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Tensorial Classification of Non-magnetic Ferroic Crystals

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Abstract

A group-theoretical method is presented to determine the tensorial classification of ferroic crystals with respect to an arbitrary macroscopic tensorial property. This method is used to derive tables of the tensorial classification in the special case where the components of the tensorial property transform as a single irreducible representation of the prototypic point group. It is also shown how these tables facilitate implementation of this method in the general case. Examples are given of the application of this method and the use of these tables in determining the tensorial classification of ferroelectric and gyrotropic ferroic crystals.

I. Introduction

A ferroic crystal contains two or more equally stable domains of the same structure but of different spatial orientation. These domains, or orientation states, can coexist in a crystal and may be distinguished by the values of components of certain macroscopic tensorial properties of the domains. Under a suitable driving force, the domain walls can be moved and the crystal switched from one orientation state to another (Aizu, 1970, 1972, 1973). Crystals in which the domains may be distinguished by spontaneous polarization, spontaneous magnetization and spontaneous strain are called primary ferroic crystals and named, respectively, ferroelectric, ferromagnetic and ferroeleastic crystals. Switching in these ferroic crystals is accomplished, respectively, by an electric field, a magnetic field and a mechanical stress. Crystals whose domains are characterized by differences in the dielectric permittivity tensor and piezoelectric tensor are examples of secondary ferroic crystals named ferrobielectric and ferroelastoelectric crystals (Aizu, 1973; Newnham & Cross, 1976). Switching is accomplished by an electric field in the former, and by a combination of an electric field and a mechanical stress in the latter. Ferroic crystals have been discussed by Newnham (1974), and secondary ferroic crystals in particular by Aizu (1973), Newnham & Cross (1974*a*, *b*) and Newnham & Skinner (1976).

Aizu (1970, 1976*a*, *b*) has introduced two point-group-classification schemes for ferroic crystals, the classes of which are named respectively 'species' and 'subspecies' of ferroic crystals. These classifications are based on relationships between the point-group symmetries of the domains of a ferroic crystal and the point-group symmetry of the non-ferroic, or 'prototypic' phase of the crystal. In addition, each class of ferroic crystals has in turn been given a tensorial classification according to a macroscopic tensorial property's ability to distinguish between the domains. Aizu has tabulated the species of ferroic crystals, using magnetic point groups, and the tensorial classification of ferroelectric, ferromagnetic and ferroelastic crystals (Aizu, 1970; see also Cracknell, 1972).

In this paper, we shall limit ourselves to consideration of the tensorial classification of non-magnetic ferroic crystals. We shall present a group-theoretical method to determine the tensorial classification of all such ferroic crystals with respect to an arbitrary macroscopic tensorial property. In § II we discuss point-group classifications of crystals with domains and list four possible point-group classifications. Physical reasons are then given for our choice of one of these, the classification corresponding to Aizu's subspecie classification, as the point-group-classification scheme for ferroic crystals to be used in this paper. The tensorial classification is then defined. The criterion to determine the tensorial classification of a ferroic crystal in the general case of an arbitrary macroscopic tensorial property is given in terms of the point groups of the point-group classification of the ferroic crystal.

In § III, a group-theoretical computational method to determine the tensorial classification of a ferroic crystal and an arbitrary macroscopic tensorial property is given. This method is based on the calculation, for a given point group, of the number of independent components of the tensorial property, and is related to the chain-subduction criterion of continuous phase transitions (Goldrich & Birman, 1968; Jaric & Birman, 1977). Tables are presented in § IV to facilitate implementation of the method of § III. Examples are given of the use of these tables in determining the tensorial classification of ferroelectric and gyrotropic ferroic crystals.

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II. Classifications of ferroic crystals

We shall first discuss possible point-group classifications of ferroic crystals. We shall then choose one of these as the point-group-classification scheme of ferroic crystals which we shall use in the remainder of the paper. We then review the additional tensorial classification of ferroic crystals.

A. Point-group classifications

Let $\mathbf{G}$ denote the point-group symmetry of the non-ferroic phase of a ferroic crystal, and let $\mathbf{H}$, a proper subgroup of $\mathbf{G}$ denote the point-group symmetry of one of the domains of the ferroic crystal. The number of domains and the point-group symmetry of each domain can be determined from the two point groups $\mathbf{G}$ and $\mathbf{H}$. Let $|\mathbf{G}|$ and $|\mathbf{H}|$ denote the order of the groups $\mathbf{G}$ and $\mathbf{H}$, respectively. The number n of domains of the ferroic crystal is given by $n = |\mathbf{G}|/|\mathbf{H}|$. The point group $\mathbf{G}$ can be written in a coset decomposition with respect to the proper subgroup $\mathbf{H}$:

$$\mathbf{G} = \mathbf{H} + G_2\mathbf{H} + \ldots + G_n\mathbf{H}. \tag{1}$$

The point-group symmetry of the ith domain is the point group $\mathbf{H}_i = G_i\mathbf{H}G_i^{-1}$, a conjugate subgroup of $\mathbf{H}$ in $\mathbf{G}$ where G_i is the ith coset representative in (1). The choice of the point group $\mathbf{H}$ is arbitrary in the sense that the point-group symmetry $\mathbf{H}$ of one domain may be replaced by the point-group symmetry $\mathbf{H}_i$ of another domain. The number of domains and their symmetry can also be determined from $\mathbf{G}$ and $\mathbf{H}_i$.

