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Symmetry relations of magnetic twin laws[1]

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Symmetry relationships between two simultaneously observed domain states (*domain pair*) are used to determine physical properties that can distinguish between the observed domains. Here the tabulation of these symmetry relationships is extended from non-magnetic cases to magnetic cases, in terms of magnetic point groups, *i.e.* all possible *magnetic symmetry groups* and *magnetic twinning groups* of domain pairs are determined and tabulated.

1. Introduction

Crystalline domains can arise in phase transitions from a high-symmetry phase of symmetry G to a low-symmetry phase of symmetry F, where F is a subgroup of G. The bulk structures of these domains in polydomain samples are referred to as *domain states*. Two domain states have the same crystal structure and differ only in their spatial orientation and consequently can exhibit different physical properties. In determining the physical properties that can distinguish between simultaneously observed pairs of domain states (*domain pair*), symmetry relationships between domains of a domain pair have been introduced in terms of two groups, the *symmetry group* of a domain pair (Janovec, 1972) and the *twinning group* of a domain pair (Fuksa & Janovec, 1995; Janovec *et al.*, 1995). We do not consider here cases where the symmetries of the phases are not related by a group–subgroup relationship. For such transitions, see Guymont (1981) or Wadhawan (2000).

Both non-magnetic symmetry groups and non-magnetic twinning groups have been tabulated (Schlessman & Litvin, 1995). Magnetic symmetry groups of domain pairs have been considered for non-ferroelastic magnetoelectric domain pairs (Litvin *et al.*, 1994) and for the so-called completely transposable domain pairs (Litvin *et al.*, 1995).

Here, using the properties of the magnetic point groups (Schlessman & Litvin, 2001), we present a computer-generated tabulation of the magnetic symmetry groups and twinning groups. For a group G, the group $m\bar{3}m1'$, $6/mmm1'$, or any subgroup of these two groups, and each subgroup F of G, we tabulate all magnetic symmetry groups and magnetic twinning groups of corresponding domain pairs. In addition, we provide the coset and double-coset decomposition of the group G with respect to F, a serial numbering and the point-group symmetry of the domain states, the permutation of the domain states under elements of G, and a classification of the domain states. In the following section, we detail the information contained in the tables of these magnetic symmetry groups and twinning groups.

2. Tables of symmetry relations of magnetic domain pairs

Three different notations can be used for the magnetic point groups: International primed notation, International $G[H]$ notation, and Schoenflies notation, *e.g.* $4_z2'_x2'_{xy}$, $4_z2_x2_{xy}[4_z]$ and $D_{4(z,x,xy)}[C_{4z}]$. We shall use here the International primed notation. For a chosen magnetic group G and subgroup F of G, the computer-generated tabulations consist of the following:[2]

Table 1
Coset and double-coset decomposition of $G = 4_z/m_zm'_xm'_{xy}$ with respect to $F = 2'_{xy}/m'_{xy}$.

Each row contains the elements of a single coset. Sets of cosets constituting a single double coset are enclosed in square brackets.

[1	$\bar{1}$	$2'_{xy}$	m'_{xy}]
[2_z	m_z	$2'_{\bar{x}y}$	$m'_{\bar{x}y}$]
[$2'_y$	$\bar{4}_z$	4_z	m'_y
$2'_x$	m'_x	4^3_z	$\bar{4}^3_z$]

(*a*) Coset and double-coset decomposition of the group G with respect to the subgroup F. The (left) coset decomposition of G with respect to F is written as

$$G = g_1F + g_2F + g_3F + \ldots + g_nF,$$

where g_i, $i = 1, 2, \ldots, n$, are the coset representatives of the coset decomposition. The number n of domain states $S_i = g_iS_1$, $i = 1, 2, \ldots, n$ that arise in a transition from G to F are in a one-to-one correspondence with the n cosets g_iF, $i = 1, 2, \ldots, n$. In Table 1, we give the coset decomposition of the group $G = 4_z/m_zm'_xm'_{xy}$ with respect to $F = 2'_{xy}/m'_{xy}$. Each line in Table 1 lists the elements of a single coset g_iF.

The double-coset decomposition of G with respect to F is written as

$$G = Fg^{dc}_1F + Fg^{dc}_2F + Fg^{dc}_3F + \ldots + Fg^{dc}_mF,$$

where g^{dc}_i, $i = 1, 2, \ldots, m$, are the double-coset representatives. The number of classes of symmetrically equivalent, with respect to G, ordered domain pairs (S_i, S_j) is equal to the number of double cosets in the double-coset decomposition of G with respect to F (Janovec, 1972). The double-coset decomposition of $G = 4_z/m_zm'_xm'_{xy}$ with respect to $F = 2'_{xy}/m'_{xy}$ is also given in Table 1. Sets of cosets which constitute a single double coset are enclosed in brackets.

(*b*) Serial numbering and point-group symmetry of domain states. Serial numbering, *i.e.* the numbering of the subindex i of a domain state $S_i = g_iS_1$ is chosen as the value of the subindex of the coset representative g_i of the coset decomposition of G with respect to F.

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[2] A computer program entitled *Symmetry Relations of Magnetic Domain Pairs* is available from the IUCr electronic archives (Reference: DR0017). Services for accessing these data are described at the back of the journal.

Table 2
Serial number i and point-group symmetry F_i of the domain states S_i in the case of $G = 4_z/m_z m'_x m'_{xy}$ and $F = 2'_{xy}/m'_{xy}$.

