values of $|B|$ in the non-isomorphous case are much smaller than those in the isomorphous case, as is shown in Table 2, resulting in the rather poor estimates. Nearly half of the seminvariants are incorrectly estimated. This implies that the traditional $\sum_1$ formula is not applicable in the macromolecular case and the comparison confirms that the ability to combine direct methods and isomorphous replacement is powerful.

## Concluding remarks

The distribution of Hauptman (1982) employing a combination of direct methods and the SIR technique has been developed to estimate the values (0 or $\pi$) of the OPSSs. The method proved to be effective with the error-free data of a pair of isomorphous structures. No heavy-atom information, neither the positions nor the content of heavy atoms, is necessary to obtain the estimates of the cosine seminvariants but, if the heavy atoms are located, better results can be obtained by making use of the heavy-atom structure information. The test calculations agree with the prediction of Fortier, Weeks & Hauptman (1984) that, even when the normalized structure factors themselves are small, reliable estimates can be obtained provided that the differences beween the structure-factor magnitudes of the native protein and the derivative are large.

The method presented here is actually equivalent to the $\sum_1$ formula combining with SIR data and provides a supplementary technique of finding individual phases in the initial stages of the phasing procedure. An obvious practical application lies in the possibility of enhancing the starting set in the standard tangent refinement by incorporating a number of the OPSSs with high reliability. In view of the fact that at least two thirds of the OPSSs can be accurately determined for the chosen example, it is not unreasonable to expect that the method may play a more important role in the solution of macromolecular structures than the $\sum_1$ formula does in the small molecule case. This work also shows that Hauptman's distribution is very promising in solving the phase problem in the SIR case, although further theoretical and experimental studies are needed for applying it to unknown structures.

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### References

CRICK, F. H. C. & MAGDOFF, B. S. (1956). *Acta Cryst.* **9**, 901–908.
FORTIER, S., MOORE, N. J. & FRASER, M. E. (1985). *Acta Cryst.* A**41**, 571–577.
FORTIER, S., WEEKS, C. M. & HAUPTMAN, H. (1984). *Acta Cryst.* A**40**, 544–548.
HAO, Q. & FAN, H.-F. (1988). *Acta Cryst.* A**44**, 379–382.
HAŠEK, J. (1977). *Z. Kristallogr.* **145**, 263–270.
HAUPTMAN, H. (1982). *Acta Cryst.* A**38**, 289–294.
HAUPTMAN, H., POTTER, S. & WEEKS, C. M. (1982). *Acta Cryst.* A**38**, 294–300.
KARLE, J. & HAUPTMAN, H. (1956). *Acta Cryst.* **9**, 635–651.
LIU, Y.-S. & HU, N.-H. (1994). *Acta Cryst.* A**50**, 595–601.
LIU, Y.-S., JIN, Z.-S. & GUO, D.-Y. (1982). *Sci. Sin. (Ser. B)*, **25**, 800–814.
TIMKOVICH, R. & DICKERSON, R. E. (1976). *J. Biol. Chem.* **251**, 4033–4046.
VELMURUGAN, D. & HAUPTMAN, H. (1989). *Acta Cryst.* A**45**, 158–163.
VELMURUGAN, D., HAUPTMAN, H. & POTTER, S. A. (1989). *Acta Cryst.* A**45**, 163–165.

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# Magnetic Completely Transposable Twin Laws and Tensor Distinction

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## Abstract

Macroscopic tensorial physical properties that are different in two domains of a ferroic crystal provide a *tensor distinction* of the two domains. This tensor distinction is determined from a symmetry relationship, called a *twin law*, between the bulk structures, the *domain states*, of the two domains. The simplest type of twin law is the so-called completely transposable twin law. We extend here the concept of completely transposable twin laws from non-magnetic to magnetic completely transposable twin laws. We establish the

structure of and tabulate the 380 classes of magnetic completely transposable twin laws. The relationship between magnetic completely transposable twin laws and double antisymmetry groups is then given. Examples of the application of magnetic completely transposable twin laws are given in the tensor distinction of non-ferroelastic magnetoelectric domain pairs.

## 1. Introduction

We consider crystalline domains that arise in a phase transition from a high-symmetry phase of symmetry **G** to a low-symmetry phase of symmetry **F**. We shall refer to the bulk structures of these domains in polydomain samples as *domain states*. Several disconnected domains of possibly different shape can have the same domain state. Consequently, domain states of a polydomain sample represent structures that appear in the sample, irrespective of in which domain and irrespective of the domain's shape. We are interested in the tensor distinction of domains, distinguishing the domains by the values of components of macroscopic tensorial physical properties. This tensor distinction of domains is identical with the tensor distinction of the domains' corresponding domain states. Because the domains, owing to their shape, are not necessarily symmetry related, while their corresponding domain states are, we consider, in what follows, the tensor distinction of domain states. As we shall consider macroscopic tensorial physical properties, we shall use the continuum description of the domain states and our symmetry analysis will be based on point-group considerations only.