To each ferroic crystal one can then associate a pair of point groups, the non-ferroic point group $\mathbf{G}$ and the point group $\mathbf{H}$ of one of its domains, which characterizes the point-group symmetries of the ferroic crystal's domains. Consequently, each ferroic crystal has been assigned a 'ferroic symbol' $\mathbf{G}F\mathbf{H}$ consisting of a symbol F to denote 'ferroic' and the two point groups $\mathbf{G}$ and $\mathbf{H}$ (Aizu, 1970).

A list of ferroic symbols can be compiled by first taking one point group $\mathbf{G}$ from each of the thirty-one classes of point groups excluding the identity point group. Each of these thirty-one point groups is then combined in turn with each proper subgroup $\mathbf{H}$ of $\mathbf{G}$ to form a ferroic symbol $\mathbf{G}F\mathbf{H}$. The identity point group has been excluded as it has no proper subgroups. In such a manner one can compile a list of 433 ferroic symbols.

We shall assume in this paper, the usual implicit assumption, that the non-ferroic point $\mathbf{G}$ of a ferroic crystal has been chosen as one of the thirty-one point groups $\mathbf{G}$ used in compiling the above list of ferroic symbols. Consequently, the ferroic symbol associated with any ferroic crystal can be found in this list of 433 ferroic symbols.

The classifications of ferroic crystals which we discuss below are defined in terms of the classifications of the proper subgroups $\mathbf{H}$ of a point group $\mathbf{G}$. Since each pair of point groups $\mathbf{G}$ and $\mathbf{H}$ determines a ferroic symbol $\mathbf{G}F\mathbf{H}$, we shall speak of classifications of ferroic symbols instead of the proper subgroups $\mathbf{H}$ of $\mathbf{G}$. Four possible classifications of ferroic symbols are as follows. Two ferroic symbols $\mathbf{G}F\mathbf{H}$ and $\mathbf{G}F\mathbf{H}'$ are said to belong to the same class of ferroic symbols if

($c1$) $\mathbf{H} = \mathbf{H}'$ the ferroic symbols are identical;

($c2$) $\mathbf{H}$ and $\mathbf{H}'$ are conjugate subgroups of $\mathbf{G}$. There is an element G of $\mathbf{G}$ such that $G\mathbf{H}G^{-1} = \mathbf{H}'$;

($c3$) 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 $R\mathbf{H}R^{-1} = \mathbf{H}'$;

($c4$) $\mathbf{H}$ and $\mathbf{H}'$ belong to the same class of point groups. There is an element of $\mathbf{R}$ such that $R\mathbf{H}R^{-1} = \mathbf{H}'$.

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

These four classifications of ferroic symbols correspond to Aizu's four classification of the proper subgroups of the thirty-one point groups $\mathbf{G}$ into, respectively, 'rigorous', 'subspecific', 'specific' and 'unique' classes of ferroic point groups (Aizu, 1979). Similar classifications of pairs of point groups have been considered in the context of 'color' point groups (Opechowski, 1980). Considering one point group $\mathbf{G}$ from each of the thirty-two classes of point groups, all proper and improper subgroups $\mathbf{H}$ of $\mathbf{G}$, and the criteria ($c2$) and ($c3$) above, lead respectively to 279 (Litvin, Kotzev & Birman, 1982) and 244 (Koptsik & Kotzev, 1974a, b; Shubnikov & Koptsik, 1974; Harker, 1976) classes of 'color' point groups.

To each ferroic crystal we assign the ferroic symbol $\mathbf{G}F\mathbf{H}$, where $\mathbf{H}$ is the point-group symmetry of one of the ferroic crystal's domains. Classifications of ferroic crystals are defined in terms of the ferroic symbols assigned to the ferroic crystals. Two ferroic crystals with assigned ferroic symbols $\mathbf{G}F\mathbf{H}$ and $\mathbf{G}F\mathbf{H}'$ are said to belong to the same class of ferroic crystals if and only if $\mathbf{G}F\mathbf{H}$ and $\mathbf{G}F\mathbf{H}'$ belong to the same class of ferroic symbols. Consequently, there are 247, 212 or 190 classes of ferroic crystals according to which criteria, ($c2$), ($c3$), ($c4$), is used to classify ferroic symbols. The criterion ($c1$) does not define classes of ferroic symbols which can be used to classify ferroic crystals, since this would lead to a classification of ferroic crystals dependent on which domain's point group is used in the ferroic symbol assigned to the crystal. The class of ferroic crystals to which a specific ferroic crystal belongs, in the three classifications ($c2$)–($c4$) defined above, does not depend on the choice of the domain whose point-group symmetry $\mathbf{H}$ is used to characterize the ferroic crystal. Aizu (1976a, b, 1979) refers to the 247 classes of ferroic crystals, using criterion ($c2$), as subspecies of ferroic crystals, and refers (Aizu, 1969, 1970, 1972) to the 212 classes of ferroic crystals, using criterion ($c3$), as species of ferroic crystals.

