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# Tensor distinction of domain pairs in ferroic crystals†

Daniel B. Litvin

*Department of Physics, The Pennsylvania State University, Penn State Berks Campus, PO Box 7006, Reading, PA 19610-6009, USA. E-mail: u3c@mail.psu.edu*

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**Abstract**

A classification of domain pairs in ferroic crystals is given in which all domain pairs in each class can be distinguished by the same set of physical property tensors. Tabulations are presented giving in which ferroic phase transitions such domain pairs arise. Whether a physical property tensor can or cannot distinguish between the domains of domain pairs of each class is given for a wide variety of physical properties.

## 1. Introduction

Consider a ferroic phase transition, a phase transition of a crystalline structure from a phase of higher symmetry **G** to a phase of lower symmetry **F** where there is a change in the point-group symmetry. In the lower-symmetry phase, *domains*, volumes of homogeneous crystalline structure oriented in space in a specific manner, arise. If a single domain appears in the lower-symmetry phase, it can appear as any one of $n = |\mathbf{G}|/|\mathbf{F}|$ *single domain states* $S_1, S_2, \ldots, S_n$, 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. The orientations of all single domain states are related by the rotational parts of elements of **G**.

In a polydomain low-symmetry phase, domains appear with the same crystalline structure and various orientations. *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 then represent the structures that appear in a polydomain sample, irrespective of which domain they are in. In nonferroelastic 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 nonferroelastic 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* (Zikmund, 1984; Janovec *et al.*, 1989) which disregards the disorientations. If we disregard the disorientations, the number and orientation of domain states in a ferroelastic polydomain sample also coincide with the number and orientations of single domain states, as in nonferroelastic polydomain samples, and are again related by the rotational parts of the elements of **G**.

Let $\boldsymbol{T_{MPP}}$ denote a macroscopic tensorial physical property. As the mathematical tensorial representation, *i.e.* vector, pseudovector, rank two tensor *etc.*, of more than a single macroscopic tensorial physical property can be the same, we denote by $\boldsymbol{T}$ the type of mathematical tensorial representation corresponding to a macroscopic tensorial physical property. We shall refer to $\boldsymbol{T}$ as a *tensor type*.

We are 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 $\boldsymbol{T}$. As the set of domain states represents the structure of all domains in a polydomain phase, we consider the tensor distinction of the domain states.

We denote by $T_i$, $i = 1, 2, \ldots, n$, the form of the tensors of a tensor type $\boldsymbol{T}$ in the set of domain states of a polydomain sample. The tensors $T_i$, $i = 1, 2, \ldots, n$, 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 $\boldsymbol{T}$ is said to be able to distinguish between two domain states, with corresponding tensors $T_i$ and $T_j$ of the type $\boldsymbol{T}$, 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 $\boldsymbol{T}$ can distinguish among all domain states.

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(*b*) *Domain pair tensor distinction*: For each pair of domain states, we consider whether or not a tensor type $\boldsymbol{T}$ can distinguish between the domain states of the domain pair.

Global tensor distinction is reviewed in §2, and domain pair distinction is presented in §§3 and 4. Both of these distinction problems consider whether or not a tensor as a whole can distinguish domain states. We do not consider whether or not individual components of the tensor distinguish domain states. This latter problem, and its relationship to the work presented in this paper, is discussed in §5.

Because we are considering the tensor distinction of domain states by macroscopic physical property tensors that depend only on the point group of the space-group symmetry of the domain state's structure, we shall now interpret the symbols $\mathbf{G}$ and $\mathbf{F}$ to be the point groups of the higher- and lower-symmetry phases, respectively. Consequently, we begin with a set of domain states $S_1, S_2, \ldots, S_n$ (for typographical simplicity, and because in the parent clamping approximation the number and orientation of the domain states is the same as for single domain states, we use the same symbols for domain states as for single domain states), where $n = |\mathbf{G}|/|\mathbf{F}|$ and where the orientation of the domain states are related by elements of $\mathbf{G}$ not in $\mathbf{F}$: We write the group $\mathbf{G}$ in a left coset decomposition with respect to $\mathbf{F}$ as

$$\mathbf{G} = \mathbf{F} + g_2\mathbf{F} + g_3\mathbf{F} + \ldots + g_n\mathbf{F}, \qquad (1)$$

where the elements $g_i$, $i = 1, 2, \ldots, n$, $g_1 = 1$, are called the *coset representatives* of the coset decomposition of $\mathbf{G}$ with respect to $\mathbf{F}$. 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 $\mathbf{F}$. Defining the domain state $S_1$ as the domain invariant under $\mathbf{F}$, the orientations of the remaining domain states are related to $S_1$ by the coset representatives of equation (1), *i.e.* $S_i = g_i S_1$, $i = 2, 3, \ldots, n$. In addition, each domain state $S_i$, $i = 1, 2, \ldots, n$, is invariant under the group $\mathbf{F}_i \equiv g_i \mathbf{F} g_i^{-1}$.

