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ON MAGNETIC DOMAIN TWIN SYMMETRY

D. B. LITVIN[a] and V. KOPSKY[b]

[a]*Department of Physics, The Pennsylvania State University Penn State - Berks Campus, P.O. Box 7009, Reading, PA 19610-6009, U.S.A;* [b]*Institute of Physics, The Academy of Sciences of the Czech Republic, Na Slovance 2, POB 24, 180 40 Prague 8, Czech Republic*

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A magnetic domain twin consists of two magnetic domains which meet along a planar transition region called a domain wall. The symmetry of a magnetic domain twin consists of those symmetry elements which 1) leave both domains invariant and also leave invariant the normal to the domain wall or 2) interexchange the domains and invert the normal. The magnetic domain symmetry is a magnetic layer group. It is shown how forthcoming tables of the non-magnetic sectional layer groups of non-magnetic crystals (International Tables for Crystallography, Volume E (Kopsky and Litvin)) can be used to determine possible magnetic domain twin symmetry.

Keywords: Magnetic domain; planar transition; crystallography

1. INTRODUCTION

The use of layer groups as sectional layer groups was introduced by Holser (1958) in the study of twin boundaries. A twin boundary is the planar interface between two semi-infinite crystal structures which have identical structures with one being misorientated and/or displaced relative to the other. These structures are referred to as *domain twins* (Janovec (1981) and Janovec, Schranz, Warhanek and Zikmund (1989)). The symmetry group of such a three-dimensional structure is called a *domain twin symmetry group*.

To determine the domain twin symmetry one first constructs a *domain pair*, i.e., a superposition of two *single domain states*. These are two infinite crystals which have the same structure, misorientation and/or displacement as the two semi-infinite crystals of the domain twin. The *domain pair symmetry group* is then determined. A plane, representing the interface, is then inserted transecting the domain pair. The domain twin is obtained by deleting from one side of the plane the atoms of one of the single domain states, and the atoms of the second single domain state from the other side of the plane.

The domain twin symmetry group is that subgroup of the domain pair symmetry group which leaves the domain twin invariant. This is the subgroup of all elements which satisfy one of the following two conditions (Janovec, Schranz, Warhanek and Zikmund (1989)):

C1) *Elements which leave invariant the structures of both single domain states and the normal to the plane.*

C2) *Elements which exchange the structures of the two single domain states and invert the normal to the plane.*

Sectional layer groups can be used in determining the domain twin symmetry group when a) the domain pair symmetry group is a three-dimensional magnetic or non-magnetic space group and b) the sectional group of the interface plane is a magnetic or non-magnetic layer group: Given a domain pair, its symmetry group and a plane transecting the domain pair. The sectional layer group of that plane is determined with respect to the domain pair symmetry group. The domain twin symmetry group is that subgroup of the sectional layer group consisting of all elements of which satisfy one of the two conditions listed above.

2. SECTIONAL LAYER GROUPS

If a crystal of magnetic or non-magnetic space group **G** is transected by a plane, the subgroup of all elements of the space group **G** which leaves the plane invariant is called the *sectional group* of the plane. Depending on the orientation of the plane, the translation subgroup of a sectional group can be two-dimensional, one-dimensional, or consist only of the identity translation. We shall consider only those planes the sectional groups of which have two-dimensional translation subgroups. These sectional groups are layer groups and consequently are referred to as *sectional layer groups*. The derivation of the sectional layers groups of planes transecting a crystal with a given non-magnetic space group symmetry has been considered by Wondratschek (unpublished), Kopsky and Litvin (1989), Kopsky (1990), Fuksa, Kopsky and Litvin (1993), and Davies and Dirl (1993). Using the method of Kopsky (1990) a complete tabulation of all sectional layer groups of planes transecting a crystal with a non-magnetic space group symmetry has been given (Kopsky and Litvin (1997)). In Table Ia, we give an example

TABLE Ia Scanning of the group $Pca2_1$

Orientation orbit (hkl)	*Conventional basis of the scanning group* a^*	b^*	d	*Scanning group*	*Translation orbit* **sd**	*Sectional layer group*
(001)	**a**	**b**	**c**	$Pca2_1$	[**sd**, (s + 1/2)**d**]	p1a1
(100)	**b**	**c**	**a**	$Pc2_1b$	[0**d**, 1/2**d**] [1/4**d**, 3/4**d**] [±**sd**, (±s + 1/2)**d**]	$P12_11$ p11b p1
(010)	**c**	**a**	**b**	$P2_1ab$	0**d**,1/2**d** [**sd**, −**sd**]	$p2_1ab$ p1a1(b^*/4)

of a part of those tables for a crystal of space group symmetry $\mathbf{G} = Pca2_1$, a listing only for those orientations with so called *fixed parameters*.

At the top of the table is the Hermann Mauguin symbol of the type of space group considered. The specific space group of that type considered, including the orientation, choice of origin, and diagram is that tabulated in The International Tables, Volume A (1983).

