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SHORT COMMUNICATIONS

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Physical-property tensors and tensor pairs in crystals.

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Abstract

The form of physical-property tensors of rank 0, 1 and 2 invariant under the 32 crystallographic point groups and their subgroups are tabulated. This constitutes the basis for the tensorial classification of domain pairs in ferroic crystals which is given *via* a group theoretical classification of the corresponding physical-property tensor pairs. We tabulate this classification of tensor pairs for all physical-property tensors of rank 0, 1 and 2, and domain point-group symmetry.

1. Introduction

A ferroic crystal contains two or more equally stable domains of the same structure but of different spatial orientation. 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 (Aizu, 1973; Newnham, 1974; Newnham & Cross, 1974; Wadhawan, 1982). Aizu (1970; see also Cracknell, 1972) has given a tensorial classification of ferroic crystals based on a rank 1 physical-property tensor's ability to distinguish some or all of the domains. This method of classification of ferroic crystals was extended by Litvin (1984) to an arbitrary physical-property tensor and used to determine the tensorial classification of non-magnetic crystals for all physical-property tensors of rank less than or equal to four (Litvin, 1985).

In the study of the mutual relationships between domains, the simplest object one can consider is a pair of domains. A classification of domain pairs *via* a tensorial classification of corresponding tensor pairs of a *full* physical-property tensor characterizing the domains, where each domain is characterized by a unique form of the physical-property tensor, was introduced by Janovec (1972). This

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Table 1. *The Jahn symbol (Jahn, 1949), rank and name is given for all physical-property tensors of rank 0, 1 and 2*

Jahn symbol	Rank	Name
e	0	Pseudoscalar
V	1	Polar vector
eV	1	Axial vector
V^2	2	Rank two polar tensor
$[V^2]$	2	Symmetric rank two polar tensor
$\{V^2\}$	2	Antisymmetric rank two polar tensor
eV^2	2	Rank two axial tensor
$e[V^2]$	2	Symmetric rank two axial tensor
$e\{V^2\}$	2	Antisymmetric rank two axial tensor

classification scheme was extended by Litvin & Wike (1989) from the case of *full* physical-property tensors to the general case of *partial* physical-property tensors, where more than a single domain is characterized by the same specific form of the physical-property tensor.

In this paper we apply the tensor classification of tensor pairs to the cases of all physical-property tensors of rank 0, 1 and 2, and domain point-group symmetry. We briefly review the physical-property tensors under consideration in § 2, and give, in § 3, the tensor pair classification.

2. Physical-property tensors

A vast amount of literature exists on the derivation and tabulation of the form of physical-property tensors invariant under the crystallographic point groups (Nye, 1957; Birss, 1964; Wooster, 1973; Fumi & Ripamonti, 1980; Sands, 1982; and references contained in these sources). A wide variety of tensors and their physical interpretation are given by Sirotin & Shaskolskaya (1975) and the form of invariant tensors up to eighth rank has been given by Smith (1970).

The tensors considered in this paper are all tensors of rank 0, 1 and 2. These tensors are listed in Table 1, where we give in the first column the Jahn (1949) symbol, the rank in the second column, and the name of the type of tensor in the third column. We have tabulated the form of these tensors invariant under each of the 32 crystallographic point groups, and under all subgroups of the 32 crystallographic point groups.*

This tabulation gives the form of the tensors invariant under all point groups and subgroups of the point groups directly without the need for any additional computations. For example, consider the form of the physical-property tensor V^2 invariant under point groups of type 3. In particular, consider the two point groups belonging to this type: the point group 3_{xyz}, a subgroup of the cubic point group $m\bar{3}m$, and the point group 3_z, a subgroup of the hexagonal point group $6/mmm$. The form of the physical property tensor V^2 invariant under 3_{xyz} and 3_z are, respectively,

$$\begin{pmatrix} A & B & C \\ C & A & B \\ B & C & A \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} A & A-C & 0 \\ C & A & 0 \\ 0 & 0 & B \end{pmatrix},$$

where the former is given in the cubic coordinate system of the point group $m\bar{3}m$, and the latter is given in the hexagonal coordinate system of the point group $6/mmm$. This is in contrast to the standard methodology of listing the form of the physical property tensor V^2 for the point group 3_z only in a Cartesian coordinate system and then requiring the reader himself to transform the coordinate system to obtain the form of the tensor invariant under 3_z in a hexagonal coordinate system or invariant under 3_{xyz}.