In the remainder of this paper we shall use the terminology 'ferroic classes' to refer to the classes of ferroic crystals determined using criterion ($c2$). We shall also denote a ferroic class of crystals by the symbol $\mathbf{G}F\mathbf{H}$ of the class of ferroic symbols to which the ferroic crystals of that ferroic class are assigned. With this classification of ferroic crystals, a ferroic crystal of prototypic point group $\mathbf{G}$ belonging to the ferroic class $\mathbf{G}F\mathbf{H}$ will have $\mathbf{H}$ as the point-group symmetry of one of its domains. Thus, a ferroic crystal belonging to the ferroic class $\mathbf{G}F\mathbf{H}$ can always be characterized by the point groups $\mathbf{G}$ and $\mathbf{H}$.

B. *Tensorial classification*

The domains of a ferroic crystal can possibly be distinguished by the values of the components of a macroscopic tensorial property associated with each of the domains. Whether or not one can distinguish some or all of the domains in such a manner has led to the additional tensorial classification of ferroic crystals (Aizu, 1969, 1970).

Consider a ferroic crystal of the ferroic class $\mathbf{G}F\mathbf{H}$, and a macroscopic tensorial property represented by a q-component tensor $\mathbf{T}$. We shall denote the components of the tensor $\mathbf{T}$ by T_j, $j=1,2,\ldots,q$. The components of the tensor $\mathbf{T}$ transform under elements of the point group $\mathbf{G}$ as basis functions of a q-dimensional representation $D^T_{\mathbf{G}}$ of $\mathbf{G}$, which we shall call a 'tensorial representation' of $\mathbf{G}$:

$$GT_j = \sum_k D^T_{\mathbf{G}}(G)_{kj} T_k. \tag{2}$$

The tensorial representation $D^T_{\mathbf{G}}$ is in general a reducible representation of the point group $\mathbf{G}$. The tensor $\mathbf{T}$ is said to be invariant under an element G of the group $\mathbf{G}$ if there exists a set $\{T_j\}$ of non-zero values of the components T_j, $j=1,2,\ldots,q$ such that $GT_j = T_j$, $j=1,2,\ldots,q$. The tensor $\mathbf{T}$ is said to be invariant under a subgroup $\mathbf{A}$ of $\mathbf{G}$, if there exists a set of non-zero components simultaneously invariant under all elements of $\mathbf{A}$.

Consider a ferroic crystal belonging to the ferroic class $\mathbf{G}F\mathbf{H}$, and a tensor $\mathbf{T}$ representing a macroscopic tensorial property invariant under $\mathbf{H}$. We shall assume that the set $\{T_j\}$ of values of the components of $\mathbf{T}$ invariant under the point-group symmetry $\mathbf{H}$ of one of the ferroic crystals' domains is the most general set of values allowed by symmetry (Nye, 1964). The sets of values of the components of the tensor $\mathbf{T}$ characterizing the n domains of the ferroic crystal are

$$\{T_j\}, \{G_2T_j\}, \ldots, \{G_nT_j\}, \tag{3}$$

where G_i, $i=2,3,\ldots,n$ are coset representatives of the coset decomposition, (1) of $\mathbf{G}$ with respect to $\mathbf{H}$, and the sets of values $\{G_iT_j\}$, $i=2,3,\ldots,n$ are obtained from the set of values $\{T_j\}$ using (2).

Ferroic crystals are classified into one of three tensorial classes with respect to a tensor $\mathbf{T}$ according to one's ability to distinguish the domains by considering only the values of the components of $\mathbf{T}$. Ferroic crystals of a ferroic class $\mathbf{G}F\mathbf{H}$ are said to belong to a

(1) 'full' ferroic class with respect to the tensor $\mathbf{T}$ if the sets of values of the components of $\mathbf{T}$ characterizing the n domains, (3), are all distinct;

(2) 'partial' ferroic class with respect to the tensor $\mathbf{T}$ if only m, $1<m<n$, of the sets in (3) are distinct;

(3) 'null' ferroic class with respect to the tensor $\mathbf{T}$ if all sets in (3) are identical.

The terminology full, partial and null was introduced by Aizu (1969, 1970).