Two domain states $S_i$ and $S_j$ form a domain pair $\{S_i, S_j\}$ (Janovec, 1972). We shall call the twin law of the domain pair $\{S_i, S_j\}$ that symmetry information that specifies the point groups of the two domain states $S_i$ and $S_j$ and their relationship. The symmetry information is provided for by the point group $\mathbf{F}_i$, the point group of the domain state $S_i$, and the element $g_{ij}$, called the twinning operation, which transforms the domain state $S_i$ into the domain state $S_j$, *i.e.* $g_{ij}S_i = S_j$. The point group of the domain state $S_j$ is given by $\mathbf{F}_j = g_{ij}\mathbf{F}_i g_{ij}^{-1}$ and the relationship between the domain states is given by the twinning operation $g_{ij}$.

The twin law of a domain pair can alternatively be given by a group $\mathbf{J} = \langle \mathbf{F}_i, g_{ij} \rangle$, the group generated by the group $\mathbf{F}_i$ and the twinning operation $g_{ij}$. In its simplest form, the twin law is of the form

$$\mathbf{J} \equiv \langle \mathbf{F}_i, g_{ij} \rangle = \mathbf{F}_i + g_{ij}\mathbf{F}_i, \tag{1}$$

where **J** consists of only two cosets of the point group $\mathbf{F}_i$. In this case, the twin law is referred to as a completely transposable twin law (Janovec, Litvin & Richterova, 1994). This is referred to as a transposable twin law [this was previously referred to as an ambivalent twin law (Janovec, 1981)] as the twinning operation $g_{ij}$ not only transforms the domain state $S_i$ into $S_j$ but in addition transforms the domain state $S_j$ into $S_i$, *i.e.*

$$S_j = g_{ij}S_i \quad \text{and} \quad S_i = g_{ij}S_j.$$

This is referred to as a completely transposable twin law because, in addition to being transposable, the point groups of the two domain states $S_i$ and $S_j$ are identical, that is

$$\mathbf{F}_j \equiv g_{ij}\mathbf{F}_i g_{ij}^{-1} = \mathbf{F}_i.$$

A ferroic phase is non-ferroelastic if all the domains have the same (zero) spontaneous deformation (Aizu, 1973). In a non-ferroelastic phase, there are $n = |\mathbf{G}|/|\mathbf{F}|$ domain states where $|\mathbf{G}|$ and $|\mathbf{F}|$ denote the order of the groups **G** and **F**, respectively, which are all related by the coset representatives of the coset decomposition of **G** with respect to **F**. The twin laws of non-ferroelastic domain pairs are of the form (1), *i.e.* are completely transposable twin laws (Janovec, Richterova & Litvin, 1993).

In a ferroelastic phase, the orientations of the domain states are controlled by disorientations, *i.e.* rotations of single domain states (domain states invariant under **F** or any conjugate subgroup of **F** in **G**) needed to achieve a coherent interface of two ferroelastic domain states along a planar wall. Consequently, the number of domain states in a ferroelastic phase is, in general, greater than $n = |\mathbf{G}|/|\mathbf{F}|$ and the twin law of a ferroelastic domain pair is, in general, not a completely transposable twin law (Janovec, Litvin & Richterova, 1994).

The tensor distinction of two domain states of a domain pair can be determined from the domain pair's twin law. The form $T_i$ of a tensor $\boldsymbol{T}$ in the domain state $S_i$ is determined by the point group $\mathbf{F}_i$ and the form $T_j$ of the tensor $\boldsymbol{T}$ in the domain state $S_j$ can be determined by transforming $T_i$ by $g_{ij}$:

$$T_j = g_{ij}T_i. \tag{2}$$

By comparing the forms $T_i$ and $T_j$ related by (2), one determines the components of the tensor $\boldsymbol{T}$ that are distinct in the two domain states, *i.e.* one determines the tensor distinction of the domain pair $\{S_i, S_j\}$.

