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Invariant Magneto-electric and Piezomagnetic Coefficients

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Invariant magneto-electric coefficients and invariant piezomagnetic coefficients are obtained for all the magnetic crystal classes.

1. Introduction

In specifying the values of the tensor components which represent physical properties of crystals, it is customary to choose a Cartesian frame of reference which has a specific orientation relative to the crystallographic axes. Such tensor coefficients, as Nowacki (1962) points out, do not determine the material constants directly since their values vary with the direction of the coordinate axes. It is, therefore, natural to seek to characterize physical properties of crystals by constants whose values do not depend upon the choice of the coordinate system, *i.e.* constants which are invariant under all coordinate transformations. Such invariants in the case of elastic constants (Srinivasan & Nigam, 1968*a*, 1969), photoelastic coefficients (Srinivasan & Nigam, 1968*b*) and piezoelectric coefficients (Srinivasan, 1970) have already been obtained.

In the present paper invariant magneto-electric coefficients and invariant piezomagnetic coefficients are found in the case of various magnetic crystal classes.

2. Form-invariant expressions

The constitutive equations governing a magneto-electric medium in which the magneto-electric tensor occurs (Dzyaloshinskii, 1959; Hornreich & Shtrikman, 1968; O'Dell, 1970) are

$$D_i = \varepsilon_{ij}E_j + \alpha_{ij}H_j \,, \tag{1}$$

$$B_i = \beta_{ij}E_j + \mu_{ij}H_j \,, \tag{2}$$

where ε_{ij} and μ_{ij} are the familiar permittivity and permeability tensor components respectively, and α_{ij} and β_{ij} are the magneto-electric tensor components. Both α_{ij} and β_{ij} are axial (or pseudo) c tensors (Birss, 1963) (*i.e.* they reverse sign under both space and time inversion) of rank two. The piezomagnetic coefficients appear in the equations (Bhagavantam, 1966; Mason, 1966)

$$M_i = d_{ijk}\sigma_{jk} \,, \tag{3}$$

where M_i are the components of the magnetization vector, σ_{jk}, the components of the stress tensor and d_{ijk}, the piezomagnetic coefficients. d_{ijk} are the components of an axial (or pseudo) c tensor of rank three.

With reference to a Cartesian frame of reference $Oxyz$, form-invariant expressions (Srinivasan & Nigam, 1968; Srinivasan, 1970) for second and third rank tensors are given by

$$\beta_{ij} = \nu_{ai}\nu_{bj}A_{ab} \,, \tag{4}$$

$$d_{ijk} = \nu_{ai}\nu_{bj}\nu_{ck}A_{abc} \,, \tag{5}$$

where summation is implied by repeated indices, and ν_{ai} *etc.* are the components of the vectors $\mathbf{v}_a$ ($a=1, 2, 3$) which are unit vectors along the crystallographic axes. Since β_{ij} and d_{ijk} are pseudo c tensors, A_{ab} and A_{abc} are pseudo scalars and also they change sign under time reversal. That is,

$$iA_{ab} = -A_{ab} \,, \quad TA_{ab} = -A_{ab} \,,$$
$$iA_{abc} = -A_{abc} \,, \quad TA_{abc} = -A_{abc} \,,$$

where i and T are space inversion and time reversal operators, respectively. Hence, they may be called pseudo c scalars. These two facts must be borne in mind while subjecting equations (4) and (5) to symmetry requirements of the magnetic point groups.

3. Invariant magneto-electric coefficients

We will now derive the form-invariant expressions for β_{ij} in the case of 58 of the 90 magnetic crystal classes in which the magneto-electric effect can be observed (Bhagavantam, 1966). To obtain similar expressions for α_{ij} we need only to replace β by α in all the expressions in which β occurs.

Triclinic system

(i) Classes 1, $\underline{\bar{1}}$

We start with the expression (4)

$$\beta_{ij} = \nu_{ai}\nu_{bj}A_{ab} \,, \tag{6}$$

where A_{ab} ($a, b=1, 2, 3$) are the 9 invariant magneto-electric coefficients for the classes 1 and $\underline{\bar{1}}$. The expressions for β_{ij} in the case of other classes are obtained from (6) by subjecting β_{ij} in (6) to appropriate symmetry requirements of the class. For the details of as to how to feed in the symmetry conditions one may refer to the earlier work (Srinivasan & Nigam, 1969). We, therefore, give below only the final results.