III. Tensorial classes

We present in this section a computational method to determine the tensorial classification of a ferroic crystal belonging to the ferroic class $\mathbf{G}F\mathbf{H}$ with respect to a tensor $\mathbf{T}$ with components T_j, $j=1,2,\ldots,q$. Let $D^T_{\mathbf{G}}$ denote the tensor representation of the point group $\mathbf{G}$ defined in (2). We denote by $N^T_{\mathbf{G}}(\mathbf{A})$ the number of independent components of the tensor $\mathbf{T}$ invariant under the subgroup $\mathbf{A}$ of $\mathbf{G}$. This number $N^T_{\mathbf{G}}(\mathbf{A})$ is equal to the number of times the identity representation of $\mathbf{A}$ is contained in the subduced representation $D^T_{\mathbf{G}}\downarrow\mathbf{A}$, that is in the tensor representation $D^T_{\mathbf{G}}$ of $\mathbf{G}$ restricted to the elements of $\mathbf{A}$. Denoting the character of the matrix $D^T_{\mathbf{G}}(G)$ by $\chi^T_{\mathbf{G}}(G)$, the number $N^T_{\mathbf{G}}(\mathbf{A})$ of components of the tensor $\mathbf{T}$ invariant under the subgroup $\mathbf{A}$ of $\mathbf{G}$ is calculated from

$$N^T_{\mathbf{G}}(\mathbf{A}) = \frac{1}{|\mathbf{A}|}\sum_A \chi^T_{\mathbf{G}}(A), \tag{4}$$

where the summation is over all elements of $\mathbf{A}$.

The tensorial classification of a ferroic crystal belong to the ferroic class $\mathbf{G}F\mathbf{H}$ can be formulated in terms of the numbers $N^T_{\mathbf{G}}(\mathbf{A})$:

($TN1$) $N^T_{\mathbf{G}}(\mathbf{H})=0$;

($TN2$) $N^T_{\mathbf{G}}(\mathbf{H})>0$ and $N^T_{\mathbf{G}}(\mathbf{H})>N^T_{\mathbf{G}}(\mathbf{H}')$ for all subgroups $\mathbf{H}'$ of $\mathbf{G}$ which contain $\mathbf{H}$ as a proper subgroup;

($TN3$) $N^T_{\mathbf{G}}(\mathbf{H})>0$ and $N^T_{\mathbf{G}}(\mathbf{H})=N^T_{\mathbf{G}}(\mathbf{H}')>N^T_{\mathbf{G}}(\mathbf{G})$ for a proper subgroup $\mathbf{H}'$ of $\mathbf{G}$ which contains $\mathbf{H}$ as a proper subgroup;

($TN4$) $N^T_{\mathbf{G}}(\mathbf{H})>0$ and $N^T_{\mathbf{G}}(\mathbf{H})=N^T_{\mathbf{G}}(\mathbf{G})$.

In ($TN1$) there are no components of the tensor $\mathbf{T}$ invariant under $\mathbf{H}$ and we consequently have a null tensorial class. The $N^T_{\mathbf{G}}(\mathbf{H})$ independent components of $\mathbf{T}$ invariant under $\mathbf{H}$ in case ($TN2$) are invariant under no additional elements of $\mathbf{G}$, and we have a full tensorial class. In ($TN3$) the $N^T_{\mathbf{G}}(\mathbf{H})$ components are invariant under additional but not all elements of $\mathbf{G}$, hence a partial tensorial class. Finally, the $N^T_{\mathbf{G}}(\mathbf{H})$ components invariant under $\mathbf{H}$ in ($TN4$) are invariant under **G** and again we have a null tensorial class.

The computations to determine the tensor classification of all ferroic classes for a given tensor **T** entails calculating the numbers $N_{\mathbf{G}}^{T}(\mathbf{A})$, (4), for all proper subgroups **A** of each of the thirty-one prototypic point groups **G**. The existence of tables of subduction numbers $N_{\mathbf{G}}^{i}(\mathbf{A})$ of irreducible representations of the point groups **G** (Birman, Berensen, Kotzev & Litvin, 1981; Litvin, Kotzev & Birman, 1981) simplifies this calculation: the tensor representation $D_{\mathbf{G}}^{T}$ is in general a reducible representation of **G**,

$$D_{\mathbf{G}}^{T}=\sum a_i^T\Gamma_i \qquad (5)$$

where the summation is over all irreducible representations Γ_i of **G**, and a_i^T denotes the number of times the irreducible representation Γ_i of **G** is contained in the reduced form of the tensor representation $D_{\mathbf{G}}^{T}$. The coefficients a_i^T are calculated from

$$a_i^T=\frac{1}{|\mathbf{G}|}\sum_{G}\chi_{\mathbf{G}}^{T}(G)\chi_i(G), \qquad (6)$$

where $\chi_i(G)$ is the character of the matrix $\Gamma_i(G)$. It follows from (4) and (5) that

$$N_{\mathbf{G}}^{T}(\mathbf{A})=\sum_{i} a_i^T N_{\mathbf{G}}^{i}(\mathbf{A}), \qquad (7)$$

where $N_{\mathbf{G}}^{i}(\mathbf{A})$ is defined by

$$N_{\mathbf{G}}^{i}(\mathbf{A})=\frac{1}{|\mathbf{A}|}\sum_{A}\chi_i(A). \qquad (8)$$

$N_{\mathbf{G}}^{i}(\mathbf{A})$ is the number of times the identity representation of **A** is contained in the subduced representation $\Gamma_i\downarrow\mathbf{A}$, the irreducible representation Γ_i of **G** restricted to the elements of the subgroup **A** of **G**.

