*Acta Cryst.* (1986). A**42**, 293-296

# Numerical Vector Representation of Physical Properties of Crystals

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(*Received 27 September* 1985; *accepted* 2 *January* 1986)

### Abstract

The idea of a *numerical vector representation* (*NVR*) *of a physical property of a crystal*, introduced in a previous paper [Fumi & Ripamonti (1980). *Acta Cryst.* A**36**, 535-551], is a convenient way to account for its rotational invariance properties. The main advantages of the NVR are the possibility of dealing with single invariance relations independently from the others and the direct display of the simplest features of the invariance relations (vanishing of components, equalities or proportionalities among components, independence of components and 'form invariance' with respect to interchange of components). The NVR also provides a *direct-expansion method* of the set of tensor components of a crystal property in terms of a minimal subset. A simple rule is reported for obtaining a NVR of any given tensorial set (*i.e.* a set of given rank and rotational and permutational symmetry) in the axial rotational groups. The use of the NVR in establishing general results such as isomorphisms between tensorial sets is also illustrated. Finally, a few examples are reported of NVR's for high-rank tensorial sets in axial rotational groups (specifically the second-order piezoelectric tensor, the second-order Pockels elastooptic tensor and the fourth-order elastic tensor).

### 1. Numerical vector representation (NVR)

The usual specification of a crystal property is by means of a tensorial set, *i.e.* a set whose components transform - under rotation - as *products* of components of a vector (*e.g.* Nye, 1985). This specification simplifies the algebra of rotational transformations that are necessary to relate different experimental measurements, but introduces redundancy. In fact, the tensorial sets specifying crystal properties are not of the most general type since they usually have additional rotational symmetry, consisting of a set of algebraic relations among their components. This is due to the usually higher rotational symmetry of a crystal property, which is fixed by the crystal structure, with respect to the intrinsic or natural rotational symmetry of a tensorial set, which is a rapidly decreasing function of rank.

To 'minimize' the tensorial specification of a crystal property one needs to expand the crystal property in terms of a minimal subset: *i.e.* each component of the tensorial set must be expanded into a sum, with proper coefficients, of the components of a minimal subset. This is the fundamental mathematical problem in the usual tensorial specification of a crystal property (*e.g.* Nye, 1985).

The expansion of tensorial sets with rotational symmetry of order 1, 2 or 4 is almost trivial as it reduces to equalities (except for sign) of pairs of components and (or) vanishing of components (Fumi, 1952). The expansion is, instead, a laborious algebraic task for high ranks in the other cases, specifically those of order 3, 6 and $\infty$.*

The NVR of a tensorial set specifying a crystal property (Fumi & Ripamonti, 1980*a*) (referred to below as I) is a one-to-one correspondence between this set and a set of numerical vectors (in a vector space of proper dimension) which preserves the rotational invariance of the tensorial set, *i.e.* all the algebraic relations of invariance among components. The NVR thus provides an account of the rotational invariance of a tensorial set without the usual recourse to an explicit form of invariance relations. In fact, the NVR accounts for rotational invariance by providing algebraic conditions for the numerical coefficients in an arbitrary invariance relation, in the form of a vector equation for the coefficients themselves.

The NVR directly displays the simplest features of the invariance relations - vanishing of components, equalities or proportionalities among components, independence of components and 'form invariance' with respect to interchange of components - and provides a means of directly checking the consistency with rotational invariance of an arbitrary relation among components. It also provides a means for direct determination of an invariance relation among any set of components: in particular, a method for direct determination of the expansion of a component in terms of a (minimal) subset of components.

The *direct-expansion method* provided by the NVR has several advantages over the existing methods:

* Group $6(6\|z)$ can be simply treated as a superposition of group $3(3\|z)$ and a symmetry axis $2(2\|z)$ (see *e.g.* Fumi & Ripamonti, 1980*b*) (referred to below as II). Group $\infty(\infty\|z)$ can also be treated as a superposition of groups $4(4\|z)$ and $3(3\|z)$ for tensors of ranks up to (but excluding) 12 (see II, Appendix *B*).