Non-magnetic completely transposable twin laws, (1), can be written as

$$\mathbf{J} = \mathbf{F} + g^*\mathbf{F}, \tag{3}$$

where **J** is a non-magnetic point group (*i.e.* a point group belonging to one of the 32 classes of crystallographic point groups) and the element $g$ has been given an asterisk to denote and emphasize that this is an element of **J** that transposes the two domain states. The non-magnetic completely transposable twin law is uniquely characterized by the point group **J** and a subgroup **F** of index 2 of **J**. Consequently, the mathematical structure of non-magnetic completely transposable twin laws is the same as that of dichromatic (black and white, anti-

symmetry) point groups (Heesch, 1930; Shubnikov, 1951). Completely transposable non-magnetic twin laws have been used in determining the macroscopic tensorial physical properties that distinguish domains of a domain pair in the cases of non-ferroelastic and ferroelectric non-ferroelastic domains (Janovec, Richterova & Litvin, 1992, 1993).

In §2, we extend the concept of completely transposable twin laws from that of non-magnetic completely transposable twin laws to magnetic completely transposable twin laws, *i.e.* to the case where in (1) **J** is a magnetic point group. The structure of magnetic completely transposable twin laws is then considered, two types of notation are introduced and all classes of magnetic completely transposable twin laws are then derived. In §3, we discuss the application of magnetic completely transposable twin laws in determining the tensor distinction of non-ferroelastic magnetoelectric domain pairs. It is shown in Appendix 1 that the mathematical structure of magnetic completely transposable twin laws is the same as that of the so-called double antisymmetry groups introduced by Zamorzaev & Sokolov (1957), see also Zamorzaev (1976) and Zamorzaev & Palistrant (1980). A third type of notation is introduced there for magnetic transposable twin laws based on the notation used for double antisymmetry groups.

In the remainder of this paper, for typographical and linguistic simplicity, we shall refer to completely transposable twin laws simply as twin laws.

## 2. Magnetic twin laws

Let **J** denote a magnetic point group, *i.e.* a point group belonging to one of the 122 classes of crystallographic magnetic point groups (Opechowski, 1986). Let **F** denote a subgroup of index two of **J**. A magnetic twin law, $\mathbf{J} = \mathbf{F} + g^*\mathbf{F}$, with a magnetic point group **J**, is uniquely characterized and can be denoted, in a double-group notation, by **J**[**F**]. A second single-group notation for a magnetic twin law can be obtained by using the Hermann–Mauguin (International) notation for the magnetic group **J**. Individual symbols in the group symbol of **J** representing elements of **J** not contained in **F** have asterisks. For example, the magnetic twin laws $\mathbf{2}_z/\mathbf{m}'_z = \mathbf{2}_z + m'^*_z\mathbf{2}_z$ and $\mathbf{4}'_z\mathbf{m}'_x\mathbf{m}_{xy} = \mathbf{m}'_x\mathbf{m}'_y\mathbf{2}_z + \mathbf{4}'^*_z\mathbf{m}'_x\mathbf{m}'_y\mathbf{2}_z$ are denoted in the double-group notation **J**[**F**] as $\mathbf{2}_z/\mathbf{m}'_z[\mathbf{2}_z]$ and $\mathbf{4}'_z\mathbf{m}'_x\mathbf{m}_{xy}[\mathbf{m}'_x\mathbf{m}'_y\mathbf{2}_z]$, respectively, and in the single-group notation as $\mathbf{2}_z/\mathbf{m}'^*_z$ and $\mathbf{4}'^*_z\mathbf{m}'_x\mathbf{m}^*_{xy}$, respectively.

The equivalence of two magnetic twin laws is defined as follows: Two magnetic twin laws $\mathbf{J}_1[\mathbf{F}_1]$ and $\mathbf{J}_2[\mathbf{F}_2]$ are said to be equivalent and belong to the same class of magnetic twin laws if there exists a Euclidian transformation that simultaneously transforms $\mathbf{J}_1$ into $\mathbf{J}_2$ and $\mathbf{F}_1$ into $\mathbf{F}_2$.

To derive the number of classes of magnetic twin laws **J**[**F**], we first introduce a notation for non-magnetic point groups and the more detailed notation for the magnetic point groups. We denote a non-magnetic point group by **Q**. There are three types of magnetic point group:

(1) $\mathbf{J} = \mathbf{Q}$. There are 32 such classes. These are the 32 classes of crystallographic non-magnetic point groups.

(2) $\mathbf{J} = \mathbf{Q1}'$. There are 32 such classes. These are direct products of a non-magnetic point group **Q** and the group $\mathbf{1}'$ consisting of the identity 1 and time inversion $1'$.

(3) $\mathbf{J} = \mathbf{H} + a'\mathbf{H}$. There are 58 such classes. Magnetic groups of this type are also denoted by **Q**(**H**), where

$$\mathbf{Q} = \mathbf{H} + a\mathbf{H}.$$

All magnetic groups $\mathbf{J} = \mathbf{Q}$, $\mathbf{J} = \mathbf{Q1}'$, and $\mathbf{J} = \mathbf{Q}(\mathbf{H})$ are said to belong to the same family of the class of the non-magnetic point group **Q**. Consequently, all 122 classes of magnetic point groups can be categorized according to their family into 32 families.