For an arbitrary tensor **T**, point groups **G** and proper subgroups **A** of **G**, the numbers $N_{\mathbf{G}}^{T}(\mathbf{A})$ can be calculated from (7). The coefficients a_i^T can be calculated using (6), or by an alternative method given in Appendix I. The numbers $N_{\mathbf{G}}^{i}(\mathbf{A})$, defined by (8), for all irreducible representations Γ_i of all point groups **G** and all subgroups **A** of **G** are known and have been tabulated (Litvin, Kotzev & Birman, 1982). To determine the tensorial classification of a ferroic crystal belonging to a ferroic class $\mathbf{G}F\mathbf{H}$ with respect to a tensor **T**, one then calculates the $N_{\mathbf{G}}^{T}(\mathbf{A})$ for all subgroups **A** of **G** from (7) and applies the criteria $(TN1)$–$(TN4)$.

IV. Tables for tensorial classification

Using the computational method of the previous section we shall tabulate below the tensorial classification of all ferroic classes $\mathbf{G}F\mathbf{H}$ and tensors **T** whose corresponding tensor representation $D_{\mathbf{G}}^{T}$ is an irreducible representation of the point group **G**. We also show how these same tables can be used in determining the tensorial classification for tensors **T** whose corresponding tensor representation $D_{\mathbf{G}}^{T}$ is a reducible representation of the point group **G**.

A. *Irreducible tensor representation*

We assume that the tensor representation $D_{\mathbf{G}}^{T}=\Gamma_i$ is an irreducible representation of the point group **G**. The tensorial classification of all ferroic crystals belonging to ferroic classes $\mathbf{G}F\mathbf{H}$ with respect to a tensor T with corresponding tensor representation $D_{\mathbf{G}}^{T}=\Gamma_i$ has been tabulated.* In Table 1 we give the subtable for $\mathbf{G}=O_h$. The tensorial classification has been determined using (7), the known values of $N_G^i(A)$ (Litvin, Kotzev & Birman, 1982), and criteria $(TN1)$–$(TN4)$.

In each subtable corresponding to a prototypic point group **G**, see Table 1 for $\mathbf{G}=O_h$, the columns are headed by a symbol for each irreducible representation Γ_i of **G** excluding the identity representation of **G**. The notation used for the irreducible representations is that of Koster, Dimmock, Wheeler & Statz (1963). The rows of each subtable are indexed by the subgroups **H** of **G** of all ferroic classes $\mathbf{G}F\mathbf{H}$. The tensorial classification of a ferroic class $\mathbf{G}F\mathbf{H}$ with respect to a tensor T with a corresponding irreducible tensor representation $D_{\mathbf{G}}^{T}=\Gamma_i$ is read off the tables as follows.

(1) If Γ_i is the identity representation of **G** then all ferroic classes $\mathbf{G}F\mathbf{H}$ are null ferroic classes.

(2) If Γ_i is not the identity representation of **G**, then the tensorial classification of the ferroic class $\mathbf{G}F\mathbf{H}$ is determined by the entry at the intersection of the Γ_ith column and the **H**th row. The ferroic class is a full, partial or null ferroic class if the entry is, respectively, the symbol F or P or if the entry is blank.

For example, for the point group $\mathbf{G}=O_h$ and a polar vector tensor **T**, the tensor representation $D_{\mathbf{G}}^{T}=\Gamma_4^-$. From Table 1 we have that $O_hFC_2^z$, $O_hFC_2^{xy}$, $O_hFC_3^{xyz}$, $O_hFC_4^z$, $O_hFC_{2v}^{(z,x,y)}$ and $O_hFC_{2v}^{(xy,\bar{x}y,z)}$ are partial ferroic classes and O_hFC_1, $O_hFC_s^z$, $O_hFC_s^{xy}$, $O_hFC_{2v}^{(xy,\bar{x}y,z)}$, $O_hFC_{3v}^{xyz}$ and $O_hFC_{4v}^z$ are full ferroic classes. The remaining ferroic classes $O_hF\mathbf{H}$ are null ferroic classes. Interpreting the polar vector tensor as a ferroelectric tensor, one refers to the ferroic classes as ferroelectric classes, and to $O_hFC_2^z$, for example, as a partial ferroelectric class. In the terminology of Aizu (1970, 1976*a*, *b*), $O_hFC_2^z$ is referred to as a partial specie or subspecie of ferroics.

