## Decomposition of tensors representing physical properties of crystals

This article has been downloaded from IOPscience. Please scroll down to see the full text article.
1998 J. Phys.: Condens. Matter 103489
(http://iopscience.iop.org/0953-8984/10/16/003)
View the table of contents for this issue, or go to the journal homepage for more

Download details:
IP Address: 171.66.16.151
The article was downloaded on 12/05/2010 at 23:21

Please note that terms and conditions apply.

# Decomposition of tensors representing physical properties of crystals 

T P Srinivasan<br>Department of Physics, Madurai Kamaraj University, Madurai 625 021, India

Received 16 October 1997, in final form 5 January 1998


#### Abstract

A recipe for generating orthonormal tensor basis is given, and as an illustration the third-rank tensor describing the piezoelectric effect is discussed. Unlike the case of the elastic stiffness (fourth-rank) tensor, the present method does not resort to the classical results of the theory of invariants in generating the tensor basis. Employing this basis it is easy to calculate the norm of the physical property and the results obtained are identical with those derived by using the decomposition in terms of the irreducible tensors. In conclusion, a detailed discussion comparing the three different methods of decomposition of tensors representing physical properties of crystals is presented.


## 1. Introduction

Tensors are the most apt mathematical entities to describe direction-dependent physical properties of condensed matter, and ipso facto the tensor components characterizing physical properties vary with the direction of the coordinate axes and hence do not determine directly the material constants (Nowacki 1962). Physical properties are intrinsic characteristics of matter and their values must, therefore, be specified without reference to any coordinate system (Srinivasan and Nigam 1968, 1969, Srinivasan 1970, Juretschke 1974, Jerphagnon et al 1978, Walpole 1981, 1984). It is, therefore, natural to seek to describe physical properties of condensed matter in terms of quantities that are independent of the coordinate system, namely, constants of matter or invariants.

In this connection, three different methods have been developed. The first method (hereinafter referred to as method I) (Smith and Rivlin 1958, Smith 1967) treats the strainenergy function as a polynomial in the strain components, and leads to the determination integrity basis for invariant (under a subgroup of the orthogonal group $O$ (3)) functions of the strain components for each one of the 32 crystallographic point groups. Using the integrity basis, and orthonormal tensor basis which spans the space of elastic (stiffness) constants is derived (Tu 1968) and an invariant norm is obtained. In the second method (hereinafter referred to as method II), a (physical property) tensor is resolved along the triad $\boldsymbol{\nu}_{1}, \boldsymbol{\nu}_{2}, \boldsymbol{\nu}_{3}$ denoting the unit vectors along the crystallographic axes (Srinivasan and Nigam 1968, 1969, Srinivasan 1970). The process of resolution yields the invariants. In the third method (hereinafter referred to as method III) (Spencer 1970, Jerphagnon et al 1978) the given tensor is decomposed into irreducible tensors occurring in the quantum theory of angular momentum. As the constituent irreducible parts of different weights are orthogonal it has been possible to define a norm which is invariant. It should be mentioned here that whereas decomposition of a tensor of any rank can be carried through (Srinivasan 1985,
1988) by methods II and III, the utility of method I seems to be restricted to the elastic stiffness tensor.

In the present paper, the results of method II are used to develop a recipe for generating orthonormal tensor bases. This is done in section 2, and section 3 comprises a discussion comparing the three methods and establishing the link between them.

## 2. Orthonormal tensor basis

We begin with a brief outline of the method II. The form-invariant expressions (Srinivasan and Nigam 1969) for the electrical susceptibility components, the piezoelectric coefficients and the elastic stiffness coefficients are, respectively,

$$
\begin{align*}
& \chi_{i j}=v_{a i} v_{b j} A_{a b}  \tag{1a}\\
& d_{i j k}=v_{a i} v_{b j} v_{c k} A_{a b c}  \tag{1b}\\
& C_{i j k m}=v_{a i} v_{b j} v_{c k} v_{d m} A_{a b c d} \tag{1c}
\end{align*}
$$

where summation is implied by repeated indices and this convention is followed throughout. These expressions are referred to a Cartesian system $\mathrm{O} x y z ; \nu_{a i}$ are the components of the unit vectors $\nu_{a}(a=1,2,3)$ along the crystallographic axes. The quantities $A_{a b}, A_{a b c}$ and $A_{a b c d}$ are invariants in the sense that when the Cartesian system is rotated to a new orientation $\mathrm{O} x^{\prime} y^{\prime} z^{\prime}$, then (1a) to (1c) take, respectively, the form