3. Tensor pairs

Let G denote the point group of the high-symmetry phase of the crystal and H the point group of one of the domains. We denote by $H^{(i)}$, $i = 1, 2, \ldots, q$, the point groups of each of the domains, with $H^{(1)} = H$. Let **T** denote a spontaneous physical-property tensor which arises in the low-symmetry phase of the crystal. We denote by $T^{(i)}$, $i = 1, 2, \ldots, q$, the specific forms of the tensor **T** characterizing each of the q domains, and denote $T^{(1)} = T$.

In studying the mutual relationships between domain pairs one can study (Janovec, 1972) the mutual relationships between the pairs of tensors which characterize the pairs of domains. All pairs of tensors having the same mutual relationship can be considered as a single class of tensor pairs, and are called a class of crystallographically equivalent tensor pairs (Litvin & Wike, 1989). A single tensor pair, called a representative tensor pair, is chosen from each class to represent the mutual relationship between all tensor pairs in that class. A listing of all representative tensor pairs will then contain all possible mutual relationships. These concepts are explained briefly in the following.

All ordered tensor pairs can be partitioned into classes of crystallographically equivalent tensor pairs: Two tensor pairs $(T^{(i)}, T^{(j)})$ and $(T^{(i')}, T^{(j')})$ are said to be crystallographically equivalent with respect to G and to belong to the same class of ordered tensor pairs, if there is an element g of G such that

$$(T^{(i)}, T^{(j)}) = (gT^{(i')}, gT^{(j')}),$$

that is, if $T^{(i)} = gT^{(i')}$ and $T^{(j)} = gT^{(j')}$.

Let G_T denote the stabilizer of T in G. This subgroup G_T of G is the set of all elements g of G which leave T invariant, *i.e.* $gT = T$. If $G_T = H$ then **T** is a *full* physical-property tensor and there are $q_T = q$ distinct forms of the tensor **T**, *i.e.* each of the q domains is characterized by a distinct form of the tensor **T**. If H is a subgroup of G_T then **T** is a *partial* physical-property tensor and there are $q_T < q$ distinct forms of the tensor **T**. We denote the $q_T \le q$ distinct forms of the tensor **T** by $T_d^{(a)}$, $a = 1, 2, \ldots, q_T$ and choose $T_d^{(1)} = T^{(1)} = T$.

All ordered distinct tensor pairs $(T_d^{(a)}, T_d^{(b)})$ can be partitioned into classes of crystallographically equivalent ordered distinct tensor pairs in the same manner as tensor pairs $(T^{(i)}, T^{(j)})$. The number of classes of ordered distinct

* A computer program on disk for IBM compatible computers titled *Physical Property Tensors and Tensor Pairs in Crystals* is available as SUP 53021 (3 diskettes) through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. This program tabulates the form of physical-property tensors of rank 0, 1 and 2 invariant under the 32 crystallographic point groups and their subgroups, and calculates the tensor pair classes for all these physical property tensors and domain point-group symmetry.

Table 2. *The tensor pair classification of a polar vector physical-property tensor is given for the case of $G = m\bar{3}m$ and $H = 4_x$*

Tensor $\mathbf{T} = V$.
Point group $G = m\bar{3}m$.
Subgroup $H = 4_x$.
Number of domains $= 12$.
Number of distinct domains $= 6$.
Number of tensor pair classes $= 3$.
Stabilizer G_T of T in $G = 4_x m_y m_{yz}$.