The first column, titled *Orientation Orbit (hkl)*, lists the Miller indices of the planes under consideration. Sets of planes have orientations which are related by rotations and rotation-inversions of the space group. Such sets of planes are called *orientation orbits*. The indices of planes in each orientation orbit are listed together and the indices of planes in different orientation orbits are separated by a horizontal line.

For a given space group and orientation of a transecting plane, the *scanning group* is that subgroup of the space group the elements of which leave invariant the orientation of the given plane. The scanning group is central in the methodology used to derive the sectional layer groups (Kopsky (1990)). In the second column, for each planar orientation given in the first column, the conventional basis vectors **a***, **b*** and **d**, of the scanning group is given in terms of the conventional basis vectors **a**, **b** and **c**, of the space group. The basis vectors **a*** and **b*** define the translation subgroup of the sectional layer groups of planes of this orientation. The vector **d** defines the *scanning direction* and is used to define the position of the plane within the crystal.

To specify a plane transecting a crystal, one must give both its orientation and its position within the crystal. The orientation of the plane is specified in the first column. The position of a plane is specified in the column under *Translation Orbit* **sd**. It is specified by the point where the plane intersects the scanning direction, the direction of the vector **d**, i.e., by specifying the value "s" of the vector s**d** of the point **O** + s**d**, where **O** is the origin of the space group.

The infinite set of all parallel planes of a specific orientation which transect a crystal can be subdivided into subsets, called *translation orbits*. All parallel planes obtained by applying all elements of the space group to any one plane of a specified orientation constitute a translation orbit. The positions of all planes in a translation orbit are specified by the set of vectors $[s_1\mathbf{d}+n\mathbf{d}, s_2\mathbf{d}+n\mathbf{d}, \ldots, s_q\mathbf{d}+n\mathbf{d}]$ where "q" is a finite number, $0 \leq s_i < 1$, $i=1,2,\ldots,q$, and because of the periodicity of the crystal in the scanning direction, $n \in Z$, the set of all integers.

In the *Translation Orbit* **sd** column the positions of the planes in each translation orbit is given, for typographical simplicity, by the position vectors $[s_1\mathbf{d}, s_2\mathbf{d}, \ldots, s_q\mathbf{d}]$ and if this set of vectors contains a single vector [s**d**] by s**d**, i.e., without the brackets. For each orientation the corresponding vector **d** found in the second column is used.

The sectional layer group of each plane is given in the fifth column on the same line as position vector s**d**.

3. SECTIONAL LAYER GROUPS OF MAGNETIC SPACE GROUPS

The action of time reversal does not change the orientation nor position of a plane transecting a crystal. Consequently, the sectional layer groups of magnetic space groups in the magnetic superfamily of a space group **G** can be easily derived from the sectional layer groups of the space group **G**. If **S** is a sectional layer group of **G**, then the corresponding sectional layer group of **G**1′ is **S**1′. The corresponding sectional layer group of magnetic space groups of the type **G**[**H**] is **S**[**K**], where **K** is a subgroup of **S** contained in **H**.

In Table Ib, a continuation of Table Ia, we list the sectional layer groups of magnetic space groups, except $Pca2_1$ which is listed in Table Ia, of the

TABLE Ib Scanning of the remaining magnetic groups of the reduced magnetic superfamily of $Pca2_1$

$Pca2_11'$	$Pc'a2_1'$	$Pca'2_1'$	$Pc'a'2_1$	$P_{2b}ca_{21}$	$P_{2b}c'a'2_1$
$p1a11'$	$p1a1$	$p1a'1$	$p1a'1$	$p_{2b}{*}1a1$	$p_{2b}{*}1a'1$
$p12_111'$	$p12_1'1$	$p12_1'1$	$p12_11$	$p_{2a}{*}12_11$	$p_{2a}{*}12_11$
$p11b1'$	$p11b'$	$p11b$	$p11b'$	$p_{2a}{*}11b$	$p_{2a}{*}11b'$
$p1'$	$p1$	$p1$	$p1$	$p_{2a}{*}1$	$p_{2a}{*}1$
$p2_1ab1'$	$p2_1'a'b$	$p2_1'ab'$	$p2_1a'b'$	$p2_1ab;p2_1'ab'$†	$p2_1a'b';p2_1'a'b^{d}$†
$p1a11'(\mathbf{b}^*/4)$	$p1a'1(\mathbf{b}^*/4)$	$p1a1(\mathbf{b}^*/4)$	$p1a'1(\mathbf{b}^*/4)$	$p1a1(\mathbf{b}^*/4)$	$p1a'1(\mathbf{b}^*/4)$

†First entry for 0**d**, second entry for 1/2 **d**.

reduced magnetic superfamily of $Pca2_1$. The first row lists the magnetic space groups with the corresponding sectional layer groups listed below each magnetic space group.