$$
\begin{align*}
& \chi_{i j}^{\prime}=v_{a i}^{\prime} v_{b j}^{\prime} A_{a b}  \tag{2a}\\
& d_{i j k}^{\prime}=v_{a i}^{\prime} v_{b j}^{\prime} v_{c k}^{\prime} A_{a b c}  \tag{2b}\\
& C_{i j k m}^{\prime}=v_{a i}^{\prime} v_{b j}^{\prime} v_{c k}^{\prime} v_{d m}^{\prime} A_{a b c d} . \tag{2c}
\end{align*}
$$

It should be remembered that $\nu_{1}, \boldsymbol{\nu}_{2}, \boldsymbol{\nu}_{3}$ form a linearly independent basis in three dimensions but are not necessarily always orthogonal. Their relative orientations in the seven crystal systems are well known (Nye 1976).

The particular form of, say, (1c) for the cubic crystals (Thomas 1966, Srinivasan and Nigam 1969) is

$$
\begin{equation*}
C_{i j k m}=\lambda \delta_{i j} \delta_{k m}+\mu\left(\delta_{i k} \delta_{j m}+\delta_{i m} \delta_{j k}\right)+\alpha v_{a i} v_{a j} v_{a k} v_{a m} \tag{3}
\end{equation*}
$$

where $\lambda$ and $\mu$ are the familiar Lamé constants of isotropic elasticity. The expression (3) can be derived by subjecting $C_{i j k m}$ in (1c) to the appropriate point group symmetries of the cubic class, and the details of the method are documented (Srinivasan and Nigam 1969) in connection with obtaining the invariant elastic constants.

A similar exercise with ( $1 b$ ) will yield, for the class 6 mm (Srinivasan 1970)

$$
\begin{equation*}
d_{i j k}=d_{1} \nu_{3 i} \nu_{3 j} \nu_{3 k}+d_{2}\left(\nu_{3 k} \delta_{i j}+\nu_{3 j} \delta_{i k}\right)+d_{3} \nu_{3 i} \delta_{j k} \tag{4}
\end{equation*}
$$

where $\nu_{3}$ is the sixfold axis. Similarly, for the uniaxial crystals, we have from (1a) (Chandrasekhar and Srinivasan 1972)

$$
\begin{equation*}
\chi_{i j}=\chi_{1} \delta_{i j}+\chi_{2} \nu_{3 i} \nu_{3 j} \tag{5}
\end{equation*}
$$

where $\nu_{3}$ is the unique axis and $\chi_{1}$ corresponds to isotropy.
The first step in the generation of orthonormal tensor basis is one of writing the Kronecker delta $\delta_{a i}$ in the place of $v_{a i}$ in (1a) to (1c). They will assume, respectively, the form

$$
\begin{align*}
& \chi_{i j}=\delta_{a i} \delta_{b j} X_{a b}  \tag{6a}\\
& d_{i j k}=\delta_{a i} \delta_{b j} \delta_{c k} X_{a b c}  \tag{6b}\\
& C_{i j k m}=\delta_{a i} \delta_{b j} \delta_{c k} \delta_{d m} X_{a b c d} \tag{6c}
\end{align*}
$$

where the coefficients $X$ are similar to the $A$ in (1). Now one can subject the expressions $(6 a)-(6 c)$ to the symmetries of any crystal class and then derive the elements of the basis appropriate to that class. Instead we can take the form-invariant expression for any given class and straightaway replace the $\nu_{a i}$ by the $\delta_{a i}$ to obtain the elements of the basis. As an illustration, let us consider the simplest example, namely, the expression (5). According to the present scheme, the elements of the basis are

$$
\begin{equation*}
\delta_{i j} \quad \delta_{3 i} \delta_{3 j} \tag{7}
\end{equation*}
$$

However, these are neither orthogonal nor normalized. The next step, therefore, is to orthonormalize them by the usual Gram-Schmidt process and the result is

$$
\begin{equation*}
T_{i j}^{I}=\frac{1}{\sqrt{3}} \delta_{i j} \quad T_{i j}^{I I}=\frac{1}{\sqrt{6}}\left(3 \delta_{3 i} \delta_{3 j}-\delta_{i j}\right) \tag{8}
\end{equation*}
$$

