TENSOR AND INTEGRITY BASES FOR THE GYROIDAL CRYSTAL CLASS

BY

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1. Introduction. A tensor $c_{ij\cdots k}$ which satisfies the equations

$$c_{ij\cdots k} = t_{ip}t_{jq} \cdots t_{kr}c_{pq\cdots r} \tag{1.1}$$

for all transformations $\mathbf{T} = ||t_{ip}||$ belonging to a group $\mathbf{\Gamma}$ is said to be invariant under $\mathbf{\Gamma}$. A set of tensors each of which is invariant under $\mathbf{\Gamma}$ and such that any tensor invariant under $\mathbf{\Gamma}$ is expressible as a linear combination of outer products of these tensors is said to form a tensor basis for $\mathbf{\Gamma}$. A function $W(\mathbf{x}_1, \mathbf{x}_2, \cdots, \mathbf{x}_N)$ of the vectors $\mathbf{x}_1, \mathbf{x}_2, \cdots, \mathbf{x}_N$ which satisfies the equations

$$W(\mathbf{Tx}_1, \mathbf{Tx}_2, \cdots, \mathbf{Tx}_N) = W(\mathbf{x}_1, \mathbf{x}_2, \cdots, \mathbf{x}_N) \tag{1.2}$$

for all transformations $\mathbf{T}$ belonging to a group $\mathbf{\Gamma}$ is said to be invariant under $\mathbf{\Gamma}$. A set of polynomials $I_p(\mathbf{x}_1, \mathbf{x}_2, \cdots, \mathbf{x}_N)$ $(p = 1, 2, \cdots, m)$, each of which is invariant under $\mathbf{\Gamma}$, is said to form an integrity basis for N vectors under $\mathbf{\Gamma}$ if any polynomial function of the N vectors which is invariant under $\mathbf{\Gamma}$ is expressible as a polynomial in $I_1, I_2, \cdots, I_m$. The I_p are referred to as elements of the integrity basis.

The tensor basis and the integrity basis for N vectors has been obtained by Smith and Rivlin [1] for each of the groups associated with the various crystal classes with the exception of the gyroidal class whose Schoenflies, Hermann–Maguin and Schubnikov symbols are 0, 43 and $\frac{3}{4}$ respectively. In this note, we fill this gap in the literature by deriving the tensor basis and the integrity basis for N vectors for the gyroidal class.

If an element I_m (say) of the integrity basis is expressible as a polynomial in the remaining elements $I_1, \cdots, I_{m-1}$, then I_m is said to be redundant. If none of the $I_1, \cdots, I_m$ are redundant, the integrity basis is said to be irreducible. We shall show in a later paper [2] that none of the multilinear elements of the integrity basis are redundant. Since the elements of the tensor basis are obtained directly from these multilinear invariants (see Sec. 3, Formula (3.1)), this will also imply the irreducibility of the tensor basis.

2. Integrity basis. The group $\mathbf{\Gamma}$ associated with the gyroidal class is comprised of the twenty-four transformations

$$(\mathbf{I}, \mathbf{D}_1, \mathbf{D}_2, \mathbf{D}_3)\cdot(\mathbf{I}, \mathbf{M}_1, \mathbf{M}_2), \quad (\mathbf{C}, \mathbf{R}_1, \mathbf{R}_2, \mathbf{R}_3)\cdot(\mathbf{T}_1, \mathbf{T}_2, \mathbf{T}_3) \tag{2.1}$$

where the transformations $\mathbf{I}, \mathbf{D}_1, \cdots, \mathbf{T}_3$ are defined in [3]. The transformations (2.1) are proper orthogonal and consequently det $(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3)$ is invariant under $\mathbf{\Gamma}$. It then follows from Peano's theorem (see [4, pp. 39–44] or [5, p. 261]) that an integrity basis for N three-dimensional vectors may be derived from det $(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3)$ and the integrity basis for two vectors by the process of polarization. Thus, if $I_1, I_2, \cdots, I_\mu$ form an integrity basis for functions of two vectors $\mathbf{x}_1, \mathbf{x}_2$ invariant under $\mathbf{\Gamma}$, then an integrity basis for N vectors is given by

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$$\det(\mathbf{x}_{K_1}, \mathbf{x}_{K_2}, \mathbf{x}_{K_3})$$

and (2.2)

$$x_{i_1}^{(K_1)} x_{i_2}^{(K_2)} \cdots x_{i_s}^{(K_s)} \frac{\partial^s I_\alpha}{\partial x_{i_1}^{(L_1)} \partial x_{i_2}^{(L_2)} \cdots \partial x_{i_s}^{(L_s)}}$$

where $\alpha = 1, \cdots, \mu$; $K_1, \cdots, K_s$ are integers chosen from $1, \cdots, N$ and $L_1, \cdots, L_s$ are appropriately chosen integers from 1, 2. The quantities $x_i^{(K)}$ represent the components of the vector $\mathbf{x}_K$.