Monoclinic system

(i) Classes 2, $\underline{m}$, $2/\underline{m}$

In class 2, $\mathbf{v}_3$ is chosen as the two-fold axis of rotation and in class m, $\mathbf{v}_1\mathbf{v}_2$-plane is chosen as the mirror plane. This is the convention followed for these two classes throughout this paper.

$$\beta_{ij}=\beta_1 v_{1i}v_{1j}+\beta_2 v_{2i}v_{2j}+\beta_3 v_{3i}v_{3j} +\beta_4 v_{1i}v_{2j}+\beta_5 v_{2i}v_{1j}\,. \quad (7)$$

(ii) Classes $\underline{2}$, m, $\underline{2}/m$

$$\beta_{ij}=\beta_1 v_{2i}v_{3j}+\beta_2 v_{3i}v_{2j}+\beta_3 v_{3i}v_{1j}+\beta_4 v_{1i}v_{3j}\,. \quad (8)$$

Orthorhombic system

(i) Classes 222, $2\underline{mm}$, $\underline{mmm}$

$$\beta_{ij}=\beta_i v_{1i}v_{1j}+\beta_2 v_{2i}v_{2j}+\beta_3 v_{3i}v_{3j}\,. \quad (9)$$

(ii) Classes $\underline{22}2$, $2mm$, $\underline{2}m\underline{m}$, $\underline{m}mm$

$$\beta_{ij}=\beta_1 v_{1i}v_{2j}+\beta_2 v_{2i}v_{1j}\,. \quad (10)$$

Tetragonal system

For the tetragonal system $\mathbf{v}_3$ is chosen as the fourfold axis of rotation. Since $\mathbf{v}_1$, $\mathbf{v}_2$, $\mathbf{v}_3$ are mutually orthogonal in tetragonal crystals, they satisfy the relation

$$v_{1i}v_{1j}+v_{2i}v_{2j}+v_{3i}v_{3j}=\delta_{ij}\,. \quad (11)$$

(i) Classes 4, $\underline{\bar{4}}$, $4/\underline{m}$

$$\beta_{ij}=\beta_1\delta_{ij}+\beta_2 v_{3i}v_{3j}+\beta_3(v_{1i}v_{2j}-v_{2i}v_{1j})\,, \quad (12)$$

where we have made use of (11), and

$$\beta_1=A_{11}\,,\quad \beta_2=(A_{33}-A_{11})\,,\quad \beta_3=A_{12}\,.$$

(ii) Classes 422, $4\underline{mm}$, $\underline{\bar{4}}2\underline{m}$, $4/\underline{mmm}$

$$\beta_{ij}=\beta_1\delta_{ij}+\beta_2 v_{3i}v_{3j}\,, \quad (13)$$

(iii) Classes $\underline{4}$, $\bar{4}$, $\underline{4}/\underline{m}$

$$\beta_{ij}=\beta_1(v_{1i}v_{1j}-v_{2i}v_{2j})+\beta_2(v_{1i}v_2+{}_j v_{2i}v_{1j})\,, \quad (14)$$

where

$$\beta_1=A_{11}=-A_{22}\,,\quad \beta_2=A_{12}=A_{21}\,.$$

(iv) Classes $\underline{4}2\underline{2}$, $\underline{4}m\underline{m}$, $\bar{4}2m$, $\bar{4}\underline{2m}$, $\underline{4}/\underline{m}m\underline{m}$

$$\beta_{ij}=\beta_1(v_{1i}v_{1j}-v_{2i}v_{2j})\,. \quad (15)$$

(v) Classes $4\underline{22}$, $4mm$, $\underline{\bar{4}2}m$, $4/\underline{m}mm$

$$\beta_{ij}=\beta(v_{1i}v_{2j}-v_{2i}v_{1j})\,. \quad (16)$$

Rhombohedral system

For rhombohedral and hexagonal systems we choose the same type of unit cell in which $\mathbf{v}_1$ and $\mathbf{v}_2$ are separated by 120° and $\mathbf{v}_3$ is perpendicular to the $\mathbf{v}_1\mathbf{v}_2$ plane. In this case the vectors $\mathbf{v}_1$, $\mathbf{v}_2$, $\mathbf{v}_3$ satisfy the identity

$$v_{1i}v_{1j}+v_{2i}v_{2j}+\tfrac{1}{2}(v_{1i}v_{2j}+v_{2i}v_{1j}) +\tfrac{3}{4}v_{3i}v_{3j}=\tfrac{3}{4}\delta_{ij}\,. \quad (17)$$

For the rhombohedral system $\mathbf{v}_3$ is chosen as the threefold axis of rotation.