The analogue of (5) for the monoclinic system, with $\boldsymbol{\nu}_{2}$ normal to the $\boldsymbol{\nu}_{3} \boldsymbol{\nu}_{1}$-plane, is (Chandrasekhar and Srinivasan 1972)

$$
\begin{equation*}
\chi_{i j}=A_{11} v_{1 i} v_{1 j}+A_{22} v_{2 i} v_{2 j}+A_{33} v_{3 i} v_{3 j}+A_{31}\left(v_{3 i} v_{1 j}+v_{1 i} v_{3 j}\right) \tag{9}
\end{equation*}
$$

Under the replacement scheme the elements are

$$
\begin{equation*}
\delta_{1 i} \delta_{1 j} \quad \delta_{2 i} \delta_{2 j} \quad \delta_{3 i} \delta_{3 j} \quad\left(\delta_{3 i} \delta_{1 j}+\delta_{1 i} \delta_{3 j}\right) \tag{10}
\end{equation*}
$$

The elements of the orthonormal basis are those given by (8) together with

$$
\begin{equation*}
T_{i j}^{I I I}=\frac{1}{\sqrt{2}}\left(2 \delta_{1 i} \delta_{1 j}+\delta_{3 i} \delta_{3 j}-\delta_{i j}\right) \quad T_{i j}^{I V}=\frac{1}{\sqrt{2}}\left(\delta_{3 i} \delta_{1 j}+\delta_{1 i} \delta_{3 j}\right) \tag{11}
\end{equation*}
$$

In constructing this basis we have made use of the identity

$$
\begin{equation*}
\delta_{1 i} \delta_{1 j}+\delta_{2 i} \delta_{2 j}+\delta_{3 i} \delta_{3 j}=\delta_{i j} \tag{12}
\end{equation*}
$$

which is a particular case of a more general identity (Srinivasan 1985)

$$
\begin{equation*}
\nu_{1 i} \nu_{1 j}+v_{2 i} \nu_{2 j}-\cos \theta\left(\nu_{1 i} \nu_{2 j}+v_{2 i} \nu_{1 j}\right)+\sin ^{2} \theta \nu_{3 i} \nu_{3 j}=\sin ^{2} \theta \delta_{i j} \tag{13}
\end{equation*}
$$

with $\nu_{a i}$ is replaced by $\delta_{a i}$ and $\theta=90^{\circ}$. In addition, if we generate the elements V and VI from IV in (11) by cyclic permutation of $\{1,2,3\}$, then the set $\{\mathrm{I}, \ldots, \mathrm{VI}\}$ will be the complete orthonormal basis for the second-rank symmetric tensor.

Next, turning our attention to the third-rank tensor, in particular, to expression (4), the elements obtained in accordance with the first step of the recipe are

$$
\begin{equation*}
\delta_{3 i} \delta_{3 j} \delta_{3 k} \quad \delta_{3 i} \delta_{j k} \quad\left(\delta_{3 j} \delta_{i k}+\delta_{3 k} \delta_{i j}\right) \tag{14}
\end{equation*}
$$

On subjecting these elements to the Gram-Schmidt process, we obtain

$$
\begin{align*}
& T_{i j k}^{I}=\delta_{3 i} \delta_{3 j} \delta_{3 k} \\
& T_{i j k}^{I I}=\frac{1}{\sqrt{2}}\left(\delta_{3 i} \delta_{j k}-\delta_{3 i} \delta_{3 j} \delta_{3 k}\right)  \tag{15}\\
& T_{i j k}^{I I I}=\frac{1}{2}\left(\delta_{3 j} \delta_{i k}+\delta_{3 k} \delta_{i j}-2 \delta_{3 i} \delta_{3 j} \delta_{3 k}\right)
\end{align*}
$$

These are the elements of the basis conforming to the symmetries of the class 6 mm .
The set given by (15) is a subset of the set comprising the elements of the basis for the most general case, namely, the noncentrosymmetric triclinic case. In the actual exercise, therefore, we start with ( $6 b$ ) and follow the recipe to construct the orthonormal tensor basis which spans the space of the third-rank tensor representing the piezoelectric effect and having the index symmetry $d_{i j k}=d_{i k j}$; the use of the identity (12) is, of course, understood. The set of elements $\{\mathrm{I}, \ldots, \mathrm{V}, \mathrm{XVI}\}$ of the basis given in table 1. Elements labelled VI

