1, S_2, ..., S_\mu\}$.

As an example, we consider the phase transition from $\mathbf{G} = \mathbf{m\bar{3}m}$ to $\mathbf{F} = \mathbf{3_{xyz}}\, m_{\bar{x}y}$ **.** Here n = 8. The indexing of the domain states, the corresponding coset representatives of the coset decomposition of **G** with respect to **F**, the symmetry groups, and the corresponding polarizations in each domain state are given in Table 5. All subsets of these domain states have been classified into classes as defined above. In Table 6 we list one subset of domain states from each class. Each subset is denoted by listing, between square brackets, the indices of the domain states contained in that subset, the indices having been given in Table 5, e.g. the subset $\{S_1, S_3, S_5\}$ is denoted by [135]. In the right-hand column is the subgroup **H** of elements of **G** which leave the corresponding subset invariant. This table, in fact, represents the list of domain-average-engineered systems which can arise in a material undergoing a phase transition from $\mathbf{m\bar{3}m}$ to **3m** .

In Table 6 only one domain is listed from each class. In the class of four domains whose representative domain, listed in Table 6, is [1368] are a total of 6 sets of four domains: (A computer program to calculate the properties of the classification of subsets of domains, including listing all subsets of each class, has been developed by Shaparenko, Schlessman, & Litvin[66] .)

Subset of Domains	Symmetry H of Subset
[1278]	$\mathbf{4_x m_y m_{yz}}$
[1368]	$\mathbf{4_z m_x m_{xy}}$
[1467]	$\mathbf{4_y m_x m_{xz}}$
[2358]	$\mathbf{4_y m_x m_{xz}}$
[2457]	$\mathbf{4_z m_x m_{xy}}$
[3456]	$\mathbf{4_x m_y m_{yz}}$

In this class of subsets of four domains is the subset [1278] with corresponding polarizations along the directions [111], $[1\bar{1}1]$, $[11\bar{1}]$ and $[1\bar{1}\bar{1}]$, the set of polarization directions of the example given above. The point group of this subset is $\mathbf{4_x m_y m_{yz}}$ **.**

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Table 1: 122 types of magnetic crystallographic point groups.

1	**11'**					
$\bar{1}$	**$\bar{1}$1'**	**$\bar{1}$'**				
2	**21'**	**2'**				
m	**m1'**	**m'**				
2/m	**2/m1'**	**2'/m**	**2/m'**	**2'/m'**		
222	**2221'**	**2'2'2**				
mm2	**mm21'**	**m'm2'**	**m'm'2**			
mmm	**mmm1'**	**m'mm**	**m'm'm**	**m'm'm'**		
4	**41'**	**4'**				
$\bar{4}$	**$\bar{4}$1'**	**$\bar{4}$'**				
4/m	**4/m1'**	**4'/m**	**4/m'**	**4'/m'**		
422	**4221'**	**4'22'**	**42'2'**			
4mm	**4mm1'**	**4'm'm**	**4m'm'**			
$\bar{4}$2m	**$\bar{4}$2m1'**	**$\bar{4}$'2'm**	**$\bar{4}$'2m'**	**$\bar{4}$2'm'**		
4/mmm	**4/mmm1'**	**4/m'mm**	**4'/mm'm**	**4'/m'm'm**	**4/mm'm'**	**4/m'm'm'**
3	**31'**					
$\bar{3}$	**$\bar{3}$1'**	**$\bar{3}$'**				
32	**321'**	**32'**				
3m	**3m1'**	**3m'**				
$\bar{3}$m	**$\bar{3}$m1'**	**$\bar{3}$'m**	**$\bar{3}$'m'**	**$\bar{3}$m'**		
6	**61'**	**6'**				
$\bar{6}$	**$\bar{6}$1'**	**$\bar{6}$'**				
6/m	**6/m1'**	**6'/m**	**6/m'**	**6'/m'**		
622	**6221'**	**6'2'2**	**62'2'**			
6mm	**6mm1'**	**6'm'm**	**6m'm'**			
$\bar{6}$m2	**$\bar{6}$m21'**	**$\bar{6}$'m'2**	**$\bar{6}$'m2'**	**$\bar{6}$m'2'**		
6/mmm	**6/mmm1'**	**6/m'mm**	**6'/mm'm**	**6'/m'm'm**	**6/mm'm'**	**6/m'm'm'**
23	**231'**					
m$\bar{3}$	**m$\bar{3}$1'**	**m'$\bar{3}$'**				
432	**4321'**	**4'32'**				
$\bar{4}$3m	**$\bar{4}$3m1'**	**$\bar{4}$'3m'**				
m$\bar{3}$m	**m$\bar{3}$m1'**	**m'$\bar{3}$'m**	**m$\bar{3}$m'**	**m'$\bar{3}$'m'**		