## 2. Global tensor distinction

Consider a ferroic phase transition of a crystalline structure from a phase of higher symmetry $\mathbf{G}$ to a phase of lower symmetry $\mathbf{F}$. Let $S_1, S_2, \ldots, S_n$ denote the domain states of the lower-symmetry phase, $\boldsymbol{T}$ a tensor type, and tensors $T_i$, $i = 1, 2, \ldots, n$, the form of the tensor type $\boldsymbol{T}$ in the domain states $S_1, S_2, \ldots, S_n$. Following the terminology of Aizu (1970), if the set of tensors $T_i$, $i = 1, 2, \ldots, n$, are all distinct, then we shall say that the tensor $\boldsymbol{T}$ provides a *full* distinction of the domain states $S_i$, $i = 1, 2, \ldots, n$, and the transition is a *full* ferroic phase transition with respect to tensor type $\boldsymbol{T}$. Each domain state is then characterized by a distinct form of tensor type $\boldsymbol{T}$, and macroscopic physical properties of this tensor type can distinguish all domain states. If the set of tensors $T_i$, $i = 1, 2, \ldots, n$, are not all distinct but not all identical, then we shall say that the tensor $\boldsymbol{T}$ provides a *partial* distinction of the domain states, and the transition is a *partial* ferroic phase transition with respect to tensor type $\boldsymbol{T}$. A tensor of type $\boldsymbol{T}$ can then distinguish among some but not all of the domain states. If the set of tensors $T_i$, $i = 1, 2, \ldots, n$, are all identical, then the tensor type $\boldsymbol{T}$ 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 $\boldsymbol{T}$.

Litvin (1984) has subdivided the 'null' case into two: The case where the set of tensors $T_i$, $i = 1, 2, \ldots, n$, are all identically zero, is referred to as *zero* distinction, and only in the case where the set of tensors are all identical and *nonzero* 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 $\mathbf{G}$ and $\mathbf{F}$. Aizu (1979) has introduced four classifications. Two ferroic phase transitions $\mathbf{G}$ to $\mathbf{F}$ and $\mathbf{G}$ to $\mathbf{F}'$ are said to belong to the same class of phase transitions if

(*c*1) $\mathbf{F} = \mathbf{F}'$;

(*c*2) $\mathbf{F}$ and $\mathbf{F}'$ are conjugate subgroups of $\mathbf{G}$ (there is an element $g$ of $\mathbf{G}$ such that $g\mathbf{F}g^{-1} = \mathbf{F}'$);

(*c*3) there is an element $r$ of the three-dimensional rotation group $\mathbf{R}$, not necessarily contained in $\mathbf{G}$, such that $r\mathbf{G}r^{-1} = \mathbf{G}$ and $r\mathbf{F}r^{-1} = \mathbf{F}'$;

(*c*4) $\mathbf{F}$ and $\mathbf{F}'$ belong to the same class of point groups (there is an element $r$ of $\mathbf{R}$ such that $r\mathbf{F}r^{-1} = \mathbf{F}'$).

According to which of the four criteria is used, there are, respectively, 433, 247, 212 or 190 classes of ferroic phase transitions.

In Litvin (1984), the classification with criterion (*c*2) was used. With this classification, it is guaranteed that a ferroic phase transition belonging to the class of $\mathbf{G}$ and $\mathbf{F}$ will have $\mathbf{F}$ as the point-group symmetry of one of its domains. Table 1 gives one example for each of the 247 classes of ferroic phase transitions using criterion (*c*2)† in which we list the groups $\mathbf{F}$ and $\mathbf{G}$. The first column gives a numerical index for the class of ferroic phase transitions and the second and third columns give the corresponding groups $\mathbf{G}$ and $\mathbf{F}$, respectively.

A general method for determining the global tensor distinction for classes of ferroic phase transitions was given by Litvin (1984). A tabulation of the global tensor distinction of all 247 classes of ferroic phase transitions for all tensor types $\boldsymbol{T}$ of rank $n \leq 4$ has been given by Litvin (1985).

† The complete tables have been deposited with the IUCr. These are available from the IUCr electronic archives (Reference: CR0536). Services for accessing these data are described at the back of the journal. The complete tables may also be downloaded from http://www.bk.psu.edu/faculty/Litvin.