Table 1. Orthonormal basis.

$$
\begin{gathered}
\hline T_{i j k}^{I}=\delta_{3 i} \delta_{3 j} \delta_{3 k} \quad T_{i j k}^{I I}=\frac{1}{\sqrt{2}}\left(\delta_{3 i} \delta_{j k}-\delta_{3 i} \delta_{3 j} \delta_{3 k}\right) \\
T_{i j k}^{I I I}=\frac{1}{2}\left(\delta_{3 j} \delta_{i k}+\delta_{3 k} \delta_{i j}-2 \delta_{3 i} \delta_{3 j} \delta_{3 k}\right) \\
T_{i j k}^{I V}=\frac{1}{\sqrt{2}}\left(2 \delta_{3 i} \delta_{1 j} \delta_{1 k}-\delta_{3 i} \delta_{j k}-\delta_{3 i} \delta_{3 j} \delta_{3 k}\right) \\
T_{i j k}^{V}=\frac{1}{2}\left[2\left(\delta_{1 i} \delta_{3 j} \delta_{1 k}+\delta_{1 i} \delta_{1 j} \delta_{3 k}+\delta_{3 i} \delta_{3 j} \delta_{3 k}\right)-\delta_{3 j} \delta_{i k}-\delta_{3 k} \delta_{i j}\right] \\
T_{i j k}^{X V I}=\frac{1}{\sqrt{2}}\left(\delta_{1 i} \delta_{2 j} \delta_{3 k}+\delta_{1 i} \delta_{3 j} \delta_{2 k}\right)
\end{gathered}
$$

Table 2. Elements of the orthonormal basis belonging to different crystal classes. For convenience the elements are referred to only by their label in Roman numerals.

| Element | Class |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: |
| I to X | $m\left(\perp x_{2}\right)^{\mathrm{a}}$ |  |  |  |  |
| VI to XV | $m\left(\perp x_{3}\right)$ |  |  |  |  |
| I to III | $4 \mathrm{~mm}, 6 \mathrm{~mm}$ | mm2 | - | - | $2\left(\\| x_{3}\right)$ |
| IV and V | - | mm2 | $\overline{4}$ | - | $2\left(\\| x_{3}\right)$ |
| XVI to XVIII | 222, $\overline{4} 2 m, 23, \overline{4} 3 m$ | - | $\overline{4}$ | $2\left(\\| x_{2}\right)^{\text {a }}$ | $2\left(\\| x_{3}\right)$ |
| XI to XV | - | - | - | $2\left(\\| x_{2}\right)$ |  |
| I to IV | - | - | 4,6 | 3 |  |
| XVI and XVII | 422, 622 | 32 | 4,6 | 3 |  |
| VI to X | - | 32 | $\overline{6}$ | 3 |  |
| XI to XV | $\overline{6} m 2\left(m \perp x_{1}\right)^{\text {a }}$ | - | $\overline{6}$ | 3 |  |
| I to III | $3 m\left(m \perp x_{1}\right)^{\mathrm{a}}$ |  |  |  |  |
| XI to XVII | $3 m\left(m \perp x_{1}\right)$ |  |  |  |  |
| I to III |  | $3 m(m$ |  |  |  |
| VI to X |  | $3 m$ (m |  |  |  |
| XVI and XVII | $\overline{6} m 2\left(m \perp x_{2}\right)$ | $3 m$ (m |  |  |  |

${ }^{\text {a }}$ Standard setting.
$\mathrm{O} x_{1} x_{2} x_{3}$ is the standard rectangular Cartesian system (Nye 1976) the choice of which with respect to the symmetry element is indicated parenthetically in those cases where alternate settings are used.
to X can be obtained, respectively, from those with labels I to V by cyclic permutation of $\{1,2,3\}$; and similarly XI to XV, respectively, from VI to X; and XVII and XVIII starting from XVI. Table 2 gives the symmetry class of the different elements of the basis.

