single-crystal work of Graf, Schneider, Freund & Lehmann (1981).

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Elastic Coefficients of Polychromatic Crystals

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Abstract

The group-theoretical method of reducing the polar (axial) tensor representation of the full rotation group has been explored and extended to obtain the second-, the third- and the fourth-order elastic coefficients for the 18 polychromatic crystal classes. The elastic coefficients obtained for all the classes are tabulated and the results obtained are briefly discussed.

1. Introduction

Many significant contributions on the study of the physical properties of crystals have been brought to light by several group-theoretical physicists during the past few decades. The number of non-vanishing as well as independent constants for the various physical properties in respect of the 32 conventional crystal classes were derived in considerable detail using group-theoretical as well as tensor methods by Bhagavantam & Venkatarayudu (1951), Wooster (1979), Nye (1985) and others. The book by Bhagavantam (1966) enhances the use of the character method in studying the magnetic properties of

these 32 classes and the 58 magnetic (double-colour) point groups derived from them. In two of the earlier papers published by the author (Rama Mohana Rao, 1987, 1988) the 18 applicationally significant polychromatic crystal classes (Indenbom, Belov & Neronova, 1960) were studied for three identified magnetic properties such as piezomagnetism and for six physical properties such as photoelasticity. The number of independent constants (n_i) required to describe a chosen magnetic/physical property was obtained using a group-theoretical procedure also established by the author (Rama Mohana Rao, 1987).

It is well known that the physical property of elasticity describes the relation between the stress field developed and the strains caused. Further, the applied stress as well as the resulting strain could be represented by second-rank symmetric tensors. Bhagavantam & Suryanarayana (1949) and Jahn (1949) successfully enumerated the second- and third-order elastic coefficients for the 32 conventional crystal classes employing group-theoretical methods. With a slightly different approach to the application of the character method, following a suggestion made by Chelam (1961), Krishnamurty (1963) and Krishnamurty & Gopala Krishna Murty (1968) also derived these coefficients for the 32 conventional crystal classes.

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It can be seen (Bhagavantam, 1966) that piezomagnetism is the appearance of a magnetic moment on the application of stress. As the physical property elasticity expresses the relation between the applied stress and the resulting strain, the connection between the two related phenomena – piezomagnetism and elasticity – is investigated in this note, in respect of the 18 polychromatic crystal classes that are piezomagnetic and the influence of stress on these magnetic classes is assessed. Accordingly the number of second-, third- and fourth-order elastic coefficients for each of the 18 classes is obtained here by extending the group-theoretical method (Jahn, 1949) of reducing the polar tensor representation of the full rotation group through formulae for the symmetrical products of representations. The non-vanishing number of elastic coefficients obtained in this paper in conjunction with the non-vanishing number of independent physical constants already obtained for these classes by the author in the preceding paper (Rama Mohana Rao, 1987) may provide a complete picture for describing their physical symmetry more elaborately.

The importance of the idea of polychromatic symmetry in deriving the similarity symmetry groups has already been explored and the utility of the colour symmetry groups in describing the stem and layer symmetry groups in higher-dimensional space has already been discussed (Roman, 1959; Zamorzaev, 1963). The procedure for deriving the desired coefficients is outlined in § 2 and is exemplified with the help of the point group 23 that induces the class $3^{(3)}/2$. Since a knowledge of the number of non-vanishing independent components of a physical property like elasticity is quite useful in identifying the class of crystals and in studying their physical properties (particularly those possessing higher symmetries), the coefficients obtained are provided in Table 2 below. The notation adopted for the polychromatic classes is due to Indenbom, Belov & Neronova (1960) and the nomenclature for the point groups is that of Hermann–Mauguin (International).

2. The method

The group-theoretical method of reducing the polar (axial) tensor representation of the full rotation group (Jahn, 1949) is extended in this section for finding the non-vanishing independent number of second-, third- and fourth-order elastic coefficients of the 18 polychromatic crystal classes that were already found to be piezomagnetic (Rama Mohana Rao, 1987). The numbers of elastic coefficients obtained here are worked out for the first time.

If V denotes the representation of a polar vector and Tisza's (1933) notation representing the symmetrical product $[V^2]$ of V with itself is employed, the reduced forms of the representation for the symmetrical second, third and fourth powers of $[V^2]$