Table 1. *The 247 classes of ferroic phase transitions*

The first column gives a numerical index. In the second and third columns, respectively, are the corresponding groups **G** and **F** of one ferroic phase transition **G** to **F** belonging to this class For each pair of groups, in the third through fifth columns, respectively, is the point group **F**, element $g_{ij}$ and twinning group $\mathbf{K}_{ij}$ of one domain pair from each double-coset class of domain pairs that can arise in the ferroic phase transition **G** to **F**. Only those classes are listed for which $\mathbf{F} = \mathbf{2_x2_y2_z}$.

| No. | G | F | $g_{ij}$ | $\mathbf{K}_{ij}$ |
|---|---|---|---|---|
| 27 | $\mathbf{m_xm_ym_z}$ | $\mathbf{2_x2_y2_z}$ | $\bar{1}$ | $\mathbf{m_xm_ym_z}$ |
| 47 | $\mathbf{4_z2_x2_{xy}}$ | $\mathbf{2_x2_y2_z}$ | $2_{\bar{x}y}$ | $\mathbf{4_z2_x2_{xy}}$ |
| 61 | $\mathbf{\bar{4}_z2_xm_{xy}}$ | $\mathbf{2_x2_y2_z}$ | $m_{\bar{x}y}$ | $\mathbf{\bar{4}_z2_xm_{xy}}$ |
| 76 | $\mathbf{4_z/m_zm_xm_{xy}}$ | $\mathbf{2_x2_y2_z}$ | $2_{\bar{x}y}$ | $\mathbf{4_z2_x2_{xy}}$ |
| | | | $\bar{1}$ | $\mathbf{m_xm_ym_z}$ |
| | | | $m_{\bar{x}y}$ | $\mathbf{\bar{4}_z2_xm_{xy}}$ |
| 184 | $\mathbf{2_z3_{xyz}}$ | $\mathbf{2_x2_y2_z}$ | $3_{xyz}$ | $\mathbf{2_z3_{xyz}}$ |
| | | | $3_{xyz}{}^2$ | $\mathbf{2_z3_{xyz}}$ |
| 190 | $\mathbf{m_z\bar{3}_{xyz}}$ | $\mathbf{2_x2_y2_z}$ | $3_{xyz}$ | $\mathbf{2_z3_{xyz}}$ |
| | | | $3_{xyz}{}^2$ | $\mathbf{2_z3_{xyz}}$ |
| | | | $\bar{1}$ | $\mathbf{m_xm_ym_z}$ |
| | | | $\bar{3}_{xyz}$ | $\mathbf{m_z\bar{3}_{xyz}}$ |
| | | | $\bar{3}_{xyz}{}^5$ | $\mathbf{m_z\bar{3}_{xyz}}$ |
| 203 | $\mathbf{4_z3_{xyz}2_{xy}}$ | $\mathbf{2_x2_y2_z}$ | $3_{xyz}$ | $\mathbf{2_z3_{xyz}}$ |
| | | | $3_{xyz}{}^2$ | $\mathbf{2_z3_{xyz}}$ |
| | | | $2_{\bar{x}y}$ | $\mathbf{4_z2_x2_{xy}}$ |
| | | | $2_{\bar{y}z}$ | $\mathbf{4_x2_y2_{yz}}$ |
| | | | $2_{\bar{x}z}$ | $\mathbf{4_y2_x2_{xz}}$ |
| 213 | $\mathbf{\bar{4}_z3_{xyz}m_{xy}}$ | $\mathbf{2_x2_y2_z}$ | $3_{xyz}$ | $\mathbf{2_z3_{xyz}}$ |
| | | | $3_{xyz}{}^2$ | $\mathbf{2_z3_{xyz}}$ |
| | | | $m_{\bar{x}y}$ | $\mathbf{\bar{4}_z2_xm_{xy}}$ |
| | | | $m_{\bar{y}z}$ | $\mathbf{\bar{4}_x2_zm_{yz}}$ |
| | | | $m_{\bar{x}z}$ | $\mathbf{\bar{4}_y2_zm_{xz}}$ |
| 239 | $\mathbf{m_z\bar{3}_{xyz}m_{xy}}$ | $\mathbf{2_x2_y2_z}$ | $3_{xyz}$ | $\mathbf{2_z3_{xyz}}$ |
| | | | $3_{xyz}{}^2$ | $\mathbf{2_z3_{xyz}}$ |
| | | | $2_{\bar{x}y}$ | $\mathbf{4_z2_x2_{xy}}$ |
| | | | $2_{\bar{y}z}$ | $\mathbf{4_x2_y2_{yz}}$ |
| | | | $2_{\bar{x}z}$ | $\mathbf{4_y2_x2_{xz}}$ |
| | | | $\bar{1}$ | $\mathbf{m_xm_ym_z}$ |

## 3. 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 $S_1, S_2, \ldots, S_n$ denote the domain states of the lower-symmetry phase, $\boldsymbol{T}$ a tensor type, and tensors $T_i$, $i = 1, 2, \ldots, n$, the form of tensor type $\boldsymbol{T}$ in the domain states $S_1, S_2, \ldots, S_n$. We now consider all *ordered domain pairs* $\{S_i, S_j\}$, $i, j = 1, 2, \ldots, n$, $i \neq j$. 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, 1957).] 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 $\{S_i, S_j\}$ is determined by the point group $\mathbf{F}_i$ and the element $g_{ij}$ of **G**.