Table 2: Physical Property Tensors

Physical Property	Tensor Type	Symbol	Phenomena
Spontaneous Polarization	V	P_i	Pyro-, Ferro-, Ferrielectricity
Spontaneous Magnetization	aeV	M_i	Pyro-, Ferro-, Ferrimagnitism

Spontaneous Deformation	$[V^2]$	ε_{ij}	Pyro-, Ferroelasticity
Electric Susceptibility	$[V^2]$	κ_{ij}	Induced Polarization, Brillouin, Raman, Raleigh scattering
Magnetic Susceptibility	$[V^2]$	χ_{ij}	Induced Magnetization
Magnetoelectric Susceptibility	aeV^2	α_{ij}	Magnetoelectric effect
Piezoelectric Coefficient	$V[V^2]$	d_{ijk}	Piezoelectricity
Piezomagnetic Coefficient	$aeV[V^2]$	g_{ijk}	Piezomagetism
Non-linear Electric Susceptibility	$[V^3]$	κ_{ijk}	Electro-Optic effect, Hyper Raman effect
Non-linear Magnetic Susceptibility	$ae[V^3]$	χ_{ijk}	Magneto-Optic effect
Magnetobielectric coefficient	$aeV[V^2]$	α_{ijk}	Second order magnetoelectric effect
Electrobimagnetic coefficient	$V[V^2]$	β_{ijk}	Second order magnetoelectric effect

Table 3: Tensor classification of domain pairs and tensor distinction.

	$\mathbf{F_i}$	g_{ij}	$\mathbf{K_{ij}}$	e	V	$e[V^2]$	$V[V^2]$	$eV[V^2]$	$[[V^2]^2]$	$[V^2]^2$
53)*	$\mathbf{2_x2_y2_z}$	$\bar{1}$	$\mathbf{m_xm_ym_z}$	Y,	Z,	Y,	Y,	N,	N,	N
54)	$\mathbf{2_x2_y2_z}$	2_{xy}	$\mathbf{4_z2_x2_{xy}}$	N,	Z,	Y,	Y,	Y,	Y,	Y
55)	$\mathbf{2_x2_y2_z}$	m_{xy}	$\mathbf{\bar{4}_z\ 2_xm_{xy}}$	Y,	Z,	Y,	Y,	Y,	Y,	Y
56)	$\mathbf{2_x2_y2_z}$	3_{xyz}	$\mathbf{2_z3_{xyz}}$	N,	Z,	Y,	Y,	Y,	Y,	Y
57)	$\mathbf{2_x2_y2_z}$	$_{xyz}$	$\mathbf{m_z\ \bar{3}_{xyz}}$	Y,	Z,	Y,	Y,	Y,	Y,	Y
58)	$\mathbf{2_{xy}2_y2_z}$	2_z	$\mathbf{4_z3_{xyz}2_{xy}}$	N,	Z,	Y,	Y,	Y,	Y,	Y
59)	$\mathbf{2_{xy}2_y2_z}$	m_z	$\mathbf{m_z\ \bar{3}_{xyz}\ m_{xy}}$	Y,	Z,	Y,	Y,	Y,	Y,	Y
60)	$\mathbf{2_x2_22_z}$	2_1	$\mathbf{6_z2_x2_1}$	N,	Z,	Y,	Y,	Y,	Y,	Y
61)	$\mathbf{2_x2_22_z}$	m_1	$\mathbf{6_z/m_zm_xm_1}$	Y,	Z,	Y,	Y,	Y,	Y,	Y
62)*	$\mathbf{m_xm_y2_z}$	$\bar{1}$	$\mathbf{m_xm_ym_z}$	Z,	Y,	Y,	Y,	N,	N,	N
63)	$\mathbf{m_xm_y2_z}$	m_{xy}	$\mathbf{4_zm_xm_{xy}}$	Z,	N,	Y,	Y,	Y,	Y,	Y
64)	$\mathbf{m_xm_y2_z}$	2_{xy}	$\mathbf{\bar{4}_z\ 2_{xy}m_x}$	Z,	Y,	N,	Y,	Y,	Y,	Y
65)	$\mathbf{m_xm_y2_z}$	2_z	$\mathbf{4_x/m_xm_ym_{yz}}$	Z,	Y,	Y,	Y,	Y,	Y,	Y
66)	$\mathbf{m_xm_y2_z}$	3_{xyz}	$\mathbf{m_z\ \bar{3}_{xyz}}$	Z,	Y,	Y,	Y,	Y,	Y,	Y