Serial number	$S_i = g_i S_1$	$F_i = g_i F g_i^{-1}$
1	$S_1 = 1S_1$	$F_1 = 2'_{xy}/m'_{xy}$
2	$S_2 = 2_z S_1$	$F_2 = 2'_{xy}/m'_{xy}$
3	$S_3 = 2'_y S_1$	$F_3 = 2'_{\bar{x}y}/m'_{\bar{x}y}$
4	$S_4 = 2'_x S_1$	$F_4 = 2'_{\bar{x}y}/m'_{\bar{x}y}$

Table 3
Permutations of the domain states under the action of elements g of G in the case of $G = 4_z/m_z m'_x m'_{xy}$ and $F = 2'_{xy}/m'_{xy}$.

Element of G	Permutation
$1, \bar{1}, 2'_{\bar{x}y}, m'_{\bar{x}y}$	1234 1234
$2'_y, 4_z, \bar{4}_z, m'_y$	1234 3421
$2_z, m_z, 2'_{xy}, m'_{xy}$	1234 2143
$2'_x, m'_x, 4_z^3, \bar{4}_z^3$	1234 4312

The symmetry group of the domain state S_i is the group $F_i = g_i F g_i^{-1}$. For $G = 4_z/m_z m'_x m'_{xy}$ and $F = 2'_{xy}/m'_{xy}$, we list in Table 2 each domain's serial numbering and symmetry group.

(c) Permutation of domain states. We tabulate the permutations of the domain states under the action of each element g of the group G, *i.e.* for each domain state S_i we tabulate $S_j = gS_i$ in the format

$$\begin{array}{cccc} S_1 & S_2 & \ldots & S_n \\ gS_1 & gS_2 & \ldots & gS_n, \end{array}$$

where, for typographical simplicity, only the subindices of the domain states S_i and $S_j = gS_i$ are explicitly listed. [For a detailed analysis of the permutations of domain states see Fuksa & Janovec (1995).] In Table 3, we list the permutations of the domain states in the case where $G = 4_z/m_z m'_x m'_{xy}$ and $F = 2'_{xy}/m'_{xy}$.

(d) Classes of domain pairs. The number of classes in the classification of the n^2 domain pairs (S_i, S_j), $i, j = 1, 2, \ldots, n$, is equal to the number of double cosets in the double-coset decomposition of G with respect to F. For $G = 4_z/m_z m'_x m'_{xy}$ and $F = 2'_{xy}/m'_{xy}$, the four classes of domain pairs are listed in Table 4. The first domain pair in each class is the representative domain pair $(S_1, g_i^{\rm dc} S_1)$ of that class.

(e) The symmetry group J_{ij} of the unordered domain pair $\{S_i, S_j\}$ is defined by $J_{ij} = F_{ij} + g^*_{ij} F_{ij}$. $F_{ij} = F_i \bigcap F_j$ consists of all elements of G that simultaneously leave both domain states invariant and is the symmetry group of the ordered domain pair (S_i, S_j) (Zikmund, 1984). An element g^*_{ij} of G, if one exists, interexchanges the two domain states, *i.e.* $g^*_{ij} S_i = S_j$ and $g^*_{ij} S_j = S_i$. The twinning group K_{ij} of a domain pair $\{S_i, S_j\}$ is defined by $K_{ij} = \langle F_i, g_{ij} \rangle$, where F_i is the point group of S_i and $g_{ij} S_i = S_j$. This is the group generated by an element g_{ij} of G and the elements of the group F_i (Janovec *et al.*, 1995). For every magnetic point group G, subgroup F and representative domain pair $\{S_1, g_i^{\rm dc} S_1\}$, except for $i = 1$, we tabulate the domain pair's symmetry group and twinning group. The case $i = 1$ is not considered as the corresponding domain pair $\{S_1, S_1\}$ consists of identical domain states. We consider only one domain pair from each class because the relative spatial orientations is the same for the two domain states in each domain pair of a single class (Litvin & Wike, 1989). For $G = 4_z/m_z m'_x m'_{xy}$ and $F = 2'_{xy}/m'_{xy}$, we list in Table 5 the symmetry groups and twinning groups of the representative domain pairs.

(f) Additional options provide the user with complete flexibility in choosing which domain pair to consider in determining domain-pair symmetry groups and twinning groups. For the domain pair $\{S_1, gS_1\}$, where g is an arbitrary element of G, and the domain pair $\{S_i, S_j\}$, for arbitrary indices i and j, the corresponding symmetry groups and twinning groups can also be calculated.

Table 4
Classes of domain pairs in the case of $G = 4_z/m_z m'_x m'_{xy}$ and $F = 2'_{xy}/m'_{xy}$.

Class number	Representative domain pair			
1	$\{S_1, S_1\}$	$\{S_2, S_2\}$	$\{S_3, S_3\}$	$\{S_4, S_4\}$
2	$\{S_1, S_2\}$	$\{S_3, S_4\}$		
3	$\{S_1, S_3\}$	$\{S_1, S_4\}$	$\{S_2, S_3\}$	$\{S_2, S_4\}$

Table 5
The symmetry group J_{1j} and twinning group K_{1j} of the representative domain pair $\{S_1, S_j\}$ in the case of $G = 4_z/m_z m'_x m'_{xy}$ and $F = 2'_{xy}/m'_{xy}$.

Representative domain pair $\{S_1, S_j\}$	J_{1j} K_{1j}	F_{1j} F_1	g^*_{1j} g_{1j}
$\{S_1, S_2\}$	$m_z m'_{xy} m'_{\bar{x}y}$ $m_z m'_{xy} m'_{\bar{x}y}$	$2'_{xy}/m'_{xy}$ $2'_{xy}/m'_{xy}$	2_z 2_z
$\{S_1, S_3\}$	$2'_y/m'_y$ $4_z/m_z m'_x m'_{xy}$	$\bar{1}$ $2'_{xy}/m'_{xy}$	$2'_y$ $2'_y$

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