In deriving the magnetic twin laws **J**[**F**], one finds that it is advantageous to subdivide the derivation according to the type of magnetic point group **J**:

(1) $\mathbf{J} = \mathbf{Q}$. **F** must then be a subgroup **H** of index 2 of the non-magnetic point group **Q**. The twin law is then of the type $\mathbf{J}[\mathbf{F}] = \mathbf{Q}[\mathbf{H}]$, *i.e.* a non-magnetic twin law, which, in the format of equation (1), is written as $\mathbf{Q} = \mathbf{H} + a^*\mathbf{H}$. The number of classes of magnetic twin law **Q**[**H**] is the same as the number of classes of magnetic point groups **Q**(**H**), that is 58. For example, for $\mathbf{Q} = \mathbf{2}_x\mathbf{2}_y\mathbf{2}_z$ and $\mathbf{H} = \mathbf{2}_z$, we have the twin law $\mathbf{2}_x\mathbf{2}_y\mathbf{2}_z = \mathbf{2}_z + \mathbf{2}^*_x\mathbf{2}_z$, which is denoted by $\mathbf{2}_x\mathbf{2}_y\mathbf{2}_z[\mathbf{2}_z]$ or $\mathbf{2}^*_x\mathbf{2}^*_y\mathbf{2}_z$.

(2) $\mathbf{J} = \mathbf{Q1}'$. There are three possibilities for **F**:

(i) If $\mathbf{F} = \mathbf{Q}$ then the twin law is $\mathbf{J}[\mathbf{F}] = \mathbf{Q1}'[\mathbf{Q}]$ and $\mathbf{J} = \mathbf{Q} + \mathbf{1}'^*\mathbf{Q} = \mathbf{Q1}'^*$. The number of classes of magnetic twin law **Q**1′[**Q**] is the same as the number of classes of magnetic point groups **Q1**′, that is 32. For example, for $\mathbf{Q} = \mathbf{2}_x\mathbf{2}_y\mathbf{2}_z$, we have the twin law $\mathbf{2}_x\mathbf{2}_y\mathbf{2}_z\mathbf{1}' = \mathbf{2}_x\mathbf{2}_y\mathbf{2}_z + \mathbf{1}'^*\mathbf{2}_x\mathbf{2}_y\mathbf{2}_z$, which is denoted by $\mathbf{2}_x\mathbf{2}_y\mathbf{2}_z\mathbf{1}'[\mathbf{2}_x\mathbf{2}_y\mathbf{2}_z]$ or $\mathbf{2}_x\mathbf{2}_y\mathbf{2}_z\mathbf{1}'^*$.

(ii) If $\mathbf{F} = \mathbf{H1}'$, where **H** is a subgroup of index 2 of **Q**, then the twin law is $\mathbf{J}[\mathbf{F}] = \mathbf{Q1}'[\mathbf{H1}']$. Since

$$\mathbf{J} = \mathbf{H1}' + a^*\mathbf{H1}' = (\mathbf{H} + a^*\mathbf{H})\mathbf{1}'$$

and $\mathbf{H} + a^*\mathbf{H}$ is a non-magnetic twin law **Q**[**H**], the above type of magnetic twin law can be denoted by **Q**[**H**]$\mathbf{1}'$. The number of classes of such magnetic twin laws is the same as the number of classes of twin laws **Q**[**H**], that is 58. For example, for $\mathbf{Q} = \mathbf{2}_x\mathbf{2}_y\mathbf{2}_z$ and $\mathbf{H} = \mathbf{2}_z$, we have the twin law $\mathbf{2}_x\mathbf{2}_y\mathbf{2}_z\mathbf{1}' = \mathbf{2}_z\mathbf{1}' + \mathbf{2}^*_x\mathbf{2}_z\mathbf{1}'$, which is denoted by $\mathbf{2}_x\mathbf{2}_y\mathbf{2}_z\mathbf{1}'[\mathbf{2}_z\mathbf{1}']$ or $\mathbf{2}^*_x\mathbf{2}^*_y\mathbf{2}_z\mathbf{1}'$.

(iii) If $\mathbf{F} = \mathbf{Q}(\mathbf{H})$, then the magnetic twin law is $\mathbf{J}[\mathbf{F}] = \mathbf{Q1}'[\mathbf{Q}(\mathbf{H})]$ and

$$\mathbf{J} = \mathbf{Q}(\mathbf{H}) + 1'^*\mathbf{Q}(\mathbf{H}) = \mathbf{Q}(\mathbf{H})\mathbf{1}'^*.$$

The number of classes of such magnetic twin laws is the

same as the number of classes of magnetic point groups **Q(H)**, that is 58. For example, for $\mathbf{Q} = 2_x2_y2_z$ and $\mathbf{H} = 2_z$, we have the twin law $2_x2_y2_z1' = 2'_x2'_y2_z + 1'^*2'_x2'_y2_z$, which is denoted by $2_x2_y2_z1'[2'_x2'_y2_z]$ or $2'_x2'_y2_z1'^*$.

