still be increasing at 97·5% TD. This suggests that discontinuous grain growth may be taking place. However, the large uncertainties in the scattering volume fraction, φ, and the effective radii, $R_{eff}(0)$ and $R_{eff}(\infty)$, preclude drawing firm conclusions.

Although the final-stage samples were originally intended for single-scattering SANS measurements, it was found that even the 97·5% TD sample was within the limit of applicability of the MSANS technique. There was significant wavelength-dependent beam broadening and even the smallest $\bar{z}$ value ($\bar{z} = 40$) is well within the MSANS formalism. However, the fact that φ is so small means that the change in r_c as a function of λ is small (see Fig. 4). This nearly flat slope makes the refinement procedure difficult, resulting in large uncertainties in the fitted $R_{eff}(0)$ and φ values. To improve the determination of $R_{eff}(0)$ during final-stage sintering, measurements of the higher-density samples are planned with a high-resolution small-angle X-ray scattering instrument (Long, Jemian, Weertman, Black, Burdette & Spal, 1991). This instrument can measure the single-scattering intensities from pores 4·0 nm to 1·0 μm in size and thus bridge the gap between those sizes which can be easily measured by conventional SANS and MSANS techniques.

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SHORT COMMUNICATIONS

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Rank 0, 1, 2 and 3 magnetic and non-magnetic physical-property tensors.

By S. Y. LITVIN* and D. B. LITVIN, *Department of Physics, The Pennsylvania State University, The Berks Campus, PO Box 7009, Reading, PA 19610-6009, USA*

Abstract

The form of 36 rank 0, 1, 2 and 3 magnetic and non-magnetic physical-property tensors invariant under each of the 236 subgroups of $6(Z)/M(Z)M(X)M(1)1'$ ($D_{6h}1'$) and each of the 420 subgroups of $M(Z)\bar{3}(XYZ)M(XY)1'$ (O_h1') is tabulated.

* Mailing address: 1701 Bern Road, Apartment B2, Wyomissing, PA 19610, USA.

1. Introduction

A vast amount of literature exists on the derivation and tabulation of the form of physical-property tensors invariant under the non-magnetic crystallographic point groups (Jahn, 1949; Nye, 1957; Birss, 1964; Wooster, 1973; Kopsky, 1979a; Fumi & Ripamonti, 1980; Sands, 1982; and references contained in these sources). A wide variety of tensors and their physical interpretation is given by Sirotin & Shaskolskaya (1975). Recently, a computer-based

tabulation of the form of 20 rank 0, 1 and 2 physical-property tensors invariant under each of the 97 subgroups of $M(Z)\bar{3}(XYZ)M(XY)$ (O_h) and the 53 subgroups of $6(Z)/M(Z)M(X)M(1)$ (D_{6h}) has been given by Litvin & Litvin (1990).

The form of physical-property tensors invariant under magnetic crystallographic point groups has also been considered (Sirotin, 1962; Birss, 1964; Tenenbaum, 1966; Kopsky, 1976, 1979b; and references contained in these sources). The usual tabulations of the form of physical-property tensors give the form invariant under a single magnetic point group from each type of magnetic point group. For example, the form of a tensor is given invariant under the magnetic point group $2(Z)/M(Z)'$ of the magnetic-point-group type $2/M'$. It is left to the reader to calculate the form of the tensor invariant under other magnetic point groups of the type $2/M'$, i.e. $2(X)/M(X)'$, $2(Y)/M(Y)'$, $2(XY)/M(XY)'$, $2(\bar{X}Y)/M(\bar{X}Y)'$, $2(YZ)/M(YZ)'$, $2(\bar{Y}Z)/M(\bar{Y}Z)'$, $2(XZ)/M(XZ)'$, $2(\bar{X}Z)/M(\bar{X}Z)'$, $2(1)/M(1)'$, $2(2)/M(2)'$ and $2(3)/M(3)'$. To bypass having to do such calculations, we consider here all subgroups of all magnetic point groups (Ascher & Janner, 1965). Consequently, we have tabulated the form of 36 rank 0, 1, 2 and 3 physical-property tensors invariant under each of the 326 subgroups of $6(Z)/M(Z)M(X)M(1)1'$ ($D_{6h}1'$) and each of the 420 subgroups of $M(Z)\bar{3}(XYZ)M(XY)1'$ (O_h1').* The physical-property tensors are discussed in § 2 and an example of this tabulation is given in § 3.