(i) Classes 3, $\underline{\bar{3}}$

$$\beta_{ij}=\beta_1\delta_{ij}+\beta_2 v_{3i}v_{3j}+\beta_3(v_{1i}v_{2j}-v_{2i}v_{1j})\,, \quad (18)$$

where (17) has been made use of, and

$$\beta_1=\tfrac{3}{4}A_{11}\,,\quad \beta_2=A_{33}-\tfrac{3}{4}A_{11}\,,\quad \beta_3=\tfrac{3}{4}(A_{12}-A_{21})\,,$$
$$A_{11}=A_{22}=(A_{12}+A_{21})\,.$$

(ii) Classes 32, $3\underline{m}$, $\underline{\bar{3}m}$

$$\beta_{ij}=\beta_1\delta_{ij}+\beta_2 v_{3i}v_{3j}\,. \quad (19)$$

(iii) Classes $3\underline{2}$, $3m$, $\underline{\bar{3}}m$

$$\beta_{ij}=\beta(v_{1i}v_{2j}-v_{2i}v_{1j})\,. \quad (20)$$

Hexagonal system

In this system $\mathbf{v}_3$ is the sixfold axis of rotation.

(i) Classes 6, $\underline{\bar{6}}$, $6/\underline{m}$

$$\beta_{ij}=\beta_1\delta_{ij}+\beta_2 v_{3i}v_{3j}+\beta_3(v_{1i}v_{2j}-v_{2i}v_{1j})\,, \quad (21)$$

where (17) has been utilized, and

$$\beta_1=\tfrac{3}{4}A_{11}\,,\quad \beta_2=(A_{33}-\tfrac{3}{4}A_{11})\,,\quad \beta_3=\tfrac{1}{2}(A_{12}-A_{21})\,,$$
$$A_{11}=A_{22}=(A_{12}+A_{21})\,.$$

(ii) Classes 622, $6\underline{mm}$, $\underline{\bar{6}}2\underline{m}$, $6/\underline{mmm}$

$$\beta_{ij}=\beta_1\delta_{ij}+\beta_2 v_{3i}v_{3j}\,. \quad (22)$$

(iii) Classes $6\underline{22}$, $6mm$, $\underline{\bar{6}}2m$, $6/\underline{m}mm$

$$\beta_{ij}=\beta(v_{1i}v_{2j}-v_{2i}v_{1j})\,. \quad (23)$$

Cubic system

(i) Classes 23, $\underline{m}3$, 432, $\underline{\bar{4}}3\underline{m}$, $\underline{m}3\underline{m}$

$$\beta_{ij}=\beta\delta_{ij}\,, \quad (24)$$

where (11) has been used, and $\beta=A_{11}=A_{22}=A_{33}$.

4. Invariant piezomagnetic coefficients

Regarding the choice of rotation axes and mirror planes in various crystal systems, we adopt the same convention as in the last section. Non-vanishing piezomagnetic coefficients exist only in 66 of the 90 magnetic crystal classes (Bhagavantam, 1966).

Triclinic system

(i) Classes 1, $\bar{1}$

We insert the condition $d_{ijk}=d_{ikj}$ in (5) and obtain

$$d_{ijk}=v_{ai}v_{bj}v_{ck}A_{abc}\,, \quad (25)$$

where $A_{abc}=A_{acb}$ (a, b, $c=1, 2, 3$) are the 18 invariant piezomagnetic coefficients for the classes 1 and $\bar{1}$.

Once again we furnish below only the final results. The method of imposing the symmetry conditions on

(25) is the same as described by Srinivasan & Nigam (1969).