Additional information is contained in these tables. If $\mathbf{G}F\mathbf{H}$ is a partial ferroic class, then the tensor characterizing the domain of symmetry **H** is invariant under a larger subgroup **H**′ of **G**. We shall refer to

* The complete tables have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 39053 (24 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 1. *Tensorial classification of ferroic classes* **G***F***H** *with* $\mathbf{G} = O_h$

The second column lists the proper subgroups **H** of all ferroic classes **G***F***H**. The third column gives the number of domains of ferroic crystals belong to the ferroic class **G***F***H**. The entry at the intersection of the **H**th row and column under the Γ_ith irreducible representation of **G** determines the tensorial classification of the ferroic class **G***F***H** with respect to a tensor representation Γ_i. *P* and *F* denote partial and full ferroic classes, respectively, and, if the entry is blank, a null ferroic class.

G	H	No	Γ_2^+	Γ_3^+	Γ_4^+	Γ_5^+	Γ_1^-	Γ_2^-	Γ_3^-	Γ_4^-	Γ_5^-
$O_h^{(x,y,z)}$	C_1	48	P	$P(1)$	$P(1)$	$P(1)$	P	P	$P(1)$	F	F
	C_2^z	24	P	$P(1)$	$P(2)$	$P(2)$	P	P	$P(1)$	$P(1)$	$P(1)$
	C_s^z	24	P	$P(1)$	$P(2)$	$P(2)$				F	F
	C_2^{xy}	24		$P(2)$	$P(3)$	$P(3)$	P		$P(2)$	$P(2)$	F
	C_s^{xy}	24		$P(2)$	$P(3)$	$P(3)$		P	$P(3)$	F	$P(C_{2v}^{(\bar{x}y,xy,z)})$
	C_3^{xyz}	16	P		$P(4)$	$P(4)$	P	P		$P(3)$	$P(2)$
	C_4^z	12		$P(2)$	$P(2)$		P		$P(2)$	$P(1)$	
	S_4^z	12		$P(2)$	$P(2)$			P	$P(3)$		$P(1)$
	$C_{2v}^{(z,x,y)}$	12	P	$P(1)$						$P(1)$	$P(1)$
	$D_2^{(z,xy,\bar{x}y)}$	12		$P(2)$		$P(2)$	P		$P(2)$		$P(1)$
	$C_{2v}^{(z,xy,\bar{x}y)}$	12		$P(2)$		$P(2)$		P	$P(3)$	$P(1)$	
	$C_{2v}^{(xy,\bar{x}y,z)}$	12		$P(2)$		$P(2)$				$F(2)$	F
	D_3^{xyz}	8				$P(4)$	P				$F(2)$
	C_{3v}^{xyz}	8				$P(4)$		P		$F(3)$	
	C_{4v}^z	6		$P(2)$						$F(1)$	
	$D_{2d}^{(z,xy,\bar{x}y)}$	6		$P(2)$							$F(1)$
	C_i	24	P	$P(1)$	$F(1)$	$F(1)$					
	C_{2h}^z	12	P	$P(1)$	$P(2)$	$P(2)$					
	C_{2h}^{xy}	12		$P(2)$	$F(3)$	$F(3)$					
	C_{3i}^{xyz}	8	P		$F(4)$	$P(4)$					
	C_{4h}^z	6		$P(2)$	$F(2)$						
	$D_{2h}^{(z,xy,\bar{x}y)}$	6		$P(2)$		$F(2)$					
	D_{3d}^{xyz}	4				$F(4)$					
	$D_2^{(x,y,z)}$	12	P	$P(1)$			P	P	$F(1)$		
	D_4^z	12		$P(2)$			P		$F(2)$		
	$D_{2d}^{(z,x,y)}$	6		$P(2)$				P	$F(3)$		
	$D_{2h}^{(z,x,y)}$	6	P	$F(1)$							
	D_{4h}^z	3		$F(2)$							
	$T^{(x,y,z)}$	4	P				P	P			
	$T_d^{(x,y,z)}$	2						F			
	$O^{(x,y,z)}$	2					F				
	$T_h^{(x,y,z)}$	2	F								

the largest such subgroup $\mathbf{H}'$ of **G** as the invariance group $\mathbf{H}'$ corresponding to the tensor T and the partial ferroic class **G***F***H**. The invariance group $\mathbf{H}'$ can be determined from the tables. If $D_{\mathbf{G}}^T = \Gamma_i$ and the entry *P* is at the intersection of the Γ_ith column and **H**th row, then $\mathbf{H}'$ is the row index of the entry *F* in the Γ_ith column. If the Γ_ith column contains more than a single *F* entry, the entries *P* are supplemented with an additional index $P(j)$, and $\mathbf{H}'$ is the row index of the entry in the Γ_ith column denoted by $F(j)$. In exceptional cases $\mathbf{H}'$ is given in parentheses following the entry *P*, that is, as $P(\mathbf{H}')$.

