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NON-FERROELASTIC MAGNETOELECTRIC TWIN LAWS

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By definition, magnetoelectric domains exhibit different tensor components of the magnetoelectric tensor when observed from the same coordinate system. Since direct detection of the magnetoelectric tensor components is difficult, it is advantageous to know in which other material tensor properties the magnetoelectric domains differ. If two magnetoelectric bulk structures (domain states) possess different spontaneous deformation, they can be simply observed in an optical microscope. Consequently, we limit our attention to non-ferroelastic magnetoelectric phases in which the domain states of different domains exhibit the same (zero) spontaneous deformation. The distinction between two non-ferroelastic magnetoelectric domains is determined by a point group generated by the point group of the domain state of the first domain and a space-time operation that relates this first domain state to the domain state of the second domain. The resulting point group is called the non-ferroelastic magnetoelectric twin law of the two domain states. Such an analysis is an extension of the recent work on tensor distinction of non-ferroelastic non-magnetic domains.[1,2] where it is shown that non-magnetic twin laws are of the same mathematical structure as antisymmetric (dichromatic) point groups. We shall show that the corresponding magnetic twin laws are of the same mathematical structure as double antisymmetry point groups.[3] We shall list all twin laws of two non-ferroelastic magnetoelectric domain states. For each of these twin laws we shall give the form of important property tensors that are different in the two magnetoelectric domain states under consideration.

Keywords: Domains, magnetoelectric, non-ferroelastic.

1. INTRODUCTION

Macroscopic properties that are different in two domains are determined by the relation between their domain states, i.e. the corresponding bulk structures of domains in polydomain samples. Two domain states S_i and S_k form a domain pair[4] $\{S_i, S_k\}$. Domain pairs $\{S_i, S_k\}$ can be divided into two types: In a *non-ferroelastic domain pair* the structures S_i and S_k possess the same (zero) spontaneous deformation, whereas in a *ferroelastic domain pair* they exhibit different spontaneous deformations. Since the tensor of spontaneous deformation transforms in the same manner as the optical indicatrix, the domain states of a ferroelastic domain pair can be easily distinguished in a polarizing microscope. The domain states of a non-ferroelastic domain pair can not be distinguished in this way.

The relationship between domain states of a domain pair $\{S_i, S_k\}$ can be expressed in terms of a group called the *twin law* of the domain pair. This group, denoted by J, for non-magnetic non-ferroelastic domain pairs, can be written as[1]

$$J = F + a^*F \tag{1}$$

where F is an invariance group of both S_i and S_k and the star on the element a of J denotes that a interexchanges the two domain states, i.e. $aS_i = S_k$ and $aS_k = S_i$. Because of the existence of an element a which interexchanges the two domain states, equation (1) is referred to as a *transposable* twin law. (In previous work on twin laws, the symbol a' was used to denote an element a of J which interexchanges the two domain states. Here we use a star notation to preserve the primed notation for magnetic group elements.)

We extend here the concept of a transposable twin law from that of a non-magnetic twin law, where J is a non-magnetic point group,[1,2] to that of a magnetic transposable twin law, where J is a magnetic point group. Magnetic transposable twin laws are then used to describe non-ferroelastic magnetoelectric domain pairs and the tensor distinction of domain states in such pairs is then considered.

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 (Here we include the 32 classes of point groups which are direct products of a non-magnetic point group and the group consisting of the identity and time inversion.) Let F denote a subgroup of index two of J. A magnetic twin law, equation (1), can be denoted, in a double group notation, by $J[F]$. An alternative single group notation can be had by using the Hermann-Mauguin (International) notation for the magnetic group J. Symbols in the group symbol representing elements of J not contained in F are stared. For example, the magnetic transposable twin laws $2_z/m_z'[2_z]$ and $4_z'm_x'm_{xy}[m_x'm_y'2_z]$ are written in the single group notation, respectively, as $2_z/m_z'^*$ and $4_z'^*m_x'm^*_{xy}$.