2. Physical-property tensors

The four types of rank 0 physical-property tensors will be denoted by 1, e, a and ae and are defined, in Table 1, by their transformation properties under the action of spatial inversion $\bar{1}$ and time inversion $1'$. The rank 0 tensor given in the ith row of the left-hand-side column transformed by the element in the jth column of the top row is given at the intersection of the ith row and jth column. The nomenclature for these four rank 0 tensors given in the right-hand-side column is that introduced by Birss (1964): *scalar* and *pseudoscalar* refer to tensors which, respectively, are invariant or change sign under spatial inversion. The prefixes i and c refer to tensors which, respectively, are invariant or change sign under time inversion.

In Table 2 we list the 36 rank 0, 1, 2 and 3 physical-property tensors considered in this paper. These tensors are given in terms of a rank 0 tensor and products of the polar vector tensor V. The symbols [ ] and { }, as in $[V^2]$, $[V^3]$ and $\{V^2\}$, denote the symmetrization and anti-symmetrization, respectively, of the tensor contained within the symbol. The Birss (1964) nomenclature of the type of each tensor is given in the top row of each column of tensors.

Table 1. *Transformation properties of rank 0 physical-property tensors under spatial inversion $\bar{1}$ and time inversion $1'$*

Transformation	1	$\bar{1}$	$1'$	$\bar{1}'$	Name
Rank 0	1	1	1	1	i scalar
physical-	e	e	$-e$	e	$-e$ i pseudoscalar
property	a	a	a	$-a$	$-a$ c scalar
tensor	ae	ae	$-ae$	$-ae$	ae c pseudoscalar

Table 2. *The 36 physical-property tensors considered in this paper*

[ ] denotes symmetrization and { } anti-symmetrization. The Birss (1964) nomenclature of the type of each tensor is given at the top of each column of tensors.

Name	i polar	i axial	c polar	c axial
Rank 0	1	e	a	ae
Rank 1	V	eV	aV	aeV
Rank 2	V^2	eV^2	aV^2	aeV^2
	$[V^2]$	$e[V^2]$	$a[V^2]$	$ae[V^2]$
	$\{V^2\}$	$e\{V^2\}$	$a\{V^2\}$	$ae\{V^2\}$
Rank 3	V^3	eV^3	aV^3	aeV^3
	$V[V^2]$	$eV[V^2]$	$aV[V^2]$	$aeV[V^2]$
	$V\{V^2\}$	$eV\{V^2\}$	$aV\{V^2\}$	$aeV\{V^2\}$
	$[V^3]$	$e[V^3]$	$a[V^3]$	$ae[V^3]$

Table 3. *The form of the magnetoelectric effect tensor, a physical-property tensor of the type aeV^2, invariant under each of the magnetic point groups of the type $\bar{3}'$ which are subgroups of the magnetic point groups $M(Z)\bar{3}(XYZ)M(XY)1'$ (O_h1') and $6(Z)/M(Z)M(X)M(1)1'$ ($D_{6h}1'$)*

$\bar{3}(Z)'$ $\begin{bmatrix} A & C & 0 \\ -C & A & 0 \\ 0 & 0 & B \end{bmatrix}$ $\bar{3}(XYZ)'$ $\begin{bmatrix} A & B & C \\ C & A & B \\ B & C & A \end{bmatrix}$

$\bar{3}(\bar{X}YZ)'$ $\begin{bmatrix} A & B & C \\ C & A & -B \\ B & -C & A \end{bmatrix}$ $\bar{3}(X\bar{Y}Z)'$ $\begin{bmatrix} A & B & -C \\ C & A & B \\ -B & C & A \end{bmatrix}$

$\bar{3}(XY\bar{Z})'$ $\begin{bmatrix} A & -B & C \\ -C & A & B \\ B & C & A \end{bmatrix}$

The form of the physical-property tensors is given in a Cartesian coordinate system with axes denoted by x, y and z which follows the convention of the *Standards on Piezoelectric Crystals* (1949) (see also Nye, 1957, p. 282). The advantage of using a Cartesian coordinate system in giving the form of the physical-property tensors is in that one then does not have to distinguish between covariant and contravariant tensor indices (Sands, 1982). This coordinate system coincides with the cubic Cartesian coordinate system X, Y, Z used to denote the subgroups of $M(Z)\bar{3}(XYZ)M(XY)1'$ (O_h1'). For the hexagonal coordinate system X, Y, Z used to denote the subgroups of $6(Z)/M(Z)M(X)M(1)1'$ ($D_{6h}1'$), the physical-property tensor Cartesian coordinate system is oriented such that

the x axis is parallel to the hexagonal X axis and the z axis is parallel to the hexagonal Z axis.