We will classify all possible domain pairs $\{S_i, S_j\}$ into classes where all domain pairs 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 **R** such that:

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

and

$$rg_{1j}r^{-1} = g_{i'j'}f_{i'}, \qquad (2b)$$

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

$$rg_{ij}\mathbf{F}_ir^{-1} = g_{i'j'}\mathbf{F}_{i'}. \qquad (2c)$$

All elements of the coset $g_{ij}\mathbf{F}_i$, *i.e.* all elements of **G** that transform the domain state $S_i$ into the domain state $S_j$, are taken by (2*c*) into all the elements of **G** that transform the domain state $S_{i'}$ into the domain state $S_{j'}$. That equation (2*c*) follows from (2*a*) and (2*b*) is shown in Appendix *A*. In Appendix *B*, we show that this classification of domain pairs is appropriate for the tensor distinction of domain pairs. That is, if two domain pairs belong to the same class of domain pairs, then, if a tensor type can (cannot) distinguish between the first pair of domains, it can (cannot) distinguish between the second pair of domains.

We shall refer to the classes of domain pairs provided by the classification scheme given by equations (2) as *equivalence tensor classes of domain pairs*, or simply as *tensor classes of domain pairs*.

This tensor classification of domain pairs is equivalent to the following classification (Janovec, 1972) of ordered domain pairs (see Appendix *C*): Two domain pairs, $\{S_i, S_j\}$ and $\{S_{i'}, S_{j'}\}$ are said to be in the same class of domain pairs if there exists an element $r$ of the full rotation group **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 $S_i$,

Table 2. *The distinct double-coset classes of domain pairs*

The tensor class, the twinning group $\mathbf{K}_{ij}$ and $\mathbf{F}$ of each double-coset class are given in the first through third columns, respectively. This is followed by an explicit listing of elements of the coset $g_{ij}\mathbf{F}$ and a list of the numerical indicies, from Table 1, of all ferroic phase transitions $\mathbf{G}$ to $\mathbf{F}$ that contain domain pairs of the double-coset class. Only those classes are listed for which $\mathbf{F} = \mathbf{2_x2_y2_z}$.

| Tensor class | $\mathbf{K}_{ij}$ | $\mathbf{F}$ | $g_{ij}\mathbf{F}$ | | | | |
|---|---|---|---|---|---|---|---|
| 53 | $\mathbf{m_xm_ym_z}$ | $\mathbf{2_x2_y2_z}$ | $\bar{1}$ | $m_x$ | $m_y$ | $m_z$ | 27,76,190,239 |
| 54 | $\mathbf{4_z2_x2_{xy}}$ | $\mathbf{2_x2_y2_z}$ | $2_{xy}$ | $2_{\bar{x}y}$ | $4_z$ | ${4_z}^3$ | 47,76,203,239 |
| 54 | $\mathbf{4_x2_y2_{yz}}$ | $\mathbf{2_x2_y2_z}$ | $2_{\bar{y}z}$ | $2_{yz}$ | $4_x$ | ${4_x}^3$ | 203,239 |
| 54 | $\mathbf{4_y2_x2_{xz}}$ | $\mathbf{2_x2_y2_z}$ | $2_{\bar{x}z}$ | $2_{xz}$ | $4_y$ | ${4_y}^3$ | 203,239 |
| 55 | $\mathbf{\bar{4}_z2_xm_{xy}}$ | $\mathbf{2_x2_y2_z}$ | $m_{\bar{x}y}$ | $m_{xy}$ | $\bar{4}_z$ | ${\bar{4}_z}^3$ | 61,76,213,239 |
| 55 | $\mathbf{\bar{4}_x2_zm_{yz}}$ | $\mathbf{2_x2_y2_z}$ | $m_{\bar{y}z}$ | $m_{yz}$ | $\bar{4}_x$ | ${\bar{4}_x}^3$ | 211,239 |
| 55 | $\mathbf{\bar{4}_y2_zm_{xz}}$ | $\mathbf{2_x2_y2_z}$ | $m_{\bar{x}z}$ | $m_{xz}$ | $\bar{4}_y$ | ${\bar{4}_y}^3$ | 213,239 |
| 56 | $\mathbf{2_z3_{xyz}}$ | $\mathbf{2_x2_y2_z}$ | $3_{xyz}$ | ${3_{\bar{x}yz}}^2$ | ${3_{x\bar{y}z}}^2$ | ${3_{xy\bar{z}}}^2$ | 184,190,203,213,239 |
| 56 | $\mathbf{2_z3_{xyz}}$ | $\mathbf{2_x2_y2_z}$ | ${3_{xyz}}^2$ | $3_{\bar{x}yz}$ | $3_{x\bar{y}z}$ | $3_{xy\bar{z}}$ | 184,190,203,213,239 |
| 57 | $\mathbf{m_z\bar{3}_{xyz}}$ | $\mathbf{2_x2_y2_z}$ | $\bar{3}_{xyz}$ | ${\bar{3}_{\bar{x}yz}}^5$ | ${\bar{3}_{x\bar{y}z}}^5$ | ${\bar{3}_{xy\bar{z}}}^5$ | 190,239 |
| 57 | $\mathbf{m_z\bar{3}_{xyz}}$ | $\mathbf{2_x2_y2_z}$ | ${\bar{3}_{xyz}}^2$ | $\bar{3}_{\bar{x}yz}$ | $\bar{3}_{x\bar{y}z}$ | $\bar{3}_{xy\bar{z}}$ | 190,239 |