67)	$\mathbf{m_{xy}m_y2_z}$	m_z	$\mathbf{\bar{4}_z\, 3_{xyz}m_{xy}}$	Z,	Y,	Y,	Y,	Y,	Y,	Y
68)	$\mathbf{m_{xy}m_y2_z}$	2_z	$\mathbf{m_z\, \bar{3}_{xyz}\, m_{xy}}$	Z,	Y,	Y,	Y,	Y,	Y,	Y
69)	$\mathbf{m_{\bar{x}y}\, m_z\, 2_{xy}}$	$m_{\bar{x}z}$	$\mathbf{m_z\, \bar{3}_{xyz}\, m_{xy}}$	Z,	Y,	Y,	Y,	Y,	Y,	Y
70)	$\mathbf{m_{\bar{x}y}\, m_z\, 2_{xy}}$	$2_{\bar{y}z}$	$\mathbf{m_z\, \bar{3}_{xyz}\, m_{xy}}$	Z,	Y,	Y,	Y,	Y,	Y,	Y
71)	$\mathbf{m_zm_y2_1}$	2_2	$\mathbf{\bar{6}_z\, m_x2_1}$	Z,	Y,	Y,	Y,	Y,	Y,	Y
72)	$\mathbf{m_zm_22_x}$	2_1	$\mathbf{6_z/m_zm_xm_1}$	Z,	Y,	Y,	Y,	Y,	Y,	Y
73)	$\mathbf{m_xm_22_z}$	m_1	$\mathbf{6_zm_xm_1}$	Z,	N,	Y,	Y,	Y,	Y,	Y
74)	$\mathbf{m_xm_22_z}$	2_1	$\mathbf{6_z/m_zm_xm_1}$	Z,	Y,	Y,	Y,	Y,	Y,	Y

Table 4: For the completely transposable magnetic twinning law $K_{ij}[F_i] = \mathbf{4_z2_x'2_{xy}'[4_z]}$ and the eight tensor types listed in the first column, the forms of the tensors T_i and $T_j = 2_x'T_i$ are given in the second and third columns, respectively. The tensor notation used is that of Sirotin & Shaskolskaya[23].