Table 1. *Reduction of the representation D_L^g for the point group 23*

T	E	C_{2m}	C_{3j}^+	C_{3j}^-	n_2	n_3	n_4	n_5	n_6	n_8
A	1	1	1	1	0	1	1	0	2	1
^1E	1	1	ω	ω^*	1	0	1	1	1	2
^2E	1	1	ω^*	ω						
T	3	-1	0	0	1	2	2	3	3	4
$\chi(D_0^g)$	5	1	-1	-1						
$\chi(D_2^g)$	7	-1	1	1						
$\chi(D_3^g)$	9	1	0	0						
$\chi(D_4^g)$	11	-1	-1	-1						
$\chi(D_5^g)$	13	1	1	1						
$\chi(D_8^g)$	17	1	-1	-1						

which represent respectively the second-, third- and fourth-order elasticity can be given by

$$[[V^2]^2] = 2D_0^g + 2D_2^g + D_4^g$$
$$[[V^2]^3] = 3D_0^g + 3D_2^g + D_3^g + 2D_4^g + D_6^g$$
$$[[V^2]^4] = 4D_0^g + 5D_2^g + D_3^g + 4D_4^g + D_5^g \quad (2.1)$$
$$+ 2D_6^g + D_8^g.$$

In (2.1), D_L^g stands for the representation of dimension $(2L+1)$ of the group R_∞^i which is even with respect to inversion.

It has already been shown that the one-dimensional (1D) complex irreducible representation (IR) Γ of a crystallographic point group G induces a polychromatic class $G^{(p)}$, $p = 3$, 4 or 6 (Rama Mohana Rao, 1985) and the number of independent constants (n_i) required to describe a magnetic/physical property in respect of the induced class $G^{(p)}$ is just the same as that number (n_i') obtained before the IR Γ that induces $G^{(p)}$, for the considered property (Rama Mohana Rao, 1987). Accordingly, the appropriate number of elastic coefficients required for the 18 polychromatic classes under consideration is obtained here by deriving the reduced form of D_L^g for each of the ten crystallographic point groups containing 1D complex IRs. The point group 23 is taken to illustrate the method.

It can be seen (Table 1) that the character table of the point group 23 contains a 1D total symmetric IR (A), a pair of 1D complex IRs $(^1E, ^2E)$ and one 3D IR (T). It is well known that either of the 1D complex IRs induce the polychromatic variant $3^{(3)}/2$ (Indenbom, Belov & Neronova, 1960; Rama Mohana Rao, 1985). The enumeration of the numbers n_i occurring before each of the distinct IRs of the group 23 is performed here by the known formula

$$n_i = (1/N) \sum_\rho h_\rho \chi_\rho^{(\Gamma)}(R) \chi_\rho^{(\Gamma_i)}(R) \quad (2.2)$$

by replacing $\chi_\rho^{(\Gamma)}(R)$ with $\chi[D_L^g(R)]$, the character for the element R provided by the even parity functions of degree L. In (2.2), N denotes the order of the group G, h_ρ represents the number of elements in the ρth conjugate class and $\chi^{(\Gamma_i)}(R)$ denotes the

Table 2. *Number of independent elastic coefficients of second-, third- and fourth-order needed by the 18 polychromatic classes*

Serial no.	Polychromatic class $G^{(p)}$	Second order	Third order	Fourth order
1	$6^{(6)}$	3	8	19
2	$\bar{3}^{(6)}$	0	0	0
3	$3^{(3)}/m'$	3	8	19
4	$6^{(3)}$	4	10	23
5	$\bar{3}^{(3)}$	7	18	42
6	$3^{(3)}/m$	4	10	23
7	$6^{(6)}/m$	0	0	0
8	$6^{(3)}/m$	4	10	23
9	$6^{(6)}/m'$	3	8	19
10	$6^{(3)}/m'$	0	0	0
11	$3^{(3)}$	7	18	42
12	$4^{(4)}$	4	12	28
13	$\bar{4}^{(4)}$	4	12	28
14	$4^{(4)}/m$	0	0	0
15	$4^{(4)}/m'$	4	12	28
16	$3^{(3)}/2$	3	6	14
17	$\bar{6}^{(3)}/2$	3	6	14
18	$\bar{6}^{(6)}/2$	0	0	0

character of the symmetry operation R in the ith IR Γ_i of G.

From Table 1, the reduced forms of D_L^g worked out for the point group 23 can be seen to be

$$D_0^g = A$$

$$D_2^g = {}^1E_1 + T$$

$$D_3^g = A + 2T$$

$$D_4^g = A + {}^1E_1 + 2T \qquad (2.3)$$

$$D_5^g = {}^1E_1 + 3T$$

$$D_6^g = 2A + {}^1E_1 + 3T$$

$$D_8^g = A + 2{}^1E_1 + 4T.$$

The above reductions of D_L^g, when substituted in the RHS of (2.1), yield

$$[[V^2]^2] = 2A + 3{}^1E_1 + 4T$$

$$[[V^2]^3] = 8A + 6{}^1E_1 + 12T \qquad (2.4)$$

$$[[V^2]^4] = 14A + 14{}^1E_1 + 28T.$$

Hence the desired elastic coefficients for the polychromatic class $3^{(3)}/2$ are readily obtained when the numerical coefficients $(3, 6, 14)$ of the 1D complex IR ${}^1E_1$ are collected from the corresponding symmetrical powers of $[V^2]$ provided by (2.4). The results obtained for the rest of the 17 classes are provided before the appropriate class in Table 2.

