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Abstract

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ANISOTROPIC TENSORS

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1. In theoretical crystal physics, anisotropic tensors play an important role ([1]), i.e., tensors invariant with respect to all operations of one or another crystallographic group K. Tensors of rank r, invariant with respect to the group K, constitute the linear space $L(K \times V^r)$. The symbol V^r in this notation characterizes tensors of rank r as quantities transformed according to the r-th power of the vector representation ([2]) $V = D_1^-$ of the orthogonal group $\infty/\infty \cdot m$ (groups are denoted according to A. V. Shubnikov ([3])). Here a method is set forth for constructing systems of generators ([4]) for such spaces.

2. Consider the operator of averaging a tensor of rank r over the group K

$$\hat{S}(K \times V^r) = \frac{1}{N(K)} \sum_k \hat{C}_k(K \times V^r),$$

where $N(K)$ is the order of the group; $C_k(\hat{K} \times V^r)$ is the operator of the representation V^r of the group K, corresponding to the element k; the summation is over all elements of the group. If this operator is applied to tensors constituting a basis in the space of all tensors of rank r, $L(V^r)$, then the transformed tensors will constitute a system of generators for the space $L(K \times V^r)$.

3. We shall use in $L(V^r)$ bases consisting of polyads (multiplicative tensors).

For the transition to groups of the lower and cubic syngonies (i.e., to groups whose vector representations split into real irreducible representations) we shall use the basis

$$\mathbf{e}_{q_1} \mathbf{e}_{q_2} \dots \mathbf{e}_{q_r} \quad (q_n = 1, 2, 3;\ n = 1, 2, \dots, r), \qquad \text{(a)}$$

where $\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3$ are the unit vectors of the axes of the crystallophysical coordinate system ([3]), and the product of vectors, like a power of a vector, is understood in the sense of dyadic (more correctly, one should say polyadic) multiplication.

For the transition to groups of the middle syngonies (i.e., to groups whose vector representations include not only real but also complex irreducible representations) we shall use the basis

$$\mathbf{j}_{q_1}\mathbf{j}_{q_2}\dots\mathbf{j}_{q_r} \quad (q_n = 1, 2, 3;\ n = 1, 2, \dots, r), \tag{ }$$

where $\mathbf{j}_1 = \frac{1}{\sqrt{2}}(\mathbf{e}_1 + i\mathbf{e}_2)$, $\mathbf{j}_2 = \frac{1}{\sqrt{2}}(\mathbf{e}_1 - i\mathbf{e}_2)$, $\mathbf{j}_3 = \mathbf{e}_3$ are the unit vectors of the so-called cyclic coordinate system ([2,5,6]).

The bases (a) and (b) include, evidently, all possible polyads of the form:

$$\mathbf{e}_1^{s_1}\mathbf{e}_2^{s_2}\mathbf{e}_3^{s_3} \quad \text{or} \quad \mathbf{j}_1^{s_1}\mathbf{j}_2^{s_2}\mathbf{j}_3^{s_3} \qquad (s_1 + s_2 + s_3 = r)$$

with all their isomers (7).

4. If the vector representation of the group K splits into one-dimensional representations (such are all groups of lower syngonies and the groups of middle syngonies belonging to the types N, $\overline{N}$, $N : m$), then the action of the operator $\widehat{S}$ on the tensors indicated in item 3 of the bases reduces to multiplying those polyads whose exponents s_i satisfy certain "selection rules" by 1 and multiplying the remaining polyads by 0. The "selection rules" for the groups of rhombic and cubic syngonies are as follows*:

$2 \cdot m$	$2 : 2,\ 3/2,\ 3/4,\ 3/\overline{4}$	$m \cdot 2 : m,\ \overline{6}/2,\ \overline{6}/4$
$s_1 \equiv s_2 \equiv 0 \pmod 2$	$s_1 \equiv s_2 \equiv s_3 \pmod 2$	$s_1 \equiv s_2 \equiv s_3 \equiv 0 \pmod 2$