we do not use a classification of unordered domain pairs. The reasons for this are discussed in §5.

There is a second classification of domain pairs (Janovec, 1972). Because of its relationship to the *double-coset decomposition* of $\mathbf{G}$ with respect to $\mathbf{F}$, we shall refer to it as the classification of domain pairs into *double-coset classes of domain pairs*. 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 $\mathbf{G}$ such that $\{gS_i, gS_j\} = \{S_{i'}, S_{j'}\}$. It follows (see Appendix *D*) that all domain pairs belonging to the same double-coset class also belong to the same tensor class of domain pairs. However, domain pairs that belong to *different* double-coset classes may also belong to the same tensor class of domain pairs. 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 pairs. 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.

To tabulate all tensor classes of domain pairs $\{S_i, S_j\}$, we shall tabulate the group $\mathbf{F}_i$ and element $g_{ij}$ of one domain pairs from each tensor class of domain pairs. However, to determine all tensor classes of domain pairs and also to provide information on which tensor classes of domain pairs arise in which classes of phase transition from a phase of higher symmetry $\mathbf{G}$ to a phase of lower symmetry $\mathbf{F}$, we proceed as follows:

We first consider each of the 247 classes of phase transition between a phase of higher symmetry $\mathbf{G}$ to a phase of lower symmetry $\mathbf{F}$. We consider one such phase transition from each class, the phase transition corresponding to the $\mathbf{G}$ and $\mathbf{F}$ tabulated in Table 1. For each pair of groups $\mathbf{G}$ and $\mathbf{F}$ listed in Table 1, we list the point group $\mathbf{F}_i$ and element $g_{ij}$ of one domain pair $(S_i, S_j)$ from each double-coset class of domain pairs that can arise in such a phase transition. [A complete analysis of the domain pairs in each double-coset class of domain pairs can be found in Schlessman & Litvin (1995).] It has been shown (Wike & Litvin, 1989) that in a phase transition from $\mathbf{G}$ to $\mathbf{F}$ one can always choose from each double-coset class a domain pair with $\mathbf{F}_i = \mathbf{F}$. We do so, and in Table 1 tabulate in the fourth column, for each $\mathbf{G}$ and $\mathbf{F}$, the element $g_{ij}$ of one domain pair from each double-coset class. In the fifth column, we give the group $\mathbf{K}_{ij} = \langle \mathbf{F}_i, g_{ij} \rangle$, the so-called *twinning group* (Janovec *et al.*, 1995) generated by the group $\mathbf{F}_i = \mathbf{F}$ and the element $g_{ij}$. The twinning group will play, as will be seen below, a central role in the computation of the tensor distinction of domain pairs.

In Table 1, many double-coset classes of domain pairs appear more than once, under different classes of phase transitions. Consequently, we give in Table 2 a tabulation of the distinct double-coset classes of domain pairs that appear in Table 1. The groups $\mathbf{K}_{ij}$ and $\mathbf{F}$ are given in the second and third columns, respectively, the sequential listing of Table 2 being given with respect to the groups $\mathbf{F}$. In the fourth column, we give not only the element $g_{ij}$ but a complete list the elements of the coset $g_{ij}\mathbf{F}$, as any element of the coset $g_{ij}\mathbf{F}$ can be taken as the twinning element of the domain pair. In the fifth column, the numerical indices, from Table 1, of all phase transitions $\mathbf{G}$ to $\mathbf{F}$ that contain the double-coset class of domain pairs are given. Not all double-coset classes belong to distinct tensor classes of domain pairs. In the first column of Table 2, we give the numerical index of the tensor class to which the double-coset class of domain pairs belongs.

A listing of the 139 tensor classes of domain pairs is given in Table 3. The tensor class's numerical index is given in the first column. An asterisk is given after the numerical index to denote that the tensor class is nonferroelastic, *i.e.* the two domain states of a domain pair belonging to a nonferroelastic tensor class have the same (zero) spontaneous deformation. The groups $\mathbf{K}_{ij}$, $\mathbf{F}$ and the elements of the coset $g_{ij}\mathbf{F}$, of one domain pair belonging to each tensor class, are given in the second, third and fourth columns, respectively.