0108-7673/86/050293-04$01.50 

(i) it deals with individual expansion relations (independently from the others);

(ii) it exploits any reduction in the number of independent expansion coefficients.

In particular, the direct-expansion method avoids both steps of the existing methods:*

($a$) the determination of a complete set of invariance relations;

($b$) the transformation of this set (by algebraic means) into the desired 'expansion' form.

To find a numerical vector representation of a tensorial set specifying a crystal property one can exploit (see I) the *contravariant* transformational properties of a component and its numerical coefficient in any invariant linear combination of tensor components. Indeed these numerical coefficients do transform under rotation as the components (by contravariance) and do have the desired invariance under the rotational group of the crystal since they enter *invariant* linear combinations. Thus any complete set of independent tensorial invariants provides a (complete) numerical vector representation of the tensorial components of a crystal property.

Consider the subset $n_z=0$,† $n_y$ even of a tensorial set of rank 4 with no permutational symmetry, invariant under the rotational symmetry group $\infty\,(\infty\|z)$. This subset consists of the following eight components: $xxxx$, $yyyy$, $(xxyy)$.‡¶

To find a NVR of the given subset one needs first a minimal set of invariant linear combinations of its components: for example (see §§ 2, 3),**

$$I^+_{++--}=xxxx-xxyy+xyxy+yxxy+xyyx+yxyx-yyxx+yyyy$$

$$I^+_{+-+-}=xxxx+xxyy-xyxy+yxxy+xyyx-yxyx+yyxx+yyyy$$

$$I^+_{-++-}=xxxx+xxyy+xyxy-yxxy-xyyx+yxyx+yyxx+yyyy.$$

One then obtains a NVR by simply associating each component with its three numerical coefficients in the three invariants (following an arbitrary but fixed order) as follows:

| NVR | $xxxx$ | $xxyy$ | $xyxy$ | $yxxy$ | $xyyx$ | $yxyx$ | $yyxx$ | $yyyy$ |
|---|---|---|---|---|---|---|---|---|
| $I^+_{++--}$ | 1 | −1 | 1 | 1 | 1 | 1 | −1 | 1 |
| $I^+_{+-+-}$ | 1 | 1 | −1 | 1 | 1 | −1 | 1 | 1 |
| $I^+_{-++-}$ | 1 | 1 | 1 | −1 | −1 | 1 | 1 | 1 . |

Inspection of the NVR reveals, first of all, the equality of components related by $x\leftrightarrow y$ exchange.

Further inspection permits one to find a minimal subset of components to be used as expansion basis. Since the NVR is three-dimensional, a minimal subset consists of any three components having (linearly) independent representative numerical vectors. Thus, for example, the three components $(xxy)y$ (*i.e.* $xxyy$, $xyxy$, $yxxy$) are independent as their representative vectors are clearly independent.

The NVR also provides almost immediately the expansion of the component $xxxx$ in the $(xxy)y$ expansion basis:

$$xxxx=C_1xxyy+C_2xyxy+C_3yxxy.$$

To determine the expansion coefficients one uses the NVR: replacing the components by their numerical vectors, one obtains a vector equation for the expansion coefficients $C_1$, $C_2$, $C_3$. However, by noting that the chosen expansion basis is closed under permutations of the first three indices, while the component $xxxx$ is invariant under these permutations, one sees that there are constraints on the form of the expansion. Indeed, this expansion must be 'form invariant' under these permutations, *i.e.* one must have $C_1=C_2=C_3=C$:

$$\begin{array}{ccccccc} xxxx & = C & (xxyy & + & xyxy & + & yxxy) \\ \downarrow & & \downarrow & & \downarrow & & \downarrow \end{array}$$

$$\begin{bmatrix}1\\1\\1\end{bmatrix}=C\left(\begin{bmatrix}-1\\1\\1\end{bmatrix}+\begin{bmatrix}1\\-1\\1\end{bmatrix}+\begin{bmatrix}1\\1\\-1\end{bmatrix}\right)=C\begin{bmatrix}1\\1\\1\end{bmatrix}.$$