(3) $\mathbf{J} = \mathbf{Q(H)}$. There are two possibilities for **F**:

(i) $\mathbf{F} = \mathbf{H}$. The magnetic twin law is **Q(H)[H]** and

$$\mathbf{J} = \mathbf{H} + a'^*\mathbf{H}.$$

The number of classes of such magnetic twin laws is the same as the number of classes of magnetic point groups **Q(H)**, that is 58. For example, for $\mathbf{Q} = 2_x2_y2_z$ and $\mathbf{H} = 2_z$, we have the twin law $2'_x2'_y2_z = 2_z + 2'^*_x2_z$, which is denoted by $2'_x2'_y2_z[2_z]$ or $2'^*_x2'^*_y2_z$.

(ii) $\mathbf{F} \neq \mathbf{H}$. The magnetic twin law is **Q(H)[K(R)]**, where **K(R)** is a magnetic subgroup of index 2 of **Q(H)** and

$$\mathbf{J} = \mathbf{R} + a'_1\mathbf{R} + a^*_2\mathbf{R} + a'^*_3\mathbf{R}.$$

$\mathbf{K} = \mathbf{R} + a_1\mathbf{R}$ and $\mathbf{H} = \mathbf{R} + a_2\mathbf{R}$ are subgroups of index 2 of **Q**. **R** is a subgroup of index 2 of both **H** and **K** and a subgroup of index 4 of **Q**. There are 116 classes of magnetic twin laws **Q(H)[K(R)]**. For example, for $\mathbf{Q} = 2_x2_y2_z$, $\mathbf{H} = 2_z$, $\mathbf{K} = 2_x$ and $\mathbf{Q} = \mathbf{1}$, we have the twin law $2'_x2'_y2_z = 2'_x + 2^*_z2'_x$ $(= \mathbf{1} + 2'_x\mathbf{1} + 2^*_z\mathbf{1} + 2'^*_y\mathbf{1})$, which is denoted by $2'_x2'_y2_z[2'_x]$ or $2'_x2'^*_y2^*_z$.

There are then six types of magnetic twin laws **J[F]**

(1) **Q[H]** (2) $\mathbf{Q1'[Q]} = \mathbf{Q1'^*}$

(3) $\mathbf{Q1'[H1']} = \mathbf{Q[H]1'}$ (4) $\mathbf{Q1'[Q(H)]} = \mathbf{Q(H)1'^*}$ (4)

(5) **Q(H)[H]** (6) **Q(H)[K(R)]**

and a total of 380 classes of magnetic twin laws.† The magnetic twin laws can be classified into 32 families according to the family of the magnetic group **J**. A representative magnetic twin law of each class of magnetic twin laws belonging to the family of $\mathbf{Q} = \mathbf{222}$ is given in Table 1. The numbers assigned to each magnetic twin law consist first of the serial number given to the magnetic twin law's family followed by a decimal point and the serial number of the class of the magnetic twin laws in that family. This is followed, in parentheses, by a number denoting the type of magnetic twin law, see equation (4). In the first column is the symbol for the magnetic twin law in double-group notation followed in the second column with the corresponding single-group notation. In the third column is a third notation based on the notation for the six types of twin law given in equation (4) and the symbols that denote double antisymmetry groups. This third notation and the relationship between the magnetic twin laws derived in this section and the double antisymmetry groups is given in Appendix 1.

† The complete tables have been deposited with the IUCr (Reference: CR0489). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 1. *Representative magnetic twin laws of classes belonging to the family of* $\mathbf{Q} = \mathbf{222}$

The type of magnetic twin law is given, in parentheses, following the magnetic twin law's serial no. Three symbols are given, the double-group symbol **J[F]**, the single-group symbol and the corresponding double antisymmetry group symbol.