In terms of this basis, the decomposition of $d_{i j k}$ is given by

$$
\begin{equation*}
d_{i j k}=\sum_{K}\left(\mathbf{d}, \mathbf{T}^{K}\right) T_{i j k}^{K} \tag{16}
\end{equation*}
$$

where

$$
\begin{equation*}
\left(\mathbf{d}, \mathbf{T}^{K}\right)=d_{i j k} T_{i j k}^{K} \tag{17}
\end{equation*}
$$

represents the inner product of $d_{i j k}$ and the $K$ th element, $T_{i j k}^{K}$, of the basis. Table 3 lists the expressions for the inner product of $d_{i j k}$ with each element of the basis. The formulae are given in terms of $d_{i j k}$ in two-suffix notation with regard to the last two indices, the replacement scheme (Nye 1976) being (11) $\rightarrow 1$, (22) $\rightarrow 2$, (33) $\rightarrow 3,(23,32) \rightarrow 4$, $(31,13) \rightarrow 5,(12,21) \rightarrow 6$; and
$d_{111}=d_{11} \quad d_{122}=d_{12} \quad d_{123}=\frac{1}{2} d_{14} \quad d_{131}=\frac{1}{2} d_{15} \quad d_{112}=\frac{1}{2} d_{16}$.

Since the basis is orthonormal, the norm is given by

$$
\begin{equation*}
\|\mathbf{d}\|=\left\{\sum_{K}\left(\mathbf{d}, \mathbf{T}^{K}\right)^{2}\right\}^{\frac{1}{2}} \tag{19}
\end{equation*}
$$

As illustration we shall consider the class $3 m$, in the standard setting (Nye 1976) of the coordinate system, for which we have

$$
\begin{equation*}
-d_{21}=d_{22}=-\frac{1}{2} d_{16} \quad d_{15}=d_{24} \quad d_{31}=d_{32} \quad d_{33} \tag{20}
\end{equation*}
$$

and all other components are zero. For this class, we see, from table 2, that the relevant elements of the basis are I to III and XI to XVII. Taking the expressions for the respective inner products from table 3, together with the relations (20), we obtain

$$
\begin{equation*}
\|\mathbf{d}\|=\left[d_{33}^{2}+2 d_{31}^{2}+d_{15}^{2}+4 d_{22}^{2}\right]^{1 / 2} \tag{21}
\end{equation*}
$$

This agrees exactly with the norm derived using the decomposition in terms of the irreducible tensors (Jerphagnon et al 1978).

Table 3. Expressions for the inner product. These are given in terms of the piezoelectric coefficients in two-suffix notation.

| $\left(\mathbf{d}, \mathbf{T}^{I}\right)=d_{33} \quad\left(\mathbf{d}, \mathbf{T}^{I I}\right)=\frac{1}{\sqrt{2}}\left(d_{31}+d_{32}\right) \quad\left(\mathbf{d}, \mathbf{T}^{I I I}\right)=\frac{1}{2}\left(d_{15}+d_{24}\right)$ |
| :---: |
| $\left(\mathbf{d}, \mathbf{T}^{I V}\right)=\frac{1}{\sqrt{2}}\left(d_{31}-d_{32}\right) \quad\left(\mathbf{d}, \mathbf{T}^{V}\right)=\frac{1}{2}\left(d_{15}-d_{24}\right)$ |
| $\left(\mathbf{d}, \mathbf{T}^{V I}\right)=$$d_{11} \quad\left(\mathbf{d}, \mathbf{T}^{V I I}\right)=\frac{1}{\sqrt{2}}\left(d_{12}+d_{13}\right) \quad\left(\mathbf{d}, \mathbf{T}^{V I I I}\right)=\frac{1}{2}\left(d_{26}+d_{35}\right)$ <br> $\left(\mathbf{d}, \mathbf{T}^{I X}\right)=\frac{1}{\sqrt{2}}\left(d_{12}-d_{13}\right) \quad\left(\mathbf{d}, \mathbf{T}^{X}\right)=\frac{1}{2}\left(d_{26}-d_{35}\right)$ <br> $\left(\mathbf{d}, \mathbf{T}^{X I}\right)=d_{22} \quad\left(\mathbf{d}, \mathbf{T}^{X I I}\right)=\frac{1}{\sqrt{2}}\left(d_{23}+d_{21}\right) \quad\left(\mathbf{d}, \mathbf{T}^{X I I I}\right)=\frac{1}{2}\left(d_{34}+d_{16}\right)$ <br> $\left(\mathbf{d}, \mathbf{T}^{X I V}\right)=\frac{1}{\sqrt{2}}\left(d_{23}-d_{21} \quad\left(\mathbf{d}, \mathbf{T}^{X V}\right)=\frac{1}{2}\left(d_{34}-d_{16}\right)\right.$ <br> $\left(\mathbf{d}, \mathbf{T}^{X V I}\right)=\frac{1}{\sqrt{2}} d_{14} \quad\left(\mathbf{d}, \mathbf{T}^{X V I I}\right)=\frac{1}{\sqrt{2}} d_{25} \quad\left(\mathbf{d}, \mathbf{T}^{X V I I I}\right)=\frac{1}{\sqrt{2}} d_{36}$ |