Through the NVR one thus obtains $C=1$. It should also be noted that whenever there is a reduction in the number of independent expansion coefficients (here from three to one) it is sufficient to use a correspondingly reduced NVR. Here one could have simply used a one-dimensional NVR, *e.g.* the NVR given by the coefficients in the first invariant:

$$\begin{array}{ccccccc} xxxx & = C\ ( & xxyy & + & xyxy & + & yxxy) \\ \downarrow & & \downarrow & & \downarrow & & \downarrow \\ 1 & = C\ ( & -1 & + & 1 & + & 1\ ). \end{array}$$

## 2. A simple rule for obtaining a NVR in axial rotational groups ($z\|$symmetry axis)

It is obviously important to have a simple rule to obtain a NVR of any given tensorial set (*i.e.* a set of given rank and rotational and permutational

* The existing methods differ essentially in the first step, of which there are basically three types:

(1) impose rotational invariance to individual components (complete but redundant set);

(2) impose that a (minimal) set of non-invariant linear combinations of components be equal to zero;

(3) expand the individual components into invariant linear combinations of components.

† $n_x$, $n_y$, $n_z$ are the partial ranks in the $x$, $y$, $z$ indices.

‡ For simplicity we denote the components by their indices.

¶ A round bracket stands for all the permutations of the enclosed indices.

** In Fumi & Ripamonti (1980$a$, $b$, 1984) we adopted a different (perhaps less transparent) notation for the tensor invariants.

symmetry). This is possible for *axial* rotational symmetries.

Since a minimal set of invariants (*i.e.* their numerical coefficients) provides a NVR, one needs actually a rule to obtain a minimal set of invariants. In general one has to recur to invariant projections of tensorial components of the given rank, but this procedure does not guarantee the independence of the generated invariants. Alternatively, invariant products (*e.g.* scalar products) of lower-rank irreducible variants (*i.e.* irreducible linear combinations of tensorial components of lower rank) can be used to avoid the use of projections, but independence is not ensured anyway.

The task is very simple, however, for axial rotational symmetries. There a minimal set of invariants is given by a special tensorial subset of Hermann's components of a vector* identified by the condition (see I)

$$n_+ = n_- \bmod N, \tag{1}$$

where $n_+$, $n_-$ are the partial ranks in the $+$, $-$ indices and $N$ is the order of the symmetry axis. For a cylindrical axis $n_+ = n_-$.

Owing to the tensorial nature of this set of invariants it is also possible to obtain the NVR through formulas (thus avoiding explicit expansion of the invariants in terms of the usual tensorial components). In fact the numerical coefficients of a (usual) tensorial component $k$ in the pertinent invariants are given by simple products (or sums of products). Specifically,

(i) for general tensorial sets (*i.e.* sets with no permutational symmetry) (see I),

$$r_{jk} = i^{n_y(k)}(-1)^{n(j,k)}, \tag{2}$$

where $j$ is a Hermann invariant, $n_y(k)$ is the $y$ partial rank of $k$ and $n(j, k)$ is the number of $(-, y)$ index correspondences between $j$ and $k$;

(ii) for tensorial sets with permutational symmetry

$$r_{(\sum j)k} = \sum_j r_{jk}, \tag{2'}$$

where $\sum j$ is an invariant with the given permutational symmetry, constructed in general by summation of permutationally related Hermann invariants.

### 3. Use of the NVR in establishing isomorphisms for general tensorial sets

Symmetrizing Hermann's invariants with respect to $+\leftrightarrow-$ exchange, one splits them into two independent subsets

$$I^+ = \tfrac{1}{2}(I + \tilde{I}),\ I^- = \tfrac{1}{2}(I - \tilde{I}), \tag{3}$$

where $\sim$ denotes $+\leftrightarrow-$ exchange. Since $+\leftrightarrow-$ exchange implies $y\leftrightarrow -y$ exchange, it follows that components having even $y$ rank ($n_y$ even) have zero coefficients in the $I^-$ invariants, while components having odd $y$ rank ($n_y$ odd) have zero coefficients in the $I^+$ invariants. Thus, components having different $n_y$ parities are independent as their representative vectors are independent.