The equivalence of two magnetic transposable twin laws is defined as follows: Two magnetic transposable twin laws $J_1[F_1]$ and $J_2[F_2]$ are said to be equivalent, and to belong to the same class of magnetic transposable twin laws, if there exists a transformation that simultaneously transforms J_1 into J_2 and F_1 into F_2. The derivation of all classes of magnetic transposable twin laws is considered elsewhere[5]

TABLE I

Magnetic twin laws of the family 222

Double Group Notation	Single Group Notation	Double Anti-symmetry Notation
$2_x2_y2_z[2_z]$	$2_x{}^*2_y{}^*2_z$	$2_x2_y2_z\{2_z\}$
$2_x2_y2_z1'[2_x2_y2_z]$	$2_x2_y2_z1'^*$	$2_x2_y2_z1'^*$
$2_x2_y2_z1'[2_z1']$	$2_x{}^*2_y{}^*2_z1'$	$2_x2_y2_z\{2_z\}1'$
$2_x2_y2_z1'[2_x'2_y'2_z]$	$2_x'2_y'2_z1'^*$	$2_x2_y2_z(2_z)1'^*$
$2_x'2_y'2_z[2_z]$	$2_x'^*2_y'^*2_z$	$2_x2_y2_z(2_z)\{2_z\}$
$2_x'2_y'2_z[2_x']$	$2_x'2_y'^*2_z{}^*$	$2_x2_y2_z(2_z)\{2_x(1)\}$

where it is shown that there are 380 such classes. A listing of representative magnetic transposable twin laws $J[F]$, one from each class, with J belonging to the family of the non-magnetic point group 222 is given in Table I. These twin laws are given in double group notation in column 1 and single group notation in column 2. In column 3, a notation based on the Zamorzaev and Sokolov[3,6] double-antisymmetry notation is given. This notation is explained in the following section.

3. RELATIONSHIP TO DOUBLE ANTISYMMETRY GROUPS

The magnetic twin laws derived above are mathematically equivalent, i.e. have the same mathematical structure, as the double-antisymmetry point groups introduced by Zamorzaev and Sokolov.[3,6] Double-antisymmetry point groups are defined in the following context: All points of a finite object are assigned two signs, each of which can take one of two values usually interpreted as a plus or minus sign. In addition to the point group transformations of the unsigned finite object, one defines transformations of the signs, a transformation $1'$ which reverses the value of the first sign, and 1^* which reverses the value of the second sign. A double-antisymmetry point group is an invariance group of such a signed finite object, i.e. the group of those point group transformations and point group transformations coupled with $1'$, 1^*, or $1'^*$ which leave the signed finite object invariant.

A magnetic transposable twin law, equation (1), as a double-antisymmetry group, contains point group transformations not coupled with $1'$ nor 1^*, and point group transformations coupled with $1'$, 1^*, or $1'^*$ where now $1'$ denotes time inversion and 1^* denotes that the point group element interexchanges the two domain states. Consequently, the mathematical structure of magnetic twin laws is the same as double-antisymmetry groups. To each magnetic transposable twin law there exists a corresponding double-antisymmetry group. However the converse is not true, as there are no magnetic transposable twin laws which contain the element 1^*.

There are two notations which have been introduced for double-antisymmetric point groups: The first is identical with the single group notation introduced above. The second notation consists of a) a symbol G of a non-magnetic point group with the symbol (H) to denote a subgroup of index two of G of elements not coupled with $1'$, and/or $\{H\}$ a subgroup of index two of G of elements not coupled with 1^*, b) such a symbol multiplied by $1'$, 1^*, or $1'^*$ or c) a symbol $G(H)\{K(R)\}$ where R is a subgroup of index 4 of G not coupled with either $1'$ or 1^*. For example, $2_x2_y2_z\{2_z\}$ denotes the group consisting of all elements of $G = 2_x2_y2_z = [1, 2_x, 2_y, 2_z]$ where the elements of G not in the subgroup $H = 2_z = [1, 2_z]$ are coupled with 1^*. This then is the group consisting of the elements $[1, 2_x^*, 2_y^*, 2_z]$. This second notation for double-antisymmetric point groups, for those double-antisymmetric point groups corresponding to the magnetic transposable twin laws listed in column 1 of Table I, is given in column 3 of that table.