3. An example: the magnetoelectric effect

The magnetoelectric effect is represented by the rank 2 c-axial physical-property tensor aeV^2 (Birss, 1964). In the tabulation given by Birss (1964) only the case corresponding to the magnetic point group $\bar{3}(Z)'$ of the magnetic-point-group type $\bar{3}'$ is given. In Table 3 we give the form of the magnetoelectric-effect tensor for all magnetic point groups which are subgroups of $M(Z)\bar{3}(XYZ)M(XY)1'$ (O_h1') and $6(Z)/M(Z)M(X)M(1)1'$ $(D_{6h}1')$ and which belong to the magnetic-point-group type $\bar{3}'$. The complete list of forms of the magnetoelectric-effect tensor invariant under all magnetic point groups is contained within the deposited tabulations.*

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* See deposition footnote.

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A comment on the asymmetric part of the translation function.

By FRANTIŠEK PAVELČÍK, Department of Inorganic Chemistry, Faculty of Natural Sciences, J. A. Komensky University, CS-842 15 Bratislava, Czechoslovakia

Abstract

The asymmetric part of the translation function is closely related to a unit cell and the symmetry of the multiple implication function. The actual asymmetric part depends on the symmetry of the fragment.

Theory

The translation function is used to locate a correctly oriented molecular fragment in the unit cell with respect to the symmetry elements. The full symmetry translation function can be given, for example, by (Pavelčík, 1988)

$$T(r) = \min_{i=1}^{F} \min_{j=1}^{F} \min_{m=1}^{S} \min_{n=1}^{S} P\{[R_n(r+r_i)+t_n]$$

$$-[R_m(r+r_j)+t_m]\}, \qquad (1)$$

where F is the number of atoms in the fragment, r_i are vectors to the atoms of the fragment, r is a search vector, R_n are rotational and t_n translational parts of the symmetry operator, respectively. S is the number of space-group operators. A search volume is given by an asymmetric part of the translation function.

In the papers of Egert & Sheldrick (1985) and Rius & Miravitlles (1987) it is stated that the asymmetric unit of the translation function is defined uniquely by the Cheshire groups (Hirshfeld, 1968). It is not clear whether this means an asymmetric unit or a unit cell of the Cheshire group. On the other hand, Wilson & Tollin (1986) state in the PATMET program instructions that the unique region is $0-\frac{1}{2}$ on each relevant axis. Both statements are only partially

correct. The Cheshire groups have limits in the application to the pure translation problem because of special treatment of chirality.

The asymmetric part of the translation function depends in general on the space group of the crystal and on the point group of the fragment. Owing to the symmetry of the Patterson function $P(r) = P(R_n r)$, (1) can be simplified to*

$$T(r) = \min_{i=1}^{F} \min_{j=1}^{F} \min_{s=1}^{S} P[(R_s - I)r + t_s + R_s r_i - r_j]. \qquad (2)$$

For the extreme case of a single (heavy) atom, the translation function is reduced to

$$T(r) = \min_{s=1}^{S} P[(R_s - I)r + t_s + (R_s - I)r_1]. \qquad (3)$$

Equation (3) is equivalent to the multiple implication (symmetry minimum) function, MIF (Ellison & Levy, 1965; Simpson, Dobrott & Lipscomb, 1965), with the origin shifted by an arbitrary vector r_1. The symmetry of the multiple implication function has recently been described by Zimmermann (1988) and Pavelčík (1990). The MIF groups are closely related to the Cheshire groups. In the case of a single atom, the asymmetric part of the translation function is given by the asymmetric part of the MIF group.

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* There is an error in equation (9) of Pavelčík (1988). It should read

$$D(r) = \left[\min_{k=1}^{n} \min_{l\geq k}^{n} \min_{j=2}^{S} \frac{Z_1 Z_1}{m_{ij} Z_k Z_l} P(r - R_j r - t_j + r_k^o - R_j r_l^o) \right]^{1/2}.$$