Double coset representative	Tensor pair	
1	$\begin{pmatrix} A \\ 0 \\ 0 \end{pmatrix}$	$\begin{pmatrix} A \\ 0 \\ 0 \end{pmatrix}$
2_y	$\begin{pmatrix} A \\ 0 \\ 0 \end{pmatrix}$	$\begin{pmatrix} -A \\ 0 \\ 0 \end{pmatrix}$
3^2_{xyz}	$\begin{pmatrix} A \\ 0 \\ 0 \end{pmatrix}$	$\begin{pmatrix} 0 \\ 0 \\ A \end{pmatrix}$

Table 3. *The tensor pair classification of a rank 2 polar physical-property tensor is given for the case of $G = 4/mmm$ and $H = m_x$*

Tensor $\mathbf{T} = V^2$.
Point group $G = 4/mmm$.
Subgroup $H = m_x$.
Number of domains $= 8$.
Number of distinct domains $= 4$.
Number of tensor pair classes $= 3$.
Stabilizer G_T of T in $G = 2_x/m$.

Double coset representative	Tensor pair	
1	$\begin{pmatrix} A & 0 & 0 \\ 0 & B & D \\ 0 & E & C \end{pmatrix}$	$\begin{pmatrix} A & 0 & 0 \\ 0 & B & D \\ 0 & E & C \end{pmatrix}$
2_y	$\begin{pmatrix} A & 0 & 0 \\ 0 & B & D \\ 0 & E & C \end{pmatrix}$	$\begin{pmatrix} A & 0 & 0 \\ 0 & B & -D \\ 0 & -E & C \end{pmatrix}$
2_{xy}	$\begin{pmatrix} A & 0 & 0 \\ 0 & B & D \\ 0 & E & C \end{pmatrix}$	$\begin{pmatrix} B & 0 & D \\ 0 & A & 0 \\ E & 0 & C \end{pmatrix}$

tensor pairs is the same as the number of classes of tensor pairs. This number is determined by the following theorem (Litvin & Wike, 1989).

Let G be the point group of the high-symmetry phase, H the point group of a domain, and T the specific form of the physical-property tensor $\mathbf{T}$ invariant under H. The number N of crystallographically equivalent ordered distinct tensor pair classes is equal to the number of double cosets in the double coset decomposition of G with respect to G_T:

$$G = G_T e G_T + G_T g_2^{(\mathrm{dc})} G_T + \ldots + G_T g_N^{(\mathrm{dc})} G_T,$$

where G_T is the stabilizer of T in G and $g_k^{(\mathrm{dc})}$, $k = 1, 2, \ldots, N$, are the double coset representatives. The double coset representatives can be found in the work of Janovec, Dvorakova, Wike & Litvin (1989). A representative ordered distinct tensor pair of each class of crystallographically equivalent ordered distinct tensor pairs is given by $(T, g_k^{(\mathrm{dc})} T)$, $k = 1, 2, \ldots, N$.

We have tabulated the representative tensor pairs $(T, g_k^{(\mathrm{dc})} T)$ for all classes of tensor pairs, for all point groups G and subgroups H and all physical-property tensors $\mathbf{T}$ of rank 0, 1 and 2.* Examples of this tabulation are given in Tables 2 and 3. In each table we list the physical tensor $\mathbf{T}$, the point group G, subgroup H, stabilizer G_T, the number of domains, the number of distinct domains and the number N of tensor pair classes. In each case we then list the coset representatives $g_k^{(\mathrm{dc})}$, $k = 1, 2, \ldots, N$, and the representative tensor pairs $(T, g_k^{(\mathrm{dc})} T)$. In the example considered in Table 2, the mutual relationships of domain pairs whose domains are characterized by a polar vector physical-property tensor are readily seen. All domain pairs have corresponding polar vectors which are parallel, anti-parallel or perpendicular.

* See deposition footnote.

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