We shall employ the notation $\sum$ to indicate the sum of the three quantities obtained by cyclic permutation of subscripts on the summand, thus:

$$\sum x_1 y_1 = x_1 y_1 + x_2 y_2 + x_3 y_3 . \tag{2.3}$$

It may be readily shown by the methods employed in [1] that the integrity basis for functions of two vectors $\mathbf{x}$ and $\mathbf{y}$ invariant under the gyroidal group is given by

$$\sum x_1^\alpha y_1^\beta , \quad \sum x_1^\gamma y_1^\delta (x_2 y_3 - x_3 y_2) \tag{2.4}$$

where α, β, γ, δ are positive integers or zero such that $\alpha + \beta = 2$, 4 or 6; $\gamma + \delta = 3$ or 5 and

$$y_{i_1} \cdots y_{i_\nu} \partial^\nu \tau / \partial x_{i_1} \cdots \partial x_{i_\nu} \qquad (\nu = 0, 1, 2, \cdots, 9) \tag{2.5}$$

where

$$\tau = \sum x_1^5 (x_2^3 x_3 - x_3^3 x_2). \tag{2.6}$$

The integrity basis for N vectors is then obtained from (2.2) upon substituting the invariants (2.4) and (2.5) for $I_1, \cdots, I_\mu$ in (2.2). We list below the typical multilinear elements of this integrity basis.

Two vectors. $\sum x_1 y_1$.

Three vectors. $\sum x_1 (y_2 z_3 - y_3 z_2)$.

Four vectors. $\sum x_1 y_1 z_1 u_1$.

Five vectors. $\theta(x, y, z, u; v)$, $\theta(v, x, y, z; u)$,

$\theta(u, v, x, y; z)$, $\theta(z, u, v, x; y)$

where

$$\theta(x, y, z, u; v) = \sum x_1 y_1 z_1 (u_2 v_3 - u_3 v_2) + \sum x_1 y_1 u_1 (z_2 v_3 - z_3 v_2) + \sum x_1 z_1 u_1 (y_2 v_3 - y_3 v_2) + \sum y_1 z_1 u_1 (x_2 v_3 - x_3 v_2).$$

Six vectors. $\sum x_1 y_1 z_1 u_1 v_1 w_1$. (2.7)

Seven vectors. $\phi(x, y, z, u, v, w; r)$, $\phi(r, x, y, z, u, v; w)$,

$\phi(w, r, x, y, z, u; v)$, $\phi(v, w, r, x, y, z; u)$,

$\phi(u, v, w, r, x, y; z)$, $\phi(z, u, v, w, r, x; y)$

where

$$\phi(x, y, z, u, v, w; r) = \sum x_1y_1z_1u_1v_1(w_2r_3 - w_3r_2) + \sum x_1y_1z_1u_1w_1(v_2r_3 - v_3r_2) + \sum x_1y_1z_1v_1w_1(u_2r_3 - u_3r_2) + \sum x_1y_1u_1v_1w_1(z_2r_3 - z_3r_2) + \sum x_1z_1u_1v_1w_1(y_2r_3 - y_3r_2) + \sum y_1z_1u_1v_1w_1(x_2r_3 - x_3r_2).$$

Nine vectors. $x_{i_1}y_{i_2}z_{i_3}u_{i_4}v_{i_5}w_{i_6}r_{i_7}s_{i_8}t_{i_9}\ \partial^9\tau/\partial x_{i_1}\,\partial x_{i_2}\cdots\partial x_{i_9}$

where

$$\tau = \sum x_1^5(x_2^3x_3 - x_3^3x_2).$$

An integrity basis for N vectors may be obtained by substituting the vectors $\mathbf{x}_1$, $\mathbf{x}_2$, $\cdots$, $\mathbf{x}_N$ in all possible combinations, repetitions allowed, for the vectors, $\mathbf{x}$, $\mathbf{y}$, $\cdots$, $\mathbf{t}$ in the invariants listed above.