Table 3. *The 139 tensor classes of domain pairs*

A numerical index is given in the first column; an asterisk denotes that the tensor class is nonferroelastic. The groups $\mathbf{K}_{ij}$ and $\mathbf{F}$ of one domain pair belonging to each tensor class are given in the second and third columns, respectively. This is followed by the elements of the coset $g_{ij}\mathbf{F}$. Only those classes are listed for which $\mathbf{F} = \mathbf{2_x2_y2_z}$.

| Tensor class | $\mathbf{K}_{ij}$ | $\mathbf{F}$ | $g_{ij}\mathbf{F}$ | | | |
|---|---|---|---|---|---|---|
| 53* | $\mathbf{m_xm_ym_z}$ | $\mathbf{2_x2_y2_z}$ | $\bar{1}$ | $m_x$ | $m_y$ | $m_z$ |
| 54 | $\mathbf{4_z2_x2_{xy}}$ | $\mathbf{2_x2_y2_z}$ | $2_{xy}$ | $2_{\bar{x}y}$ | $4_z$ | $4_z^3$ |
| 55 | $\mathbf{\bar{4}_z2_xm_{xy}}$ | $\mathbf{2_x2_y2_z}$ | $m_{\bar{x}y}$ | $m_{xy}$ | $\bar{4}_z$ | $\bar{4}_z^3$ |
| 56 | $\mathbf{2_z3_{xyz}}$ | $\mathbf{2_x2_y2_z}$ | $3_{xyz}$ | $3_{\bar{x}yz}^2$ | $3_{x\bar{y}z}^2$ | $3_{xy\bar{z}}^2$ |
| 57 | $\mathbf{m_z\bar{3}_{xyz}}$ | $\mathbf{2_x2_y2_z}$ | $\bar{3}_{xyz}$ | $\bar{3}_{\bar{x}yz}^5$ | $\bar{3}_{x\bar{y}z}^5$ | $\bar{3}_{xy\bar{z}}^5$ |

## 4. Tensor distinction of domain pairs

In Table 4, for each of the 139 tensor classes of domain pairs and 22 tensor types of rank $n \leq 4$, we list whether or not tensors of these types can distinguish between the domains of the domain pair. An extensive list of the physical properties corresponding to these tensor types is given in Sirotin & Shaskolskaya (1975).

At the intersection of a row corresponding to a tensor class and a column corresponding to a tensor type is one of three entries:

(i) $Y$, meaning that tensors of that tensor type distinguish between the domains of domain pairs belonging to that tensor class, *i.e.* the tensors $T_i$ and $T_j$ of the domain states $S_i$ and $S_j$ of the tensor pair $\{S_i\, S_j\}$ are nonzero and distinct.

(ii) $N$, meaning that the tensors of the domains of the domain pair are nonzero and identical and cannot distinguish between the domains.

(iii) $Z$, meaning that the tensors of the domains of the domain pair are both identically zero and cannot distinguish between the domains.

For visual simplicity, only $N$ and $Z$ are explicitly given, $Y$ being replaced by an empty entry.

This trichotomy can be determined according to the invariance of the tensor of the type $\boldsymbol{T}$ under the groups $\mathbf{F}$ and $\mathbf{K}$. The tensor $T_i$ is invariant under $\mathbf{F}$ and $T_j = g_{ij}T_i$. If $T_i$ is also invariant under the element $g_{ij}$, it is invariant under the elements of the group $\mathbf{K} = \langle \mathbf{F}, g_{ij} \rangle$. Consequently, the three entries can be interpreted as follows:

(i) $Y$ means that the tensor of type $\boldsymbol{T}$ invariant under $\mathbf{F}$ is not invariant under $\mathbf{K}$.

(ii) $N$ means that the tensor of type $\boldsymbol{T}$ invariant under $\mathbf{F}$ is not identically zero and is also invariant under $\mathbf{K}$.

(iii) $Z$ means that the tensor of type $\boldsymbol{T}$ invariant under $\mathbf{F}$ is identically zero.

## 5. Tensor component distinction

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 $\mathbf{F}$ and $\mathbf{K}$ 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 $\boldsymbol{P}$ and two domain pairs: (i) a domain pair of tensor class 69 with

$$\mathbf{F}_i = \mathbf{m_{\bar{x}y}m_z2_{xy}}, \quad g_{ij} = m_{\bar{x}z} \quad \text{and} \quad \mathbf{K} = \mathbf{m_z\bar{3}_{xyz}m_{xy}}$$
$$P_i = (P, P, 0) \quad \text{and} \quad P_j = (0, P, P);$$

and (ii) a domain pair of tensor class 70 with

$$\mathbf{F}_i = \mathbf{m_{\bar{x}y}m_z2_{xy}}, \quad g_{ij} = 2_{\bar{y}z} \quad \text{and} \quad \mathbf{K} = \mathbf{m_z\bar{3}_{xyz}m_{xy}}$$
$$P_i = (P, P, 0) \quad \text{and} \quad P_j = (-P, 0, -P).$$

While polarization does distinguish between the domains in both domain pairs, since both have the same $\mathbf{F}$ and $\mathbf{K}$, the tensor-component distinction is distinct. Comparing the polarization tensors in the domains of the domain pair of tensor class No. 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 No. 70 all three components change.