| (6) 222 | | | |
|---|---|---|---|
| 6.1(1) | $2_x2_y2_z[2_z]$ | $2^*_x2^*_y2_z$ | $2_x2_y2_z\{2_z\}$ |
| 6.2(2) | $2_x2_y2_z1'[2_x2_y2_z]$ | $2_x2_y2_z1'^*$ | $2_x2_y2_z1'^*$ |
| 6.3(3) | $2_x2_y2_z1'[2_z1']$ | $2^*_x2^*_y2_z1'$ | $2_x2_y2_z\{2_z\}1'$ |
| 6.4(4) | $2_x2_y2_z1'[2'_x2'_y2_z]$ | $2'_x2'_y2_z1'^*$ | $2_x2_y2_z(2_z)1'^*$ |
| 6.5(5) | $2'_x2'_y2_z[2_z]$ | $2'^*_x2'^*_y2_z$ | $2_x2_y2_z(2_z)\{2_z\}$ |
| 6.6(6) | $2'_x2'_y2_z[2'_x]$ | $2'_x2'_y2^*_z$ | $2_x2_y2_z(2_z)\{2_x(1)\}$ |

## 3. Tensor distinction

We consider the tensor distinction of a non-ferroelastic magnetoelectric domain pair (Litvin, Janovec & Litvin, 1994). In such domain pairs, the domains states $S_i$ and $S_j$ have the same (zero) spontaneous deformation and their magnetic twin laws $\mathbf{J} = \mathbf{F} + g^*\mathbf{F}$ are completely transposable. We denote a physical property tensor by $\boldsymbol{T}$ and the form of this tensor in the two domain states $\mathbf{S}_i$ and $\mathbf{S}_j$, respectively, by $T_i$ and $T_j$. The components of the tensor $T_i$ will be denoted by $T_i^{\alpha\beta\gamma\cdots}$.

The types of physical property tensors considered are denoted by symbols for their transformational properties. Each symbol consists of the symbol $V^n$, which denotes the $n$th product of a polar vector tensor, possibly preceded by $a$ and/or $e$, symbols that denote rank-zero tensors that change sign under time inversion $1'$ and spatial inversion $\bar{1}$, respectively. The physical meaning of many types of these tensors is given by Sirotin & Shaskolskaya (1975). We list eight tensor types in the first column of Table 2.

We consider a domain pair related by the magnetic twin law $\mathbf{J[F]} = 4_z2'_x2'_{xy}[4_z]$, *i.e.* by the twin law $4_z2'_x2'_{xy} = 4_z + 2'^*_x4_z$. In this case, the point group of the domain $S_i$ is $\mathbf{F} = 4_z$ and the domain $S_j$ is related to the domain $S_i$ by the element $2'_x$, *i.e.* $S_j = 2'_xS_i$. Consequently, the form of the tensor $T_i$ is invariant under the point group $4_z$ and the form of the tensor $T_j$ is related to the form of the tensor $T_i$ by the element $2'_x$, *i.e.* $T_j = 2'_xT_i$. The form of non-magnetic physical property tensors invariant under non-magnetic point groups for a wide variety of tensor types can be found in Sirotin & Shaskolskaya (1975). The same tables can also be used to determine the form of a magnetic physical property tensor invariant under magnetic point groups (Litvin, 1994). For the magnetoelectric effect tensor, a tensor of the type $aeV^2$, the form of the tensor $T_i$, invariant under $4_z$ is

$$T_i^{\alpha\beta} = \begin{pmatrix} A & C & 0 \\ -C & A & 0 \\ 0 & 0 & B \end{pmatrix}.$$

Table 2. *For the magnetic twin law* $\mathbf{J[F]} = \mathbf{4}_z\mathbf{2}'_x\mathbf{2}'_{xy}[\mathbf{4}_z]$ *and the eight types of tensors listed in the first column, the forms of the tensors* $T_i$ *and* $T_j = 2'_xT_i$ *are given in the second and third columns, respectively*

The tensor notation used is that of Sirotin & Shaskolskaya (1975).

| Tensor type | Domain state $S_i$ $T_i$ | Domain state $S_j$ $T_j$ |
|---|---|---|
| $V$ | $\begin{matrix}0\\0\\A\end{matrix}$ | $\begin{matrix}0\\0\\-A\end{matrix}$ |
| $aeV$ | $\begin{matrix}0\\0\\A\end{matrix}$ | $\begin{matrix}0\\0\\A\end{matrix}$ |
| $[V^2]$ | $\begin{matrix}A&0&0\\0&A&0\\0&0&B\end{matrix}$ | $\begin{matrix}A&0&0\\0&A&0\\0&0&B\end{matrix}$ |
| $aeV^2$ | $\begin{matrix}A&C&0\\-C&A&0\\0&0&B\end{matrix}$ | $\begin{matrix}-A&C&0\\-C&-A&0\\0&0&-B\end{matrix}$ |
| $V[V^2]$ | $\begin{matrix}0&0&0&B&A&0\\0&0&0&A&-B&0\\C&C&D&0&0&0\end{matrix}$ | $\begin{matrix}0&0&0&B&-A&0\\0&0&0&-A&-B&0\\-C&-C&-D&0&0&0\end{matrix}$ |
| $aeV[V^2]$ | $\begin{matrix}0&0&0&B&A&0\\0&0&0&A&-B&0\\C&C&D&0&0&0\end{matrix}$ | $\begin{matrix}0&0&0&-B&A&0\\0&0&0&A&B&0\\C&C&D&0&0&0\end{matrix}$ |
| $[V^3]$ | $\begin{matrix}0&0&0&0\\0&0&0\\A&A&B\end{matrix}$ | $\begin{matrix}0&0&0&0\\0&0&0\\-A&-A&-B\end{matrix}$ |
| $ae[V^3]$ | $\begin{matrix}0&0&0&0\\0&0&0\\A&A&B\end{matrix}$ | $\begin{matrix}0&0&0&0\\0&0&0\\A&A&B\end{matrix}$ |