Tensor Type	Domain State S_i T_i	Domain State S_j T_j
V	$\begin{matrix} 0 \\ 0 \\ A \end{matrix}$	$\begin{matrix} 0 \\ 0 \\ -A \end{matrix}$
aeV	$\begin{matrix} 0 \\ 0 \\ A \end{matrix}$	$\begin{matrix} 0 \\ 0 \\ A \end{matrix}$
$[V^2]$	$\begin{matrix} A & 0 & 0 \\ 0 & A & 0 \\ 0 & 0 & B \end{matrix}$	$\begin{matrix} A & 0 & 0 \\ 0 & A & 0 \\ 0 & 0 & B \end{matrix}$
aeV^2	$\begin{matrix} A & C & 0 \\ -C & A & 0 \\ 0 & 0 & B \end{matrix}$	$\begin{matrix} -A & C & 0 \\ -C & -A & 0 \\ 0 & 0 & -B \end{matrix}$
$V[V^2]$	$\begin{matrix} 0 & 0 & 0 & B & A & 0 \\ 0 & 0 & 0 & A & -B & 0 \\ C & C & D & 0 & 0 & 0 \end{matrix}$	$\begin{matrix} 0 & 0 & 0 & B & -A & 0 \\ 0 & 0 & 0 & -A & -B & 0 \\ -C & -C & D & 0 & 0 & 0 \end{matrix}$

$$\mathrm{aeV}[V^2] \qquad \begin{array}{cccccc} 0 & 0 & 0 & B & A & 0 \\ 0 & 0 & 0 & A & -B & 0 \\ C & C & D & 0 & 0 & 0 \end{array} \qquad \begin{array}{cccccc} 0 & 0 & 0 & -B & A & 0 \\ 0 & 0 & 0 & A & B & 0 \\ C & C & D & 0 & 0 & 0 \end{array}$$

$$[V^3] \qquad \begin{array}{cccc} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \\ A & A & B & \end{array} \qquad \begin{array}{cccc} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \\ -A & -A & -B & \end{array}$$

$$\mathrm{ae}[V^3] \qquad \begin{array}{cccc} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \\ A & A & B & \end{array} \qquad \begin{array}{cccc} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \\ A & A & B & \end{array}$$

Table 5: Domain state index, coset representative, symmetry group and polarization.

Index i	Coset Representative g_i	$F_i = g_i F_1 g_i^{-1}$	$P_i = g_i P_1$
1	1	$\mathbf{3_{xyz}\, m_{\bar{x}y}}$	(A, A, A)
2	2_x	$\mathbf{3_{\bar{x}yz}\, m_{\bar{y}z}}$	(A, -A, -A)
3	2_z	$\mathbf{3_{xy\bar{z}}\, m_{\bar{x}y}}$	(-A, -A, A)
4	2_y	$\mathbf{3_{x\bar{y}z}\, m_{\bar{x}z}}$	(-A, A, -A)
5	$\bar{1}$	$\mathbf{3_{xyz}\, m_{\bar{x}y}}$	(-A, -A, -A)
6	m_x	$\mathbf{3_{\bar{x}yz}\, m_{\bar{y}z}}$	(-A, A, A)
7	m_z	$\mathbf{3_{xy\bar{z}}\, m_{\bar{x}y}}$	(A, A, -A)
8	m_y	$\mathbf{3_{x\bar{y}z}\, m_{\bar{x}z}}$	(A, -A, A)

Table 6: Representative subsets of domain states for the species $\mathbf{m\bar{3}m}$ to $\mathbf{3m}$ and the subgroups of $\mathbf{m\bar{3}m}$ which leave them invariant.

Representative subset	Symmetry **H** of the subset
[1] or [2345678]	$\mathbf{3_{xyz}m_{\bar{x}y}}$
[13] or [245678]	$\mathbf{m_{xy}m_{\bar{x}y}2_z}$
[15] or [234678]	$\mathbf{\bar{3}_{xyz}m_{\bar{x}y}}$
[16] or [234578]	$\mathbf{m_x m_{\bar{y}z} 2_{yz}}$
[123] or [45678]	$\mathbf{3_{xyz}m_{xz}}$
[135] or [24678]	$\mathbf{m_{\bar{x}y}}$
[136] or [24578]	$\mathbf{m_{xy}}$
[1234]	$\mathbf{\bar{4}3m}$
[1235]	$\mathbf{m_{\bar{x}z}}$
[1238]	$\mathbf{3_{x\bar{y}z}m_{\bar{x}z}}$
[1356]	$\mathbf{2_{\bar{x}z}}$
[1357]	$\mathbf{m_{xy}m_{\bar{x}y}m_z}$
[1368]	$\mathbf{4_z m_x m_{xy}}$