## 3. Discussion

The present method of constructing orthonormal tensor basis can easily be extended to (physical property) tensor of any rank. On the other hand, method I works on the invariance of the elastic strain-energy function under a finite group of transformations defining the symmetry class of the crystal and appears to be applicable only to elastic constants. It treats the strain-energy function as a polynomial in strain components $e_{i j}$, for which the theory of invariants (Weyl 1946) ensures the existence of a finite integrity basis. Smith and Rivlin (1958, Smith 1967) have determined the integrity basis for invariant functions of $e_{i j}$ for each of the 32 crystallographic point groups; and Tu (1968) used the integrity basis to construct an orthonormal tensor basis for second-order as well as third-order elastic constants.

The same orthonormal basis for the elastic stiffness tensor $C_{i j k m}$ can be generated with the help of form-invariant expressions for $C_{i j k m}$ reported (Srinivasan and Nigam 1969) earlier. In this basis, the elements of the isotropic case (Tu 1968) need special consideration for reasons which the following discussion will reveal.

The three isotropic tensors (Temple 1960) of rank four are

$$
\begin{equation*}
\delta_{i j} \delta_{k m} \quad \delta_{i k} \delta_{j m} \quad \delta_{i m} \delta_{j k} \tag{22}
\end{equation*}
$$

which due to the symmetry

$$
\begin{equation*}
C_{i j k m}=C_{j i k m}=C_{i j m k}=C_{j i m k} \tag{23}
\end{equation*}
$$

reduce to two

$$
\begin{equation*}
\alpha_{i j k m}=\delta_{i j} \delta_{k m} \quad \beta_{i j k m}=\left(\delta_{i k} \delta_{j m}+\delta_{i m} \delta_{j k}\right) \tag{24}
\end{equation*}
$$

where we have used the same notation as Tu (1968). When these are orthonormalized they become

$$
\begin{equation*}
A_{i j k m}^{I}=\frac{1}{3} \alpha_{i j k m} \quad A_{i j k m}^{I I}=\frac{1}{6 \sqrt{5}}\left(3 \beta_{i j k m}-2 \alpha_{i j k m}\right) \tag{25}
\end{equation*}
$$

With these two elements the nearest isotropic tensor for any crystal class is defined ( Tu 1968) by

$$
\begin{equation*}
C_{i j k m}^{0}=\sum_{K=I}^{I I}\left(\mathbf{C}, \mathbf{A}^{K}\right) A_{i j k m}^{K} \tag{26}
\end{equation*}
$$

where the inner products in (26) are

$$
\begin{equation*}
\left(\mathbf{C}, \mathbf{A}^{I}\right)=(A+2 B) \quad\left(\mathbf{C}, \mathbf{A}^{I I}\right)=\frac{2}{\sqrt{5}}(A-B+3 C) \tag{27}
\end{equation*}
$$

and

$$
\begin{equation*}
A=\frac{1}{3}\left(C_{11}+C_{22}+C_{33}\right) \quad B=\frac{1}{3}\left(C_{12}+C_{23}+C_{31}\right) \quad C=\frac{1}{3}\left(C_{44}+C_{55}+C_{66}\right) \tag{28}
\end{equation*}
$$