Furthermore, since (see I, Appendix)

$$r_{j^-\tilde{k}} = f r_{j^+k} \text{ if } (n_x + n_y) \text{ is odd} \tag{4}$$

[where $f$ is a constant depending only on $(n_x + n_y)$, $\sim$ denotes $x\leftrightarrow y$ exchange and $j^+, j^-$ are symmetrized Hermann invariants constructed from a given invariant $j$], it follows that subsets of odd $(n_x + n_y)$ rank, having different $n_y$ parities, have a common NVR (besides being independent). Alternatively, the NVR is invariant with respect to $x\leftrightarrow y$ exchange (except for an irrelevant factor $f$). Accordingly, it is sufficient to deal with only one of these subsets.

This result can be extended to even $(n_x + n_y)$ rank by limiting $x\leftrightarrow y$ exchange to an odd number of indices, say $(n_x + n_y) - 1$, and by taking into account the effect of the fixed index: since (see I, Appendix)

$$r_{j^-\tilde{k}} = \pm f r_{j^+k} \tag{5}$$

[where $\sim$ denotes $x\leftrightarrow y$ exchange on $(n_x + n_y - 1)$ indices, and the minus sign holds if the fixed index is $y$], it follows that the NVR is invariant with respect to the $x\leftrightarrow y$ exchange in $(n_x + n_y - 1)$ indices when accompanied by a change of sign if the fixed (*i.e.* unexchanged) index is $y$.

In conclusion, general tensorial subsets of different $n_y$ parities, besides being independent, are formally identical (*i.e.* they have the same formal algebraic structure). The correspondence that preserves such a formal structure is the $x\leftrightarrow y$ exchange over all the indices for $(n_x + n_y)$ odd and over all indices but one (plus a sign change if the fixed index is $y$) for even $(n_x + n_y)$.

Another important result for even $(n_x + n_y)$ which follows from the NVR (see I, Appendix) is that for $n_y$ even the coefficients of pairs of general tensorial components totally exchanged in $x$ and $y$ are equal when taken from Hermann invariants for which $n_+ = n_- \bmod 4$, and opposite otherwise: for $n_y$ odd the opposite is true.

The NVR is a powerful tool for establishing general results such as isomorphisms between tensorial sets (including sets with permutational symmetry).

### 4. Examples of NVR's

(*a*) *Rank* 5

Rotational symmetry group: $3(3\|z)$

* The Hermann components of a vector are given by $v_+ = v_x + iv_y$, $v_- = v_x - iv_y$, $v_0 = v_z$, where $v_x$, $v_y$, $v_z$ are the usual orthogonal components of a vector.

Permutational symmetry group: $i[[jk][lm]]$;* *second-order piezoelectric tensor*

Tensorial subset: $n_z = 0$, $n_y$ even.

This subset consists of the following six components:† 111, 112, 122, 166, 216, 226.

A minimal set of invariants is given by the five invariants (see §§2, 3) $I^+_{(-++++)}$. Of these $I^+_{-++++}$ has the desired permutational symmetry and another one can be constructed by summing the other four:

$$I^+_{+[-+++]} = \sum_{i=1}^{4} I^+_{+(-+++)_i}. \qquad (6)$$

Thus a NVR of the given permutational symmetry is two-dimensional. By using (2) for the coefficients in the individual Hermann invariants and by summing over the four Hermann invariants in (6), one obtains the following NVR:‡

| NVR | 111 | 112 | 122 | 166 | 216 | 226 |
|---|---|---|---|---|---|---|
| $I^+_{-++++}$ | 1 | −1 | 1 | −1 | 1 | −1 |
| $I^+_{+[-+++]}$ | 4 | 0 | −4 | 0 | −2 | −2 |

(*b*) *Rank* 6

Rotational symmetry group: $\infty(\infty\|z)$

Permutational symmetry group: $[ij][[kl][mn]]$; *second-order Pockels elastooptic tensor*