The invariant of (2.7) involving nine vectors is also expressible as the sum of the 504 distinct expressions obtained from

$$\sum x_1y_1z_1u_1v_1(w_2r_2s_2t_3 - w_3r_3s_3t_2) \tag{2.8}$$

by permuting the letters x, $\cdots$, t in all possible ways. We note that $\theta(x, y, z, u; v)$ is symmetric in the first four letters and that

$$\theta(x, y, z, u; v) + \theta(v, x, y, z; u) + \theta(u, v, x, y; z) + \theta(z, u, v, x; y) + \theta(y, z, u, v; x) = 0. \tag{2.9}$$

Similarly, $\phi(x, y, z, u, v, w; r)$ is symmetric in the first six letters and satisfies the equation

$$\phi(x, y, z, u, v, w; r) + \phi(r, x, y, z, u, v; w) + \phi(w, r, x, y, z, u; v) + \phi(v, w, r, x, y, z; u) + \phi(u, v, w, r, x, y; z) + \phi(z, u, v, w, r, x; y) + \phi(y, z, u, v, w, r; x) = 0. \tag{2.10}$$

3. Tensor basis. Let $L_1, \ldots, L_R$ denote the elements (2.7) of the integrity basis for N vectors which are multilinear in the first p, $\cdots$, first q vectors respectively. Then, the tensor basis is given [6] by the tensors

$$\frac{\partial^p L_1}{\partial x_i^{(1)}\,\partial x_j^{(2)}\cdots\partial x_k^{(p)}}, \cdots, \frac{\partial^q L_R}{\partial x_i^{(1)}\,\partial x_j^{(2)}\cdots\partial x_k^{(q)}}. \tag{3.1}$$

We shall employ the notation

$$\begin{aligned} c_{ijklm} &= \sum \delta_{1i}\delta_{1j}\delta_{1k}(\delta_{2l}\delta_{3m} - \delta_{3l}\delta_{2m}),\\ \theta_{ijklm} &= c_{ijklm} + c_{lijkm} + c_{klijm} + c_{jklim},\\ d_{ijklmnp} &= \sum \delta_{1i}\delta_{1j}\delta_{1k}\delta_{1l}\delta_{1m}(\delta_{2n}\delta_{3p} - \delta_{3n}\delta_{2p}),\\ \phi_{ijklmnp} &= d_{ijklmnp} + d_{nijklmp} + d_{mnijklp}\\ &\quad + d_{lmnijkp} + d_{klmnijp} + d_{jklmnip} \end{aligned} \tag{3.2}$$

where the term δ_{1i} is equal to one if $i = 1$ and is equal to zero otherwise. Further, let $\tau_{ijklmnpqr}$ denote the sum of the 504 distinct terms arising from

$$\sum \delta_{1i}\delta_{1j}\delta_{1k}\delta_{1l}\delta_{1m}(\delta_{2n}\delta_{2p}\delta_{2q}\delta_{3r} - \delta_{3n}\delta_{3p}\delta_{3q}\delta_{2r}) \tag{3.3}$$

by permuting the subscripts i, j, $\cdots$, r in all possible ways. We note that there are only five distinct tensors arising from θ_{ijklm} upon permuting the subscripts due to the symmetry of θ_{ijklm} in the first four subscripts. Only four of these five tensors are independent since

$$\theta_{ijklm} + \theta_{mijkl} + \theta_{lmijk} + \theta_{klmij} + \theta_{jklmi} = 0. \tag{3.4}$$

Similarly there are only seven distinct tensors arising from $\phi_{ijklmnp}$ upon permutation of the subscripts due to the symmetry of $\phi_{ijklmnp}$ in the first six subscripts. Only six of these seven tensors are independent since

$$\phi_{ijklmnp} + \phi_{pijklmn} + \phi_{npijklm} + \phi_{mnpijkl} + \phi_{lmnpijk} + \phi_{klmnpij} + \phi_{jklmnpi} = 0. \tag{3.5}$$

With (3.4) and (3.5) in mind, we see from (2.7), (3.1), (3.2) and (3.3) that the tensor basis for the gyroidal group is given by

$$\begin{gathered}
\delta_{ij}\ ;\ e_{ijk}\ ;\ \sum \delta_{1i}\delta_{1j}\delta_{1k}\delta_{1l}\ ; \\
\theta_{ijklm}\ ,\ \theta_{mijkl}\ ,\ \theta_{lmijk}\ ,\ \theta_{klmij}\ ; \\
\sum \delta_{1i}\delta_{1j}\delta_{1k}\delta_{1l}\delta_{1m}\delta_{1n}\ ; \\
\phi_{ijklmnp}\ ,\ \phi_{pijklmn}\ ,\ \phi_{npijklm}\ ,\ \phi_{mnpijkl}\ ,\ \phi_{lmnpijk}\ ,\ \phi_{klmnpij}\ ; \\
\tau_{ijklmnpqr}\ .
\end{gathered} \tag{3.6}$$

The tensors δ_{ij} and e_{ijk} appearing in (3.6) are the Kronecker delta and the alternating tensor respectively. The tensors θ_{ijklm} , $\phi_{ijklmnp}$ and $\tau_{ijklmnpqr}$ are defined above.

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