In (28) we have used the well-known two-suffix notation for the elastic constants. On using (27) and (28) in (26) to find expressions for $C_{1111}^{0}=C_{11}^{0}, C_{1122}^{0}=C_{12}^{0}$, and $C_{2323}^{0}=C_{44}^{0}$, we obtain

$$
\begin{align*}
& C_{11}^{0}=\frac{1}{5}(3 A+2 B+4 C) \quad C_{12}^{0}=\frac{1}{5}(A+4 B-2 C) \\
& C_{44}^{0}=\frac{1}{5}(A-B+3 C)=\frac{1}{2}\left(C_{11}^{0}-C_{12}^{0}\right) \tag{29}
\end{align*}
$$

These are precisely the expressions derived by Voigt (1889) for the orientational averages of the components of elastic stiffness tensor for polycrystalline aggregates. If one uses the elastic compliance tensor $S_{i j k m}$ instead of $C_{i j k m}$ in (26), then one will obtain the analogue of (29) for the compliance tensor, and those agree exactly with the orientational averages derived by Reuss (1929) for the elastic compliance coefficients.

Next, when we take the contraction of $C_{i j k m}$, respectively, with $\alpha_{i j k m}$ and $\beta_{i j k m}$ in (24) we have

$$
\begin{equation*}
\left(C_{i j k m}, \alpha_{i j k m}\right)=3(A+2 B) \quad\left(C_{i j k m}, \beta_{i j k m}\right)=3(A+2 C) \tag{30}
\end{equation*}
$$

These two can be identified as the two scalar (irreducible tensor of weight zero) parts of method II (Jerphagnon et al 1978) but for the presence of the numerical factor of 3 in (30). This difference arises due to the definition of the scalar part in which a factor of $1 / 3$ is introduced. Similarly, the nearest isotropic tensor for a second-rank tensor can be worked out using the element I in (8). The only independent component of the nearest isotropic tensor will be proportional to the trace of the second-rank tensor.

The nearest isotropic tensor, for obvious reasons, does not exist in the case of the piezoelectric effect. However, the choice of the appropriate elements of the basis in a given coordinate system can be illustrated as follows. Let us consider AT-cut quartz (Mason 1950) belonging to the point group 32, for which, in the standard setting the $z$-axis is the threefold axis and the $x$-axis, the twofold axis. Let this coordinate system be rotated through an
angle $-\theta\left(=35^{\circ}\right)$ about the $x$-axis, so that the new $z$-axis is perpendicular to the plane of the AT-cut plate. The non-vanishing piezoelectric coefficients in the new system are

$$
\left(\begin{array}{cccccc}
d_{11}^{\prime} & d_{12}^{\prime} & d_{13}^{\prime} & d_{14}^{\prime} & \cdot & \cdot  \tag{31}\\
\cdot & \cdot & \cdot & \cdot & d_{25}^{\prime} & d_{26}^{\prime} \\
\cdot & \cdot & \cdot & \cdot & d_{35}^{\prime} & d_{36}^{\prime}
\end{array}\right)
$$

The form (31) corresponds to the class 2 with the difference that the $x$-direction is along the twofold axis instead of the $y$-direction (cf table 2). Hence the basis comprises the elements VI to X and XVI to XVIII. Using the respective expressions from table 3, the norm is

$$
\begin{gather*}
\|\mathbf{d}\|=\left[d_{11}^{\prime 2}+\frac{1}{2}\left(d_{12}^{\prime}+d_{13}^{\prime}\right)^{2}+\frac{1}{4}\left(d_{26}^{\prime}+d_{35}^{\prime}\right)^{2}+\frac{1}{2}\left(d_{12}^{\prime}-d_{13}^{\prime}\right)^{2}\right. \\
 \tag{32}\\
\left.+\frac{1}{4}\left(d_{26}^{\prime}-d_{36}^{\prime}\right)^{2}+\frac{1}{2}\left(d_{14}^{\prime 2}+d_{25}^{\prime 2}+d_{13}^{\prime 2}\right)\right]^{\frac{1}{2}} .
\end{gather*}
$$

On expressing the primed coefficients in terms of the unprimed ones (in the standard setting) and using the relations (Nye 1976)

$$
\begin{equation*}
d_{11}=-d_{12}=-\frac{1}{2} d_{26} \quad d_{14}=-d_{25} \tag{33}
\end{equation*}
$$

the equation (32) assumes the form

$$
\begin{equation*}
\|\mathbf{d}\|=\left[4 d_{11}^{2}+d_{14}^{2}\right]^{\frac{1}{2}} . \tag{34}
\end{equation*}
$$

This is exactly what we would have obtained had we chosen the basis for the class 32 from table 2.