For example, in Table 1 for the partial ferroelectric class $O_hFC_2^z$, the entry at the intersection of the Γ_4^- column and C_2^z row is $P(1)$. In the Γ_4^- column, the entry $F(1)$ is in the C_{4v}^z row. Consequently, a polar tensor invariant under the subgroup $\mathbf{H} = C_2^z$ of $\mathbf{G} = O_h$ is in fact invariant under the larger subgroup $\mathbf{H}' = C_{4v}^z$ of $\mathbf{G} = O_h$.

B. Reducible tensor representation

We assume that the tensor representation $D_{\mathbf{G}}^T$ is reducible and that the irreducible representations Γ_i of **G** contained in the reduced form, (5), of the tensor representation are known. We define the set $\{\Gamma_i\}$ of irreducible representations as the set of all irreducible representations of **G** excluding the identity representation, contained in the reduced form of the tensor representation. Each irreducible representation Γ_i appears once in this set if the corresponding coefficient a_i^T of (5) is equal to or greater than one.

The tensorial classification of ferroic crystals belonging to the ferroic class **G***F***H** with respect to a tensor **T** with a reducible tensor representation is determined from Table 1 as follows. If the set $\{\Gamma_i\}$ is empty, *i.e.* only the identity representation is contained in the tensor representation, **G***F***H** is a null ferroic class. If the set $\{\Gamma_i\}$ is not empty, then there are four cases to be distinguished. To distinguish between these cases we define the set of entries as the set of all *P* and *F* entries in the **H**th row of the **G**th subtable at the intersections of the columns corresponding to all irreducible representations in $\{\Gamma_i\}$. The four cases are:

(1) if the set of entries is empty, then **G***F***H** is a null ferroic class;

(2) if at least one of the set of entries is an *F*, then **G***F***H** is a full ferroic class;

(3) if the set of entries consists of a single *P*, then **G***F***H** is a partial ferroic class;

(4) if the set of entries consists of two or more *P*'s, then one determines from the table the corresponding invariance groups $\mathbf{H}_1', \mathbf{H}_2', \ldots$ and the intersection **I**

of these point groups. If $\mathbf{I}=\mathbf{H}$, then $\mathbf{G}F\mathbf{H}$ is a full ferroic class, otherwise, $\mathbf{G}F\mathbf{H}$ is a partial ferroic class.

An example: gyrotropic ferroic classes have been discussed by Konak, Kopsky & Smutny (1978) and Wadhawan (1979). According to Wadhawan (1979), the ferroelectric phase of dicalcium strontium propionate belongs to the ferroic class O_hFC_4, and O_hFC_4 is a partial gyrotropic class. The optical gyration tensor is a symmetric second-rank axial tensor (Nye, 1964). The tensor representation $D^T_{\mathbf{G}}$ for the optical gyration tensor and $\mathbf{G}=O_h$ is, see Appendix 1, reducible and $D^T_{\mathbf{G}}=\Gamma_1^-+\Gamma_3^-+\Gamma_5^-$. From subtable $\mathbf{G}=O_h$ of Table 1, for $\mathbf{H}=C_4$ and the set $\{\Gamma_1^-,\Gamma_3^-,\Gamma_5^-\}$ of irreducible representations of $\mathbf{G}=O_h$, the corresponding set of entries consists of two P's. The corresponding invariance groups are O and D_4, and the intersection I of these two groups is D_4. Since $\mathbf{H}=C_4$ is contained in $\mathbf{I}=D_4$, O_hFC_4 is a partial gyrotropic class in agreement with Wadhawan (1979).

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APPENDIX I
Reduction of the tensor representation

In this Appendix we discuss an alternative method to equation (6) to determine the coefficients a_i^T, the number of times the Γ_ith irreducible representation of a point group $\mathbf{G}$ is contained in the reduced form, equation (5), of a tensor representation $D^T_{\mathbf{G}}$ of $\mathbf{G}$. We shall limit our discussion to tensors whose transformational properties under the full rotation group $\mathbf{R}$, the group of all proper and improper three-dimensional rotations, are known.

Let $D^T_{\mathbf{R}}$ denote the tensor representation of $\mathbf{R}$ defined by

$$RT_j=\sum_k D^T_{\mathbf{R}}(R)_{kj}T_k, \qquad (A\text{-}1)$$

where $T_j, j=1,2,\ldots,q$, are the components of a tensor T. The tensor representation $D^T_{\mathbf{R}}$ is in general reducible and

$$D^T_{\mathbf{R}}=\sum_j b_jD^j_{\mathbf{R}}, \qquad (A\text{-}2)$$

where b_j denotes the number of times the irreducible representation $D^j_{\mathbf{R}}$ of $\mathbf{R}$ is contained in the reduced form of the tensor representation $D^T_{\mathbf{R}}$. The tensor representation $D^T_{\mathbf{G}}$ of a point group $\mathbf{G}$ is

$$D^T_{\mathbf{G}}=D^T_{\mathbf{R}}\downarrow\mathbf{G} \qquad (A\text{-}3)$$

equal to the tensor representation of $\mathbf{R}$ subduced onto $\mathbf{G}$. From (A–2) and (A-3) it follows that

$$D^T_{\mathbf{G}}=\sum_j b_j(D^j_{\mathbf{R}}\downarrow\mathbf{G}). \qquad (A\text{-}4)$$