Monoclinic system

(i) Classes 2, m, $2/m$

$$\begin{aligned} d_{ijk} = {} & d_1 v_{3i}v_{3j}v_{3k} + d_2(v_{1i}v_{1j}v_{3k} + v_{1i}v_{3j}v_{1k}) + d_3 v_{3i}v_{1j}v_{1k} \\ & + d_4(v_{2i}v_{2j}v_{3k} + v_{2i}v_{3j}v_{2k}) + d_5 v_{3i}v_{2j}v_{2k} \\ & + d_6(v_{1i}v_{2j}v_{3k} + v_{1i}v_{3j}v_{2k}) + d_7(v_{2i}v_{3j}v_{1k} + v_{2i}v_{1j}v_{3k}) \\ & + d_8(v_{3i}v_{1j}v_{2k} + v_{3i}v_{2j}v_{1k}) . \end{aligned} \tag{26}$$

(ii) Classes $\underline{2}$, $\underline{m}$, $\underline{2}/\underline{m}$

$$\begin{aligned} d_{ijk} = {} & d_1 v_{1i}v_{1j}v_{1k} + d_2 v_{2i}v_{2j}v_{2k} + d_3(v_{1i}v_{1j}v_{2k} + v_{1i}v_{2j}v_{1k}) \\ & + d_4 v_{2i}v_{1j}v_{1k} + d_5(v_{2i}v_{2j}v_{1k} + v_{2i}v_{1j}v_{2k}) + d_6 v_{1i}v_{2j}v_{2k} \\ & + d_7(v_{3i}v_{3j}v_{1k} + v_{3i}v_{1j}v_{3k}) + d_8 v_{1i}v_{3j}v_{3k} \\ & + d_9(v_{3i}v_{3j}v_{2k} + v_{3i}v_{2j}v_{3k}) + d_{10} v_{2i}v_{2j}v_{3k} . \end{aligned} \tag{27}$$

Orthorhombic system

(i) Classes 222, $2mm$, mmm

$$\begin{aligned} d_{ijk} = {} & d_1(v_{1i}v_{2j}v_{3k} + v_{1i}v_{3j}v_{2k}) + d_2(v_{2i}v_{3j}v_{1k} + v_{2i}v_{1j}v_{3k}) \\ & + d_3(v_{3i}v_{1j}v_{2k} + v_{3i}v_{2j}v_{1k}) . \end{aligned} \tag{28}$$

(ii) Classes $\underline{2}\underline{m}m$, $2\underline{mm}$, $\underline{22}2$, $\underline{mm}m$

$$\begin{aligned} d_{ijk} = {} & d_1 v_{3i}v_{3j}v_{3k} + d_2(v_{1i}v_{1j}v_{3k} + v_{1i}v_{3j}v_{1k}) + d_3 v_{3i}v_{1j}v_{1k} \\ & + d_4(v_{2i}v_{2j}v_{3k} + v_{2i}v_{3j}v_{2k}) + d_5 v_{3i}v_{2j}v_{2k} . \end{aligned} \tag{29}$$

Tetragonal system

(i) Classes 4, $\bar{4}$, $4/m$

$$\begin{aligned} d_{ijk} = {} & d_1 v_{3i}v_{3j}v_{3k} + d_2(v_{3k}\delta_{ij} + v_{3j}\delta_{ik}) + d_3 v_{3i}\delta_{jk} \\ & + d_4[v_{3k}(v_{1i}v_{2j} - v_{2i}v_{1j}) + v_{3j}(v_{1i}v_{2k} - v_{2i}v_{1k})] , \end{aligned} \tag{30}$$

where we have made use of (11) and

$$d_1 = (A_{333} - 2A_{113} - A_{311}) , \quad d_2 = A_{113} = A_{223} ,$$
$$d_3 = A_{311} = A_{322} , \quad d_4 = A_{123} .$$

Suppose we choose a Cartesian system whose x, y, and z axes coincide with $\mathbf{v}_1$, $\mathbf{v}_2$, $\mathbf{v}_3$ respectively, then (30) gives the correct number of non-vanishing coefficients d_{ijk} satisfying the relations (Bhagavantam, 1966)

$$\begin{aligned} & d_{311} = d_{322} = d_3 , \quad d_{333} = d_1 + 2d_2 + d_3 , \\ & d_{123} = -d_{231} = d_4 , \quad d_{113} = d_{223} = d_2 , \end{aligned} \tag{31}$$

where we have used the fact that for the *special* (which is also the conventional) choice of the Cartesian system made $v_{11} = v_{22} = v_{33} = 1$ and all others vanish.