The form of the tensor $T_j = 2'_xT_i$ is calculated *via* the standard transformation of a second-rank tensor

$$T_j^{\alpha\beta} = -D^{1-}(2_x)_{\alpha\alpha'}D^{1-}(2_x)_{\beta\beta'}T_i^{\alpha'\beta'},$$

where the additional minus sign is present since the tensor type is $aeV^2$, which changes sign under time inversion and $g^* = 2'_x$ is a primed element. The form of the tensor $T_j$ is then

$$T_j^{\alpha\beta} = \begin{pmatrix} -A & C & 0 \\ -C & -A & 0 \\ 0 & 0 & -B \end{pmatrix}.$$

The two domains can be distinguished by the $T^{xx}$, $T^{yy}$ and $T^{zz}$ components of the magnetoelectric effect tensor.

In the second and third columns of Table 2, we give the component forms of the tensors $T_i$ and $T_j$ for the tensor types listed in the first column. By comparing the forms of the tensors in the two domains of the domain pair related by this magnetic twin law, we have that five tensor types distinguish between the two domains and three do not.

This domain pair is magnetoelectric as the form of the magnetoelectric effect tensor (a tensor of type $aeV^2$) is different in the two domains and non-ferroelastic as the ferroelasticity effect tensor (of the type $[V^2]$) is identical in the two domains. From Table 2, we have that the domains of this domain pair can also be distinguished by spontaneous polarization ($V$), piezoelectric and second non-linear magnetoelectric tensors ($V[V^2]$), piezomagnetic and first non-linear magnetoelectric tensors ($aeV[V^2]$) and non-linear electric tensors ($[V^3]$). [See Schmid (1975) for a complete discussion of these magnetoelectric phenomena.] The domains cannot be distinguished by spontaneous magnetization ($aeV$), their electric and magnetic susceptibility ($[V^2]$) or by their non-linear magnetic susceptibility ($ae[V^3]$).

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## APPENDIX 1
## Double antisymmetry groups

The magnetic twin laws, derived in §2, have the same mathematical structure as the double antisymmetry point groups introduced by Zamorzaev & Sokolov (1957). Double antisymmetry point groups can be defined as follows. All points of a finite object are assigned two signs, each of which can be a positive or negative sign. In addition to the point-group transformations of the unsigned object, one defines transformations of the signs, a transformation $1'$ that reverses the value of the first sign and $1^*$ that reserves the value of the second sign. [In Zamorzaev & Sokolov (1957), the star is placed to the left of the symbol, *i.e.* *1.] A double antisymmetry group is an invariance group of such a signed finite object, the group of those point-group transformations and point-group transformations coupled with $1'$, $1^*$ or $1'^*$ that leave the signed finite object invariant. Of the twelve types of double antisymmetry point groups, six correspond to the six types of magnetic twin laws. Listed in order corresponding to the types of magnetic twin laws given in equation (4), these are:

$$\begin{array}{ll} (1)\ \mathbf{Q\{H\}} & (2)\ \mathbf{Q1'^*} \\ (3)\ \mathbf{Q\{H\}1'} & (4)\ \mathbf{Q(H)1'^*} \\ (5)\ \mathbf{Q(H)\{H\}} & (6)\ \mathbf{Q(H)\{K\} = Q(H)\{K(R)\}}. \end{array} \qquad (A1)$$

**Q** denotes a point group and **H** and **K** subgroups of index 2 of **Q**. **R** is a subgroup of index 2 of both **H** and **K** and a subgroup of index 4 of **Q**.