Incidentally, the general invariance of the norm has been demonstrated. It is most suitable for comparing the strength or the magnitude of any property in different materials belonging to the same crystal class (Jerphagnon et al 1978); or different phases of the same material. For example, the norms of the elastic stiffness tensor (in GPa) and the piezoelectric tensor (in $\mathrm{pC} \mathrm{N}{ }^{-1}$ ), respectively, in the two phases of quartz are

|  | Class | $\\|\mathbf{C}\\|$ | $\\|\mathbf{d}\\|$ |
| :--- | :---: | :---: | :---: |
| $\alpha$-quartz | 32 | 253 | 4.65 |
| $\beta$-quartz | 622 | 255 | 1.89 |

where the data for the calculation of the norm have been taken from the Landolt-Börnstein tables (1979). We find that $\alpha$-quartz is more piezoelectric than $\beta$-quartz, whereas the elastic stiffness is almost the same in the two phases. The norm is very useful for selecting suitable materials for electro-optic devices, transducers, modulators, acousto-optic devices and acoustic delay lines.

To summarize, we have developed a recipe for generating an orthonormal tensor basis for the decomposition of any tensor representing a physical property. This has been accomplished without using the approach based on the theory of invariants (Weyl 1946). As illustration we have considered an odd-rank tensor like the piezoelectric tensor, because odd-rank tensors describing physical properties like piezoelectricity, acoustic gyrotropy may not lend themselves to decomposition by the use of method I. It is very clear that the present approach will work very easily for tensor of any rank. Whereas the calculation of the norm using the decomposition of method II, although possible in principle but not attempted so far, is very tedious and cumbersome, the present procedure based on the results of method II appears to be simple and direct.

The norm provides the link between the three different methods of decomposing a tensor describing a physical property. Regarding the advantages of different approaches, they are well documented elsewhere (Jerphagnon et al 1978, Srinivasan 1985, 1988) and they will not be discussed here.

## Acknowledgments

The author gratefully acknowledges financial support under UGC-DRS scheme. He also expresses his sincere thanks to Professor K Srinivasa Rao, Institute of Mathematical Sciences, Chennai (Madras), for having introduced him to document preparation using $\mathrm{LAT}_{\mathrm{E}} \mathrm{X}$.

## References

Chandrasekhar P and Srinivasan T P 1972 Acta Crystallogr. A 28 594-7
Jerphagnon J, Chemla D S and Bonneville R 1978 Adv. Phys. 27 609-50
Juretschke H J 1974 Crystal Physics (London: Benjamin)
Landolt-Börnstein New Series 1979 Group III, vol 11 (Berlin: Springer)
Mason W P 1950 Piezoelectric Crystals and their Applications to Ultrasonics (New York: Van Nostrand)
Nowacki W 1962 Thermoelasticity (London: Pergamon) p 586
Nye J F 1976 Physical Properties of Crystals (Oxford: Clarendon)
Reuss A 1929 Z. Angew. Math. Mech. 9 49-58
Smith G F 1967 Q. Appl. Math. 25 218-21
Smith G F and Rivlin R S 1958 Trans. Am. Math. Soc. 88 175-93
Spencer A J M 190 Int. J. Eng. Sci. 8 475-81
Srinivasan T P 1970 Phys. Status Solidi 41 615-20
——1985 J. Phys. C: Solid State Phys. 18 3263-71
_-1988 J. Phys. C: Solid State Phys. 21 4207-19
Srinivasan T P and Nigam S D 1968 Phys. Status Solidi 28 K71-73
_- 1969 J. Math. Mech. 19 311-20
Temple G 1960 Cartesian Tensors (London: Methuen)
Thomas T Y 1966 Proc. Natl Acad. Sci., USA 55 235-9
Tu Yih-O 1968 Acta Crystallogr. A 24 273-82
Voigt W 1889 Ann. Phys., Lpz. 38 573-87
Walpole L J 1981 Advances in Applied Mechanics vol 21, ed Chia-Shun Yih (New York: Academic) 1984 Proc. R. Soc. A 391 149-79
Weyl H 1946 The Classical Groups (Princeton, NJ: Princeton University Press)