## APPENDIX *A*

We show here that equation (2*c*) follows from equations (2*a*) and (2*b*): We first show that, for any element $g_{ij}f_i$ of

$g_{ij}\mathbf{F}_i$, $rg_{ij}f_ir^{-1}$ is contained in $g_{i'j'}\mathbf{F}_{i'}$, *i.e.* that the element $rg_{ij}f_ir^{-1}$ transforms the domain state $S_{i'}$ into the domain state $S_{j'}$:

$$\begin{aligned} rg_{ij}f_ir^{-1}S_{i'} &= rg_{ij}r^{-1}rf_ir^{-1}S_{i'} \\ &= (rg_{ij}r^{-1})(rf_ir^{-1})S_{i'} \\ &= (g_{i'j'}f_{i'})(f'_{i'})S_{i'} \\ &= g_{i'j'}S_{i'} \\ &= S_{j'}. \end{aligned}$$

Consequently, every element of the coset $g_{ij}\mathbf{F}_i$ is transformed by the element $r$ into an element of the coset $g_{i'j'}\mathbf{F}_{i'}$. We next show that every element $g_{i'j'}f_{i'}$ of the coset $g_{i'j'}\mathbf{F}_{i'}$ is obtained from some element of the coset $g_{ij}\mathbf{F}_i$ by a transformation with the element $r$. To do this, we show that $r^{-1}g_{i'j'}f_{i'}r$ is an element of $g_{ij}\mathbf{F}_i$, *i.e.* is an element which transforms the domain state $S_i$ into the domain state $S_j$:

$$\begin{aligned} r^{-1}g_{i'j'}f_{i'}rS_i &= r^{-1}g_{i'j'}rr^{-1}f_{i'}rS_i \\ &= (r^{-1}g_{i'j'}r)(r^{-1}f_{i'}r)S_i \\ &= (g_{ij}r^{-1}f'^{-1}_{i'}r)(r^{-1}f_{i'}r)S_i \\ &= g_{ij}f'_if_iS_i \\ &= g_{ij}S_i \\ &= S_j. \end{aligned}$$

It follows that $rg_{ij}\mathbf{F}_ir^{-1} = g_{i'j'}\mathbf{F}_{i'}$.

## APPENDIX *B*

To show that the classification of domain pairs given by equations (2) is appropriate for the tensor distinction of domain pairs, we show that, if a tensor type can (cannot) distinguish between the first pair of domains, then it can (cannot) distinguish between the second pair of domains:

Assume that two domain pairs $\{S_i, S_j\}$ and $\{S_{i'}, S_{j'}\}$ belong to the same class of domain pair. For a specific tensor type $\boldsymbol{T}$, $T_i$ is invariant under the point group $\mathbf{F}_i$ and $T_j = g_{ij}T_i$. The tensor $rT_i$ is invariant under the point group $\mathbf{F}_{i'}$:

$$f_{i'}(rT_i) = rf_ir^{-1}rT_i = rf_iT_i = rT_i$$

and, consequently, $T_{i'} = rT_i$. In addition, $T_{j'} = rT_j$ since

$$T_{j'} = g_{i'j'}T_{i'} = g_{i'j'}f_{k'}T_{i'} = rg_{ij}r^{-1}rT_i = rg_{ij}T_i = rT_j.$$

Since $T_{i'} = rT_i$ and $T_{j'} = rT_j$, it follows that if $T_i$ and $T_j$ are (are not) distinct, then $T_{i'}$ and $T_{j'}$ are (are not) distinct, and if a tensor type $\boldsymbol{T}$ can (cannot) distinguish between the first pair of domains, then it can (cannot) distinguish between the second pair of domains.