4. NON-FERROELASTIC MAGNETOELECTRIC TWIN LAWS AND TENSOR DISTINCTION

Let V^n denote the n-th product of a polar vector tensor, and "a" and "e" rank zero tensors that change sign, respectively, under time inversion $1'$ and spatial inversion $\bar{1}$. The magnetoelectric effect tensor transforms as a second rank tensor of the type aeV^2. The spontaneous deformation tensor transforms as $[V^2]$ where the brackets denote symmetrization of the indices. Of the 380 magnetic transposable twin laws, 140 are non-ferroelastic magnetoelectric twin laws, i.e. where the two domains have the same (zero) spontaneous deformation tensor and distinct magnetoelectric tensors. Of the six magnetic transposable twin laws listed in Table I, only the second and fourth are non-ferroelastic magnetoelectric twin laws.

From the Taylor expansion of the density of stored free enthalpy, the polarization P, magnetization M, and mechanical deformation s can be written in a third order expansion in terms of the electric field E, magnetic field H, and stress tensor T as[7]

$$P_i = \kappa_i^0 + \kappa_{ij}E_j + (\tfrac{1}{2})\kappa_{ijk}E_jE_k + \alpha_{ij}H_j + \alpha_{jik}H_jE_k + (\tfrac{1}{2})\beta_{ijk}H_jH_k + d_{ijk}T_{jk}$$

$$M_i = \chi_i^0 + \chi_{ij}H_j + (\tfrac{1}{2})\chi_{ijk}H_jH_k + \alpha_{ij}E_j + \beta_{jik}E_jH_k + (\tfrac{1}{2})\alpha_{ijk}E_jE_k + g_{ijk}T_{jk}$$

$$s_{ij} = s_{ij}^0 + d_{kij}E_k + g_{kij}H_k$$

where the names of the coefficients in the above equations and their transformational properties are given in Table II.

For each non-ferroelastic magnetoelectric twin law we have considered which of the above physical property tensors are different in the two magnetoelectric domain states under consideration.[8] For example, for the non-ferroelastic magnetoelectric twin law $2_x2_y2_z1'[2_x'2_y'2_z]$, among those tensors listed in Table II, the types of tensors

TABLE II
Transformation properties of coefficients

	Name of Coefficient	Transformation
κ_i^0	*Spontaneous polarization*	V
χ_i^0	*Spontaneous magnetization*	aeV
s_{ij}^0	*Spontaneous deformation*	[V²]
κ_{ij}	*Electric susceptibility*	[V²]
χ_{ij}	*Magnetic susceptibility*	[V²]
α_{ij}	*Magnetoelectric susceptibility*	aeV²
d_{ijk}	*Piezoelectric coefficient*	V[V²]
g_{ijk}	*Piezomagnetic coefficient*	aeV[V²]
κ_{ijk}	*non-linear electric susceptibility*	[V³]
χ_{ijk}	*Non-linear magnetic susceptibility*	ae[V³]
α_{ijk}	*First non-linear magnetoelectric susceptibility*	aeV[V²]
β_{ijk}	*Second non-linear magnetoelectric susceptibility*	V[V²]

TABLE III

Tensor distinction for $2_x2_y2_z1'[2'_x2'_y2_z]$

Tensor	First Domain	Second Domain
aeV	0	0
	0	0
	A	-A
aeV²	0 A 0	0 -A 0
	B 0 0	-B 0 0
	0 0 0	0 0 0
aeV[V²]	0 0 0 0 A 0	0 0 0 0 -A 0
	0 0 0 B 0 0	0 0 0 -B 0 0
	C D E 0 0 0	-C -D -E 0 0 0
ae[V³]	0 0 0 0	0 0 0 0
	0 0 0	0 0 0
	A B C	-A -B -C

which are different in the two magnetoelectric domain states are listed in Table III in the notation of reference (11). The form of various tensors invariant under magnetic point groups can be found in references (9) and (10). However, the forms of the tensors in Table III have been derived as follows: The form of the tensors in the first domain are invariant under $2'_x2'_y2_z$. These have been derived using tables of the form of tensors invariant under non-magnetic point groups[11] and a general method, reference (12), to determine the form of tensors invariant under magnetic point groups from known tables of the form of tensors invariant under non-magnetic point groups. The form of the tensors in the second domain have been derived by transforming the corresponding tensor in the first domain by $a^* = 1'$.

In this case, the two domains with distinct magnetoelectric effect tensors can also be distinguished by their spontaneous magnetization, piezomagnetic coefficient, and by their non-linear magnetic and first non-linear magnetoelectric susceptibilities.

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