(ii) Classes $4\underline{22}$, $4\underline{mm}$, $\bar{4}\underline{2m}$, $4/m\underline{mm}$

$$d_{ijk} = d_1 v_{3i}v_{3j}v_{3k} + d_2(v_{3k}\delta_{ij} + v_{3j}\delta_{ik}) + d_3 v_{3i}\delta_{jk} . \tag{32}$$

(iii) Classes $\underline{4}$, $\underline{\bar{4}}$, $\underline{4}/m$

$$\begin{aligned} d_{ijk} = {} & d_1[v_{3k}(v_{1i}v_{1j} - v_{2i}v_{2j}) + v_{3j}(v_{1i}v_{1k} - v_{2i}v_{2k})] \\ & + d_2 v_{3i}(v_{1j}v_{1k} - v_{2j}v_{2k}) + d_3[v_{3k}(v_{1i}v_{2j} + v_{2i}v_{1j}) \\ & + v_{3j}(v_{1i}v_{2k} + v_{2i}v_{1k})] + d_4 v_{3i}(v_{1j}v_{2k} + v_{2j}v_{1k}) . \end{aligned} \tag{33}$$

(iv) Classes $\underline{4}2\underline{2}$, $\underline{4}m\underline{m}$, $\underline{\bar{4}}2\underline{m}$, $\underline{\bar{4}}\underline{2}m$, $\underline{4}/m\underline{m}m$

$$\begin{aligned} d_{ijk} = {} & d_3[v_{3k}(v_{1i}v_{2j} + v_{2i}v_{1j}) + v_{3j}(v_{1i}v_{2k} + v_{2i}v_{1k})] \\ & + d_4 v_{3i}(v_{1j}v_{2k} + v_{2j}v_{1k}) . \end{aligned} \tag{34}$$

(v) Classes 422, $4mm$, $\bar{4}2m$, $4/mmm$

$$d_{ijk} = d[v_{3k}(v_{1i}v_{2j} - v_{2i}v_{1j}) + v_{3j}(v_{1i}v_{2k} - v_{2i}v_{1k})] . \tag{35}$$

Rhombohedral system

(i) Classes 3, $\bar{3}$

$$\begin{aligned} d_{ijk} = {} & d_1 v_{3i}v_{3j}v_{3k} + d_2(v_{3k}\delta_{ij} + v_{3j}\delta_{ik}) + d_3 v_{3i}\delta_{jk} \\ & + d_4[v_{3k}(v_{1i}v_{2j} - v_{2i}v_{1j}) + v_{3j}(v_{1i}v_{2k} - v_{2i}v_{1k})] \\ & + d_5(v_{1i}v_{1j}v_{1k} - v_{2i}v_{2j}v_{2k} + v_{1i}v_{1j}v_{2k} + v_{1i}v_{2j}v_{1k} \\ & + v_{2i}v_{1j}v_{1k}) + d_6(v_{2i}v_{2j}v_{2k} - v_{1i}v_{1j}v_{1k} + v_{2i}v_{2j}v_{1k} \\ & + v_{2i}v_{1j}v_{2k} + v_{1i}v_{2j}v_{2k}) , \end{aligned} \tag{36}$$

where we have used (17), and

$$\begin{aligned} & d_1 = A_{333} - \tfrac{3}{2}(A_{123} + A_{231}) - \tfrac{3}{2}A_{312} , \\ & d_2 = \tfrac{3}{4}(A_{123} + A_{231}) , \quad d_3 = \tfrac{3}{2}A_{312} , \\ & d_4 = \tfrac{1}{2}(A_{123} - A_{231}) , \quad d_5 = A_{112} , \quad d_6 = A_{221} . \end{aligned}$$