3. Discussion

It has already been established (Rama Mohana Rao, 1987) that the 18 polychromatic crystal classes are magnetic and they exhibit magnetic properties like piezomagnetism. It is shown in this paper that 13 out of these 18 classes exhibit the physical property elas-

ticity. The occurrence of the number of non-vanishing coefficients indicates that the presence of spin in the magnetic state of a crystal does not necessarily affect their physical property.

It can be observed that the five polychromatic classes $\bar{3}^{(6)}$; $6^{(6)}/m$, $6^{(3)}/m'$; $4^{(4)}/m$; $\bar{6}^{(6)}/2$ induced by the 1D complex IR of the point groups $\bar{3}$; $6/m$; $4/m$; $m3$ in each of which the centre of inversion (i) is associated with the character -1 do not give rise to elastic coefficients of any order. It was observed that the same five classes did not require any piezomagnetic coefficients (Rama Mohana Rao, 1987). This coincidence is due to the fact that the elastic coefficients are characterized by polar tensors of even rank while the piezomagnetic coefficients are represented by axial tensors of odd rank, both of which are centrosymmetric.

The values of the elastic coefficients of various orders obtained here increase with the order. It is interesting to note that, in so far as the number of non-vanishing elastic coefficients is concerned, the polychromatic classes divide themselves into five sets with the groups contained in each set requiring the same number of coefficients. Also the six classes $6^{(3)}$, $6^{(6)}$; $6^{(3)}/m$, $6^{(6)}/m'$; $3^{(3)}/m$, $3^{(3)}/m'$ generated by the point groups 6; $6/m$; $3/m$ of the hexagonal system have split themselves into two sets requiring different numbers of elastic coefficients. Whereas the three classes $6^{(3)}$; $6^{(3)}/m$; $3^{(3)}/m$ require $(4, 10, 23)$ coefficients, the other three classes $6^{(6)}$; $6^{(6)}/m'$; $3^{(3)}/m'$ require $(3, 8, 19)$ coefficients. This is because, in the first category, the symmetry operations c_2 and σ_h of $6/m$; σ_h of $3/m$ and c_2 of 6 are associated with the character $+1$ in the inducing IR, whereas in the second set these very symmetry elements are associated with the character -1 in the inducing IR.

The elastic coefficients derived and tabulated in this paper were also obtained by the author simultaneously utilizing the character method and the coefficients obtained were found to be identical with those derived in this paper. However, the group-theoretical method adopted in this work has the merit of avoiding the character calculations encountered in the later method.

In the case of polychromatic crystal classes, from what has already been established earlier by this author (Rama Mohana Rao, 1987) and from the results obtained here, it can be concluded that the exhibition of piezomagnetic phenomena implies the exhibition of elasticity. The converse of the above statement can also be seen to hold good in respect of the polychromatic crystals, though it cannot be contended in general. That the converse need not always be true is evident from the elastic and piezomagnetic coefficients of crystals corresponding to the point groups 432, $\bar{4}3m$, $m3m$ (Bhagavantam & Pantulu, 1964; Bhagavantam & Suryanarayana, 1949).

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Analysis of Neutron Diffraction Data in the Case of High-Scattering Cells

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Abstract

A data reduction procedure is presented to analyse neutron diffraction intensities from low-scattering-power systems contained in high-scattering cells. A careful analysis of the cell contribution is carried out and a numerical program to treat absorption and multiple scattering also due to the cell is developed.

1. Introduction

The purpose of a neutron diffraction experiment from non-crystalline samples is to obtain the static structure factor $S(Q)$ from the measured intensity. However, the scattered neutron flux contains some background (scattering from container and environment) and is affected by absorption, multiple processes and inelasticity contributions apart from instrumental effects like beam inhomogeneity, counter efficiency and resolution.

In the case of high-scattering-power samples or for low container contribution to the total scattered intensity, the data reduction can be done by following standard procedures like that outlined by Paalman & Pings (1962) after a subtraction of the multiple scattering due to the sample only according to Blech & Averbach (1965). On the other hand, when such experimental conditions do not prevail, *i.e.* when the container contribution is an appreciable fraction of the total measured intensity (over 10%), the simplifying approximation of a negligible-thickness cell in evaluating the multiple scattering no longer holds.

One of the most widely employed approaches to the problem of multiple scattering from the sample and/or the container makes use of Monte Carlo (MC) procedures (Bischoff, Yeater & Moore, 1972; Copley, 1974, 1981; Copley, Verkerk, van Well & Fredrikze, 1986; Meardon, 1973; Johnson, 1974) which allow for a simulation of the real experiment by following a given number of neutron histories. By using this