Tensorial subset: $n_z = 0$, $n_y$ even.

| NVR | 111 | 112 | 122 | 166 | 211 | 212 | 222 | 266 | 616 | 626 |
|---|---|---|---|---|---|---|---|---|---|---|
| $I^+_{+-[[++][--]]}$ | 2 | −2 | 2 | 2 | 2 | −2 | 2 | 2 | 0 | 0 |
| $I^+_{+-[[+-][+-]]}$ | 4 | 4 | 4 | 0 | 4 | 4 | 4 | 0 | 0 | 0 |
| $I^+_{++[+---]}$ | 4 | 0 | −4 | 0 | −4 | 0 | 4 | 0 | 2 | 2 |

The representative vectors of 122, 212, 222, 266 and 626 follow directly from the representative vectors of 211, 112, 111, 166 and 616 owing to the last two paragraphs of § 3.

(*c*) *Rank* 8

Rotational symmetry group: $3(3\|z)$

Permutational symmetry group: $[[ij][kl][mn][pq]]$;* *fourth-order elastic tensor*

(i) Tensorial subset: $n_z = 0$, $n_y$ odd.

| NVR | 1116 | 1126 | 1226 | 1666 | 2226 | 2666 |
|---|---|---|---|---|---|---|
| $i^{-1}I^-_{[+++++++-]}$ | 6 | −2 | −2 | −2 | 6 | −2 |

The representatives of 1226, 2226 and 2666 follow directly from the representatives of 1126, 1116 and 1666 owing to the last two paragraphs of § 3.

(ii) Tensorial subset: $n_z = 1$, $n_y$ even.†‡

| NVR | 1115 | 1125 | 1225 | 1146 | 1246 | 1566 | 2225 | 2246 | 2566 | 4666 |
|---|---|---|---|---|---|---|---|---|---|---|
| $I^+_{[[++][++][--]]+z}$ | 3 | −3 | 3 | −1 | 1 | 1 | −3 | −1 | −1 | −3 |
| $I^+_{[[++][++][+-]]-z}$ | 6 | −2 | −2 | 4 | 0 | −2 | 6 | −4 | −2 | 0 |
| $I^+_{[[++][+-][+-]+z}$ | 12 | 4 | −4 | −4 | −4 | 0 | −12 | −4 | 0 | 0 |

The reported NVR's give expansions that agree with those reported in the literature by Nelson (1979) for case (*a*), Vedam and Srinivasan (1967) for case (*b*)§ and Brendel (1979) and Markenskoff (1979) for cases (*c*) (i) and (ii).

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* A square bracket stands for symmetry with respect to permutations of the enclosed indices.

† The abbreviated standard notation is: $i = x(\equiv 1), y(\equiv 2), z(\equiv 3)$; $[jk]$ or $[lm] = xx[\equiv 1), yy(\equiv 2), xy(\equiv 6)$.

‡ Pairs of components related by $1 \leftrightarrow 2$ exchange in the last two indices have vectors with identical corresponding entries (except for sign). Accordingly a convenient expansion basis is one that is closed under such an exchange (*e.g.* 111 and 122) and then the resulting expansion relations are 'form invariant' under the exchange.

*The abbreviated standard notation is: $[ij]$ or $[kl]$, $[mn]$, $[pq] = xx\ (\equiv 1)$, $yy\ (\equiv 2)$, $yz\ (\equiv 4)$, $zx\ (\equiv 5)$, $xy\ (\equiv 6)$.

† The tensorial invariants with the index $z$ in different positions are independent.

‡ Pairs of components related by $1 \leftrightarrow 2$ exchange have vectors with identical corresponding entries (except for sign). A convenient expansion basis is thus one closed under such an exchange (*e.g.* 1115, 2225, 1246) and then the resulting expansion relations are 'form invariant' under the exchange.

§ In fact the pertinent expansions for isotropy 0(3) reported by these *AA* follow by symmetrization with respect to *x*, *y*, *z* of the expansions for $\infty(\infty\|z)$ (see II, Appendix *B*).