The subduced representation $D^j_{\mathbf{R}}\downarrow\mathbf{G}$ is in general a reducible representation of the point group $\mathbf{G}$:

$$D^j_{\mathbf{R}}\downarrow\mathbf{G}=\sum_i c_{ji}\Gamma_i \qquad (A\text{-}5)$$

and substituting into (A-4) we have

$$D^T_{\mathbf{G}}=\sum_i(\sum b_jc_{ji})\Gamma_i. \qquad (A\text{-}6)$$

Comparing this with (5), one has that the number a_i^T of times the Γ_ith irreducible representation of the point group $\mathbf{G}$ is contained in the reduced form of the tensor representation of $\mathbf{G}$ is given by

$$a_i^T=\sum b_jc_{ji}. \qquad (A\text{-}7)$$

The computation of the coefficients a_i^T using (A-7), in place of (6) is simplified by the existence of tables of the coefficients b_i and c_{ji}. Koster, Dimmock, Wheeler & Statz (1963) have tabulated the coefficients c_{ji}, (A-5), for all irreducible representations D^j_R and all point groups $\mathbf{G}$. The coefficients b_j, see (A-2), for twenty-six tensor representations, corresponding to tensors of second, third and fourth rank whose components are of various intrinsic symmetry, have been tabulated by Tenenbaum (1966).

For example, the optical gyration tensor is a symmetric second-rank axial tensor (Nye, 1964). Equation (A-2) is then, according to the tables of Tenenbaum, $D^T_{\mathbf{R}}=D_0^-+D_2^-$. For the point group $\mathbf{G}=O_h$ using the tables of Koster, Dimmock, Wheeler & Statz (1963), (A-5) for these two irreducible representations of $\mathbf{R}$ becomes $D_0^-\downarrow O_h=\Gamma_1^-$ and $D_2^-\downarrow O_h=\Gamma_3^-+\Gamma_5^-$. Consequently, using ($A$-7), the reduced-form equation (5) of the optical gyration tensor representation for the point group $\mathbf{G}=O_h$ is $D_0^T=\Gamma_1^-+\Gamma_3^-+\Gamma_5^-$.

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Secondary Extinction and Absolute Structure Factors in X-ray Diffraction: Determination by Polarization Variation

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Abstract

If a rocking curve is measured in symmetric Laue geometry for two different X-ray polarizations, and the incident beam meets the geometrical conditions for diffraction, *i.e.* the incident beam is much less divergent than the sample mosaic, then the intensity ratio $R_{\rm obs}$, for the intensities measured with each polarization, will depend upon the reflectivity at each point on the rocking curve. From the variation of $R_{\rm obs}$ *vs* the observed intensity, $I_{\rm obs}$, the absolute reflectivities and secondary extinction can be determined. If absorption is properly treated, then all data taken in this geometry should lie on a single curve of $R_{\rm obs}$ *vs* $I_{\rm obs}$. Failure to fit this curve is evidence that the sample has other processes occurring such as multiple scattering or primary extinction.

Introduction

A major advantage of high-intensity synchrotron X-ray sources, which have recently been constructed or will soon become operational, is the ability to vary the polarization of a monochromatic beam falling on a diffracting sample, while still keeping sufficient intensity for easy data collection. One use to which the polarization dependence can be put is in the study of primary extinction (Suortti, 1982*a*, *b*), since the extinction length is inversely proportional to the polarization. A second advantage of the synchrotron source is the high intensity available in a very narrow angular and wavelength band. Unlike conventional X-ray sources, with synchrotrons it should be possible to restrict the divergence of the beam in both angle and energy, so that the divergence of the beam is less than that of the sample (for all but the most perfect specimens), while preserving reasonable intensity on the sample.

In two recent papers (Yelon, van Laar, Kaprzyk & Maniawski, 1984; Yelon, van Laar, Maniawski & Kaprzyk, 1984) it has been shown that absolute reflectivity measurements with a beam meeting the above divergence conditions could give good secondary extinction corrections in polarized neutron scattering, free from any parametrization or fitting. In the present paper we propose an inverse method in which measurement of the intensity ratio for X-ray scattering with two different beam polarizations can be used to determine the absolute reflectivity as well as to give the secondary extinction corrections for a measured rocking curve.

Theory

The present method is based on the Zachariasen (1967) solutions to the intensity transfer equations (Darwin, 1922) in symmetric Laue geometry, which

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