**Q{H}** denotes a group where the elements of **Q** not contained in the subgroup **H** are coupled with $1^*$. **Q(H)** denotes a group where the elements of **Q** not contained in the subgroup **H** are coupled with $1'$. **Q(H){K}** denotes a group where the elements of **Q** not contained in **H** are coupled with $1'$ and the elements of **Q** not contained in **K**

are coupled with 1*. In groups $\mathbf{Q}(\mathbf{H})\{\mathbf{H}\}$, the elements of $\mathbf{Q}$ not contained in $\mathbf{H}$ are coupled with $1'^*$. In groups $\mathbf{Q}(\mathbf{H})\{\mathbf{K}\}$, with $\mathbf{H} \neq \mathbf{K}$, there are elements of $\mathbf{Q}$ coupled with $1'$, coupled with 1* and coupled with $1'^*$. Those elements of $\mathbf{Q}$ not coupled with any of these constitute a subgroup $\mathbf{R}$ which is a subgroup of index 2 of both $\mathbf{H}$ and $\mathbf{K}$, and a subgroup of index 4 of $\mathbf{Q}$. Elements of $\mathbf{K}$ that are not in $\mathbf{R}$ are coupled with $1'$ and consequently double antisymmetry point groups of this type can be denoted by $\mathbf{Q}(\mathbf{H})\{\mathbf{K}(\mathbf{R})\}$. The mathematical equivalence of the magnetic twin laws given in equation (4) with the double antisymmetry groups listed in equation (A1) can now be easily seen: One can interchange the corresponding types of magnetic twin laws and double antisymmetry groups by interchanging the square brackets [] with the curly brackets {}. In the third column of symbols in Table 1, we give the double antisymmetry group symbol, equation (A1), of each of the listed magnetic twin laws.

### References


AIZU, K. (1973). *J. Phys. Soc. Jpn*, **34**, 121–128.

HEESCH, H. (1930). *Z. Kristallogr.* **73**, 325–345.

JANOVEC, V. (1972). *Czech J. Phys.* B**22**, 974–994.

JANOVEC, V. (1981). *Ferroelectrics*, **35**, 105–110.

JANOVEC, V., LITVIN, D. B. & RICHTEROVA, L. (1994). *Ferroelectrics*, **157**, 75–80.

JANOVEC, V., RICHTEROVA, L. & LITVIN, D. B. (1992). *Ferroelectrics*, **126**, 287–292.

JANOVEC, V., RICHTEROVA, L. & LITVIN, D. B. (1993). *Ferroelectrics*, **140**, 95–100.

LITVIN, D. B. (1994). *Acta Cryst.* A**50**, 406–408.

LITVIN, D. B., JANOVEC, V. & LITVIN, S. Y. (1994). *Ferroelectrics*, **162**, 275–280.

OPECHOWSKI, W. (1986). *Crystallographic and Metacrystallographic Groups*. Amsterdam: North-Holland.

SCHMID, H. (1975). *Magnetoelectric Interaction Phenomena in Crystals*, edited by A. J. FREEMAN & H. SCHMID, pp. 121–145. New York: Gordon and Breach.

SHUBNIKOV, A. V. (1951). *Symmetry and Antisymmetry of Finite Figures*. Moscow: Academy of Sciences. [English translation in *Color Symmetry* (1964), edited by W. T. HOLSER. New York: Macmillan.]

SIROTIN, YU. & SHASKOLSKAYA, M. P. (1975). *Osnovi Kristallogfiziki*. Moscow: Nauka. [English translation: *Fundamentals of Crystal Physics* (1982). Moscow: Mir.]

ZAMORZAEV, A. M. (1976). *The Theory of Simple and Multiple Antisymmetry*. Kishinev: Shtiintsa.

ZAMORZAEV, A. M. & PALISTRANT, A. F. (1980). *Z. Kristallogr.* **151**, 231–248.

ZAMORZAEV, A. M. & SOKOLOV, E. I. (1957). *Sov. Phys. Crystallogr.* **2**, 9–14.


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# On the Use of Crenel Functions for Occupationally Modulated Structures


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## Abstract

The use of a crenel function, *i.e.* a difference between two Heaviside functions of amplitude 1, for strong occupation modulation waves and its influence on the refinement of accompanying displacive modulation waves is discussed. The basic set of harmonic functions that is usually employed for the modelling of the displacive modulation wave is no longer orthogonal on the interval where the crenel function takes the value 1. This causes severe correlations between different displacive modulation amplitudes during refinement. The best solution to prevent these correlations is to select functions for inclusion in the refinement according to the criterion that their generalized cosine to the subspace of already selected functions has to be smaller than a certain threshold value. A quality-of-selection parameter is used to estimate the completeness of the selected functions. Finally, the selected functions are orthogonalized. One artificial illustration and one real example are given to demonstrate the use and application of the proposed methods.


## Introduction

The theory of $(3 + d)$ superspace groups, introduced by de Wolff (1974, 1977), Janner & Janssen (1977) and de

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