(ii) Classes $3\underline{2}$, $3\underline{m}$, $\bar{3}\underline{m}$

$$\begin{aligned} d_{ijk} = {} & d_1 v_{3i}v_{3j}v_{3k} + d_2(v_{3k}\delta_{ij} + v_{3j}\delta_{ik}) + d_3 v_{3i}\delta_{jk} \\ & + d_5(2v_{1i}v_{1j}v_{1k} - 2v_{2i}v_{2j}v_{2k} + v_{1i}v_{1j}v_{2k} + v_{1i}v_{2j}v_{1k} \\ & + v_{2i}v_{1j}v_{1k} - v_{2i}v_{2j}v_{1k} - v_{2i}v_{1j}v_{2k} - v_{1i}v_{2j}v_{2k}) . \end{aligned} \tag{37}$$

(iii) Classes 32, $3m$, $\bar{3}m$

$$\begin{aligned} d_{ijk} = {} & d_4[v_{3k}(v_{1i}v_{2j} - v_{2i}v_{1j}) + v_{3j}(v_{1i}v_{2k} - v_{2i}v_{1k})] \\ & + d_5(v_{1i}v_{1j}v_{2k} + v_{1i}v_{2j}v_{1k} + v_{2i}v_{1j}v_{1k} + v_{2i}v_{2j}v_{1k} \\ & + v_{2i}v_{1j}v_{2k} + v_{1i}v_{2j}v_{2k}) . \end{aligned} \tag{38}$$

Hexagonal system

(i) Classes 6, $\bar{6}$, $6/m$

$$\begin{aligned} d_{ijk} = {} & d_1 v_{3i}v_{3j}v_{3k} + d_2(v_{3k}\delta_{ij} + v_{3j}\delta_{ik}) + d_3 v_{3i}\delta_{jk} \\ & + d_4[v_{3k}(v_{1i}v_{2j} - v_{2i}v_{1j}) + v_{3j}(v_{1i}v_{2k} - v_{2i}v_{1k})] , \end{aligned} \tag{39}$$

where (17) has been utilized, and

$$\begin{aligned} & d_1 = A_{333} - \tfrac{3}{2}(A_{123} + A_{231}) - \tfrac{3}{2}A_{312} , \\ & d_2 = \tfrac{3}{2}(A_{123} + A_{231}) , \quad d_3 = A_{312} , \quad d_4 = \tfrac{1}{2}(A_{123} - A_{231}) . \end{aligned}$$

(ii) Classes $6\underline{22}$, $6\underline{mm}$, $\bar{6}\underline{2m}$, $6/m\underline{mm}$

$$d_{ijk} = d_1 v_{3i}v_{3j}v_{3k} + d_2(v_{3k}\delta_{ij} + v_{3j}\delta_{ik}) + d_3 v_{3i}\delta_{jk} . \tag{40}$$

(iii) Classes $\underline{6}$, $\underline{\bar{6}}$, $\underline{6}/\underline{m}$

$$\begin{aligned} d_{ijk} = {} & d_1(v_{1i}v_{1j}v_{1k} - v_{2i}v_{2j}v_{2k} + v_{1i}v_{1j}v_{2k} + v_{1i}v_{2j}v_{1k} \\ & + v_{2i}v_{1j}v_{1k}) + d_2(v_{2i}v_{2j}v_{2k} - v_{1i}v_{1j}v_{1k} + v_{2i}v_{2j}v_{1k} \\ & + v_{2i}v_{1j}v_{2k} + v_{1i}v_{2j}v_{2k}) . \end{aligned} \tag{41}$$

(iv) Classes $\underline{6}\underline{2}2$, $\underline{6}\underline{m}m$, $\underline{\bar{6}}\underline{2}m$, $\underline{\bar{6}}2\underline{m}$, $\underline{6}/\underline{m}m\underline{m}$

$$\begin{aligned} d_{ijk} = {} & d_1(v_{1i}v_{1j}v_{2k} + v_{1i}v_{2j}v_{1k} + v_{2i}v_{1j}v_{1k} + v_{2i}v_{2j}v_{1k} \\ & + v_{2i}v_{1j}v_{2k} + v_{1i}v_{2j}v_{2k}) . \end{aligned} \tag{42}$$

(v) Classes 622, $6mm$, $\bar{6}2m$, $6/mmm$

$$d_{ijk}=d[v_{3k}(v_{1i}v_{2j}-v_{2i}v_{1j})+v_{3j}(v_{1i}v_{2k}-v_{2i}v_{1k})]\,. \tag{43}$$