Table 4. *For 22 tensor types and each of the 139 tensor classes is given whether or not physical property tensors of the tensor type can distinguish between domains of domain pairs belonging to the tensor class*

The tensor types are listed in the first column and each column is headed by the index of a tensor class. Only those classes are listed for which $\mathbf{F} = \mathbf{2_x2_y2_z}$. A blank entry denotes that the tensor type can distinguish between the domains. *N* denotes that the tensors are nonzero and cannot distinguish between the domains. *Z* denotes that the tensors are identically zero and cannot distinguish between the domains. $\varepsilon$ denotes a pseudoscalar and *V* denotes a polar vector tensor.

| Tensor type | Tensor class of domain pair | | | | |
|---|---|---|---|---|---|
| | 53* | 54 | 55 | 56 | 57 |
| $\varepsilon$ | | *N* | | *N* | |
| $V$ | *Z* | *Z* | *Z* | *Z* | *Z* |
| $\varepsilon V$ | *Z* | *Z* | *Z* | *Z* | *Z* |
| $[V^2]$ | *N* | | | | |
| $\{V^2\}$ | *Z* | *Z* | *Z* | *Z* | *Z* |
| $V^2$ | *N* | | | | |
| $\varepsilon[V^2]$ | | | | | |
| $\varepsilon\{V^2\}$ | *Z* | *Z* | *Z* | *Z* | *Z* |
| $\varepsilon V^2$ | | | | | |
| $[V^3]$ | | | *N* | *N* | |
| $V[V^2]$ | | | | | |
| $\{V^2\}V$ | | | | | |
| $V^3$ | | | | | |
| $\varepsilon V[V^2]$ | *N* | | | | |
| $\varepsilon\{V^2\}V$ | *N* | | | | |
| $[V^4]$ | *N* | | | | |
| $V[V^3]$ | *N* | | | | |
| $[[V^2]^2]$ | *N* | | | | |
| $[V^2]^2$ | *N* | | | | |
| $[(V^2)^2]$ | *N* | | | | |
| $[V^2]V^2$ | *N* | | | | |
| $V^4$ | *N* | | | | |

## APPENDIX *C*

If $(S_i, S_j)$ and $(S_{i'}, S_{j'})$ belong to the same tensor class of domain pair, then there exists an element $r$ of $\mathbf{R}$ such that $r\mathbf{F}_ir^{-1} = \mathbf{F}_{i'}$, $rg_{ij}r^{-1} = g_{i'j'}f_{i'}$ and $rg_{ij}\mathbf{F}_ir^{-1} = g_{i'j'}\mathbf{F}_{i'}$. Since $r\mathbf{F}_ir^{-1} = \mathbf{F}_{i'}$, we have $rS_i = S_{i'}$ and $rS_j = S_{j'}$ since

$$\begin{aligned} rF_jr^{-1} = r(g_{ij}\mathbf{F}_ig_{ij}^{-1})r^{-1} &= rg_{ij}\mathbf{F}_ir^{-1}rg_{ij}^{-1}r^{-1} \\ = g_{i'j'}\mathbf{F}_{i'}rg_{ij}^{-1}r^{-1} &= g_{i'j'}\mathbf{F}_{i'}g_{i'j'}^{-1}g_{i'j'}rg_{ij}^{-1}r^{-1} \\ = \mathbf{F}_{j'}g_{i'j'}rg_{ij}^{-1}r^{-1} &= \mathbf{F}_{j'}g_{i'j'}f_{i'}^{-1}g_{i'j'}^{-1} \\ = \mathbf{F}_{j'}f_{j'} &= \mathbf{F}_{j'}. \end{aligned}$$

Consequently, $(rS_i, rS_j) = (S_{i'}, S_{j'})$.

Conversely, if $(rS_i, rS_j) = (S_{i'}, S_{j'})$, then $r\mathbf{F}_ir^{-1} = \mathbf{F}_{i'}$ and $rg_{ij}r^{-1} = g_{i'j'}f_{i'}$ since

$$rg_{ij}r^{-1}S_{i'} = rg_{ij}r^{-1}(rS_i) = rg_{ij}S_i = rS_j = S_{j'}.$$

Consequently, $(S_i, S_j)$ and $(S_{i'}, S_{j'})$ belong to the same tensor class of domain pairs.

## APPENDIX *D*

Two domain pairs $\{S_i, Sj\}$ and $\{S_{i'}, S_{j'}\} = \{gS_i, gS_j\}$, which belong to the same double-coset class of domain pair, belong to the same tensor class of domain pair: Let $\mathbf{F}_i$ be the point group of $S_i$ and $g_{ij}S_i = S_j$. From the definition $\{S_{i'}, S_{j'}\} = \{gS_i, gS_j\}$, it follows that $\mathbf{F}_{i'} = g\mathbf{F}_i g^{-1}$ and $g_{i'j'} = gg_{ij}g^{-1}$. Consequently, equation (2*a*) is automatically satisfied, and since

$$gg_{ij}\mathbf{F}_i g^{-1} = (gg_{ij}g^{-1})(g\mathbf{F}_i g^{-1}) = g_{i'j'}\mathbf{F}_{i'},$$

equation (2*c*) is also satisfied. The two domain pairs $\{S_i, S_j\}$ and $\{S_{i'}, S_{j'}\} = \{gS_i, gS_j\}$ then belong to the same tensor class of domain pair.

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