For the remaining groups the "selection rules" are expressed by the formulas

$N,\quad N : 2,\quad N \cdot m$	$\overline{N},\quad \overline{N} \cdot m$	$N : m,\quad m \cdot N : m$
$s_1 \equiv s_2 \pmod N$	$s_1 - s_2 \equiv \frac{N}{2} s_3 \pmod N$	$s_1 \equiv s_2 \pmod N,\quad s_3 \equiv 0 \pmod 2$

5. Knowing the "selection rules," it is easy to write down integral rational bases (5) of the spaces $L(K \times V^r)$, where K is some group whose vector representation splits into one-dimensional representations**. In this case all tensor spaces of the given group K have one and the same integral rational basis. The integral rational bases of the groups of lower syngonies are as follows:

1	$\mathbf{e}_1,\ \mathbf{e}_2,\ \mathbf{e}_3$	$2 : m$	$\mathbf{e}_1^2,\ \mathbf{e}_2^2,\ \mathbf{e}_3^2,\ \mathbf{e}_1\mathbf{e}_2$
$\overline{2}$	$\mathbf{e}_1^2,\ \mathbf{e}_2^2,\ \mathbf{e}_3^2,\ \mathbf{e}_2\mathbf{e}_3,\ \mathbf{e}_3\mathbf{e}_1,\ \mathbf{e}_1\mathbf{e}_2$	$2 : 2$	$\mathbf{e}_1^2,\ \mathbf{e}_2^2,\ \mathbf{e}_3^2,\ \mathbf{e}_1\mathbf{e}_2\mathbf{e}_3$
2	$\mathbf{e}_1^2,\ \mathbf{e}_2^2,\ \mathbf{e}_3,\ \mathbf{e}_1\mathbf{e}_2$	$2 \cdot m$	$\mathbf{e}_1^2,\ \mathbf{e}_2^2,\ \mathbf{e}_3$
m	$\mathbf{e}_1,\ \mathbf{e}_2,\ \mathbf{e}_3^2$	$m \cdot 2 : m$	$\mathbf{e}_1^2,\ \mathbf{e}_2^2,\ \mathbf{e}_3^2$

Introduce the notation:

$$\mathrm{I} = \mathbf{e}_1^2 + \mathbf{e}_2^2 + \mathbf{e}_3^2,$$

$$\mathrm{E} = \mathbf{e}_1\mathbf{e}_2\mathbf{e}_3 + \mathbf{e}_2\mathbf{e}_3\mathbf{e}_1 + \mathbf{e}_3\mathbf{e}_1\mathbf{e}_2 - \mathbf{e}_1\mathbf{e}_3\mathbf{e}_2 - \mathbf{e}_2\mathbf{e}_1\mathbf{e}_3 - \mathbf{e}_3\mathbf{e}_2\mathbf{e}_1,$$

$$\tilde{\mathrm{I}} = \mathbf{e}_1^2 + \mathbf{e}_2^2, \qquad \hat{\mathrm{E}} = \mathbf{e}_1\mathbf{e}_2 - \mathbf{e}_2\mathbf{e}_1,$$

$$\mathrm{T}^{\langle m\cdot 2:m\rangle} = \Gamma = \mathbf{e}_1^2 - \mathbf{e}_2^2, \qquad \mathrm{T}^{\langle 2:m\rangle} = \mathrm{H} = \mathbf{e}_1\mathbf{e}_2,$$

$$\mathrm{T}^{\langle m\cdot 3:m\rangle} = \mathbf{e}_1^3 - \overline{\mathbf{e}_1\mathbf{e}_2\mathbf{e}_2}, \qquad \mathrm{T}^{\langle 3:m\rangle} = \mathbf{e}_2^3 - \overline{\mathbf{e}_2\mathbf{e}_1\mathbf{e}_1},$$

$$\mathrm{T}^{\langle m\cdot 4:m\rangle} = \Gamma^2 - \mathrm{H}^2, \qquad \mathrm{T}^{\langle 4:m\rangle} = \overline{\Gamma\mathrm{H}},$$

$$\mathrm{T}^{\langle m\cdot 6:m\rangle} = \Gamma^3 - \overline{\Gamma\mathrm{H}\mathrm{H}}, \qquad \mathrm{T}^{\langle 6:m\rangle} = \mathrm{H}^3 - \overline{\mathrm{H}\Gamma\Gamma}.$$