Cubic system

(i) Classes $\underline{23}$, $\underline{m3}$, $\underline{432}$, $\underline{\bar{4}3m}$, $\underline{m3m}$

$$d_{ijk}=d(v_{1i}v_{2j}v_{3k}+v_{1i}v_{3j}v_{2k}+v_{2i}v_{3j}v_{1k}+v_{2i}v_{1j}v_{3k}+v_{3i}v_{1j}v_{2k}+v_{3i}v_{2j}v_{1k})\,. \tag{44}$$

The form-invariant expressions for β_{ij} and d_{ijk} obtained in the case of various magnetic crystal classes are referred to a Cartesian coordinate system with respect to which the triad $\mathbf{v}_1$, $\mathbf{v}_2$, $\mathbf{v}_3$ has an arbitrary orientation. However, when conventional choice (Bhagavantam, 1966) of the Cartesian system is made, the form-invariant expression furnished above gives the appropriate number of non-vanishing components d_{ijk}, as demonstrated in the case of (30). A similar check can be made in the case of expressions for β_{ij} and d_{ijk} corresponding to other classes.

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References

BHAGAVANTAM, S. (1966). *Crystal Symmetry and Physical Properties*. New York: Academic Press.
BIRSS, R. R. (1963). *Rep. Prog. Phys.* **26**, 307.
DZYALOSHINSKII, I. E. (1959). *Sov. Phys. JETP*, **10**, 628.
HORNREICH, R. M. & SHTRIKMAN, S. (1968). *Phys. Rev.* **171**, 1065.
MASON, W. P. (1966). *Crystal Physics of Interaction Processes*. New York: Academic Press.
NOWACKI, W. (1962). *Thermoelasticity*, p. 586. Oxford: Pergamon Press.
O'DELL, T. H. (1970). *The Electrodynamics of Magneto-Electric Media*. Amsterdam: North Holland.
SRINIVASAN, T. P. (1970). *Phys. Stat. Sol.* **41**, 615.
SRINIVASAN, T. P. & NIGAM, S. D. (1968*a*). *Phys. Stat. Sol.* **28**, K71.
SRINIVASAN, T. P. & NIGAM, S. D. (1968*b*). *J. Math. Phys. Sci.* **2**, 311.
SRINIVASAN, T. P. & NIGAM, S. D. (1969). *J. Math. Mech.* **19**, 411.

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Shubnikov Point Groups and the Property of 'Ferroelasticity'

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Previously the concept of ferroelasticity, introduced by Aizu, has only been studied in connexion with classical point groups. In this paper the use of this concept is extended to the Shubnikov point groups; this is important in connexion with ferroelectric phase transitions and various kinds of magnetic phase transition. Tables are given which enable all ferroelastic species to be identified.

1. Introduction

The concept of a 'ferroelastic' crystal was introduced by Aizu (1969) and it is relevant to the discussion of displacive phase transitions. By the term 'displacive' phase transition we mean a phase transition which does not involve any major structural rearrangement of the atomic positions in a crystal, but involves only rather small displacements of the equilibrium positions of the atoms. These displacements will generally be accompanied by a reduction in the symmetry of the crystal and displacive phase transitions may also be ferroelectric transitions but need not necessarily be so. The concept of ferroelasticity, its relationship to the phenomenon of ferroelectricity, and the examination of the symmetries of ferroelastic crystals described by Aizu (1969) was restricted to materials with the symmetry of one of the 32 classical point groups. It seemed to be desirable to extend Aizu's work to the Shubnikov point groups for two reasons. First, there are many possible ferroelectric symmetries which are described by Shubnikov point groups (Neronova & Belov, 1959; Ascher, 1970; Schelkens, 1970; Zheludev, 1971). Secondly, it would seem to be profitable to extend the use of the concept of 'ferroelasticity' in connexion with magnetic phase transitions, which would also involve the use of Shubnikov point groups.

In many magnetic crystals the onset of magnetic ordering is accompanied by a magnetostrictive distortion of the crystal structure, with a consequent reduction in the symmetry of the crystal. There may be several possible choices of direction for the preferred orientation associated with the magnetic ordering, with the resultant occurrence of magnetic domains even within a crystal that was a single crystal in its non-magnetic phase. The relevance of the concept of ferro-