(Brackets over a product of tensors denote summation over all actually distinct permutations of the tensors being multiplied; for example,

$$\overline{\Gamma\mathrm{H}\mathrm{H}} = \Gamma\mathrm{H}^2 + \mathrm{H}\Gamma\mathrm{H} + \mathrm{H}^2\Gamma.$$

) Using this notation,

* On the "selection rules" for groups whose vector representations do not split into one-dimensional ones, see

** The existence of integral rational tensor bases for all crystallographic groups was proved by Smith and Riv

can, in general form, write down the integral rational bases for the aforementioned groups of the middle systems in the crystallophysical system:

N	$\tilde{\mathbf{I}},\ \tilde{\mathbf{E}},\ \mathbf{e}_3,\ \mathbf{T}^{\langle m\cdot N:m\rangle},\ \mathbf{T}^{\langle N:m\rangle}$
$\overline{N}$	$\tilde{\mathbf{I}},\ \tilde{\mathbf{E}},\ \mathbf{e}_3^2,\ \mathbf{T}^{\langle m\cdot N:m\rangle},\ \mathbf{T}^{\langle N:m\rangle},\ \mathbf{e}_3\mathbf{T}^{\langle m\cdot \frac{N}{2}:m\rangle},\ \mathbf{e}_3\mathbf{T}^{\langle \frac{N}{2}:m\rangle}$
$N:m$	$\tilde{\mathbf{I}},\ \tilde{\mathbf{E}},\ \mathbf{e}_3^2,\ \mathbf{T}^{\langle m\cdot N:m\rangle},\ \mathbf{T}^{\langle N:m\rangle}$

Knowing an integral rational tensor basis, it is easy to construct a system of generators for any of the spaces $L(K \times V^r)$. It will contain all possible products of basis tensors having rank r, and all isomers of these products.

6. If the vector representation of the group K does not split into one-dimensional representations (such are the groups of the cubic system and the groups of the middle systems belonging to the types $N:2,\ N\cdot m,\ \overline{N}\cdot m,\ m\cdot N:m$), then the operator $\hat{S}$, acting on the polyads indicated in Sec. 3 of the bases, not only annihilates some of these polyads, but also transforms the remaining polyads into their linear combinations (sums or differences)*. Thus, $\hat{S}$ is regarded as the product of two operators: the first, as in Sec. 4, is characterized by "selection rules" ; the second we shall call the combination operator. The "selection rules" were written out in Sec. 4. We shall write the combination operators in the form of sums (or differences) of operators $\hat{P}_i$ and $\hat{Q}_i$, which perform the replacement of indices in the basis polyads according to the corresponding substitutions, namely:

$\hat{P}_1$	$\hat{P}_2$	$\hat{P}_3$	$\hat{Q}_1$	$\hat{Q}_2$	$\hat{Q}_3$
(1)(2)(3)	(123)	(132)	(1)(23)	(13)(2)	(12)(3)

The combination operators for the groups of the types under consideration are as follows:

$N\cdot m,\ m\cdot N:m$	$\hat{P}_1+\hat{Q}_3$	$3/4$	$\sum_{i=1}^{3}\left[\hat{P}_i+(-1)^r\hat{Q}_i\right]$
$N:2,\ \overline{N}\cdot m$	$\hat{P}_1+(-1)^{s_3}\hat{Q}_3$		
$3/2,\ \overline{6}/2$	$\sum_{i=1}^{3}\hat{P}_i$	$\overline{3}/4,\ \overline{6}/4$	$\sum_{i=1}^{3}\left(\hat{P}_i+\hat{Q}_i\right)$

7. On the basis of known results (8), one can write down integral rational bases of the limiting crystallographic symmetry groups:

$\infty/\infty\cdot m$	$\mathbf{I}$		
∞/∞	$\mathbf{I},\ \mathbf{E}$	$\infty:2$	$\tilde{\mathbf{I}},\ \tilde{\mathbf{E}}\mathbf{e}_3,\ \mathbf{e}_3^2$
$m\cdot\infty:m$	$\tilde{\mathbf{I}},\ \mathbf{e}_3^2$	$\infty:m$	$\tilde{\mathbf{I}},\ \tilde{\mathbf{E}},\ \mathbf{e}_3^2$
$\infty\cdot m$	$\tilde{\mathbf{I}},\ \mathbf{e}_3$	∞	$\tilde{\mathbf{I}},\ \tilde{\mathbf{E}},\ \mathbf{e}_3$

The groups ∞ and $\infty:m$, whose vector representations split into one-dimensional ones, also have integral rational bases consisting of the polyads:

$$\mathbf{j}_3,\quad \mathbf{j}_1\mathbf{j}_2 \quad \text{and} \quad \mathbf{j}_3^2,\quad \mathbf{j}_1\mathbf{j}_2$$

* The transformed tensors, of course, are not all multiplicative. It can be proved that, for the possibility of constructing a basis of the space $L(K\times V^r)$ from polyads alone, it is necessary and sufficient that the vector representation of the group K split into one-dimensional ones.

§. Let us illustrate what has been said by examples. A system of generators for $L(\bar{4} \cdot m \times V^7)$ consists of the tensors*

$$(\mathbf{j}_1^6 - \mathbf{j}_2^6)\mathbf{j}_3 \sim \mathrm{T}^{(6:m)}\mathbf{e}_3,$$

$$(\mathbf{j}_1^4\mathbf{j}_2^2 - \mathbf{j}_2^4\mathbf{j}_1^2)\mathbf{j}_3 \sim (\mathrm{T}^{(4:m)}\Gamma - \mathrm{T}^{(m\cdot 4:m)}\mathrm{H})\mathbf{e}_3,$$

$$(\mathbf{j}_1^3\mathbf{j}_2 - \mathbf{j}_2^3\mathbf{j}_1)\mathbf{j}_3^3 \sim (\mathrm{T}^{(3:m)}\mathbf{e}_1 - \mathrm{T}^{(m\cdot 3:m)}\mathbf{e}_2)\mathbf{e}_3^3,$$

$$(\mathbf{j}_1^2 - \mathbf{j}_2^2)\mathbf{j}_3^5 \sim \mathrm{H}\mathbf{e}_3^5$$

and their isomers, and for $L(3/\bar{4} \times V^9)$—of the tensors

$$\mathbf{e}_1^7\overline{\mathbf{e}_2\mathbf{e}_3} + \mathbf{e}_2^7\overline{\mathbf{e}_3\mathbf{e}_1} + \mathbf{e}_3^7\overline{\mathbf{e}_1\mathbf{e}_2},$$

$$\mathbf{e}_1^5(\mathbf{e}_2^3\mathbf{e}_3 + \mathbf{e}_3^3\mathbf{e}_2) + \mathbf{e}_2^5(\mathbf{e}_3^3\mathbf{e}_1 + \mathbf{e}_1^3\mathbf{e}_3) + \mathbf{e}_3^5(\mathbf{e}_1^3\mathbf{e}_2 + \mathbf{e}_2^3\mathbf{e}_1),$$

$$\overline{\mathbf{e}_1^3\mathbf{e}_2^3\mathbf{e}_3^3}$$

and their isomers.

For $L(m \cdot \infty : m \times V^6)$ the system of generators, according to item 7, is found in the form

$$\tilde{\Gamma}^3, \quad \tilde{\Gamma}^2\mathbf{e}_3^2, \quad \tilde{\Gamma}\mathbf{e}_3^4, \quad \mathbf{e}_3^6,$$

and for $L(\infty : 2 \times V^7)$—in the form

$$\tilde{\Gamma}^2\widetilde{\mathrm{E}}\mathbf{e}_3, \quad \tilde{\Gamma}\widetilde{\mathrm{E}}\mathbf{e}_3^3, \quad \widetilde{\mathrm{E}}\mathbf{e}_3^5.$$

Thus, the method set forth makes it possible to construct easily anisotropic tensors of a given crystallographic symmetry—a problem that occurs very often in crystal physics and, for a tensor of high rank, is rather laborious.

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* The tilde $\sim$ denotes proportionality.

Note: Figure translations are in progress. See original paper for figures.