4. MAGNETIC DOMAIN TWIN SYMMETRY

Given a domain pair symmetry, the domain twin symmetry depends on the orientation and position of the domain twin boundary. The domain twin symmetry also depends on the structure of the domain pair symmetry: The domain pair symmetry **J** has the structure $\mathbf{J} = \mathbf{F} + g\mathbf{F}$ where **F** is the subgroup of symmetry elements which leaves both domains invariant and $g\mathbf{F}$ are those elements which exchange, the two domains. For the magnetic domain pair symmetry $Pca2_11'$, there are fifteen possible structures listed, in Table II, corresponding to the fifteen maximal subgroups of index two of the magnetic space group $Pca2_11'$ (Litvin, 1996). The magnetic domain twin symmetry for these fifteen cases and for the orientations and positions listed in Table Ia are given in Table III. The numbering in the first row refers to the numbering of these fifteen cases given in Table II. As an example of the use of such tables, we consider the phase transition in manganese iodine boracite where the change in magnetic symmetry is from $Pca2_11'$ to $Pc'a2_1'$ (Crottaz *et al.*, 1996). The two domains have magnetic domain pair symmetry $Pca2_11'$ corresponding to case #6 in Table II. The magnetic twin groups for orientations with fixed parameters are given column 6 of Table III. A complete listing for all orientations is given in Table IV. For variable parameter orientations, e.g., $(mn0)$, the integers m and n are variable.

TABLE II Domain symmetry groups $\mathbf{J} = \mathbf{F} + g\mathbf{F}$ with $\mathbf{J} = Pca2_11'$

1)	$Pca2_1$	+	$(1\|0, 0, 0)'$ $Pca2_1$
2)	$P112_11'$	+	$(m_x\|1/2, 0, 1/2)$ $P112_11'$
3)	$P1a11'$	+	$(m_x\|1/2, 0, 1/2)$ $P1a11'$
4)	$Pc111'$	+	$(2_z\|0, 0, 1/2)$ $Pc111'$
5)	$Pc'a'2_1$	+	$(1\|0, 0, 0)'$ $Pc'a'2_1$
6)	$Pc'a2_1'$	+	$(1\|0, 0, 0)'$ $Pc'a2_1'$
7)	$Pca'2_1'$	+	$(1\|0, 0, 0)'$ $Pca'2_1'$
8)	$P_{2b}ca2_1$	+	$(1\|0, 0, 0)'$ $P_{2b}ca2_1$
9)	$P_{2b}ca'2_1'$	+	$(1\|0, 0, 0)'$ $P_{2b}ca'2_1'$
10)	$P_{2b}c'a'2_1$	+	$(1\|0, 0, 0)'$ $P_{2b}c'a'2_1$
11)	$P_{2b}c'a2_1'$	+	$(1\|0, 0, 0)'$ $P_{2b}c'a2_1'$
12)	$P(a, 2b, c)$ $ca2_11'$	+	$(1\|010)$ $P(a, 2b, c)$ $ca2_11'$
13)	$P(a, 2b, c)$ $ca2_11'(b/2)$	+	$(1\|010)$ $P(a, 2b, c)$ $ca2_11'(b/2)$
14)	$P(a, 2b, c)$ $na2_11'$	+	$(1\|010)$ $P(a, 2b, c)$ $na2_11'$
15)	$P(a, 2b, c)$ $na2_11'(b/2)$	+	$(1\|010)$ $P(a, 2b, c)$ $na2_11'(b/2)$

TABLE III Domain twin symmetry groups for the domain pair symmetry group $Pca2_11'$

	1	*2*	*3*	*4*	*5*
(001)	p1a1	p1'	p1a11'	p1'	p1a'1
(100)	$p12_1'1$ p11b' p1	p1' p11b1' p1'	$p12_111'$ p11b1' p1'	$p12_111'$ p1' p1'	$p12_1'1$ p11b p1
(010)	$p2_1'ab'$ p1a1	p11b1' p1'	$p2_1111'$ p1'	$p2_1ab1'$ pc111'	$p2_1'a'b$ p1a'1
	6	7	8	9	10
	p1a1	p1a'1	$p_{2b^*}1a1$	$p_{2b^*}a'1$	$p_{2b^*}1a'1$
	$p12_11$ p11b p1	$p12_11$ p11b' p1	$p_{2a^*}12_1'1$ $p_{2a^*}11b'$ $p_{2a^*}1$	$p_{2a^*}12_11$ $p_{2a^*}11b'$ $p_{2a^*}1$	$p_{2a^*}12_1'1$ $p_{2a^*}11b$ $p_{2a^*}1$
	$p2_1'ab'$ p1a'1	$p2_1ab$ p1a1	$p2_1'ab'$ p1a1	$p2_1ab$ p1a1	$p2_1'a'b$ p1a'1
	11	12	13	14	15
	$p_{2b^*}1a$	$^{\alpha}p1a11'$	$^{\alpha}p1a11'(b^*/2)$	$^{\alpha}p1a11'(b^*/2)$	$^{\alpha}p1a11'$
	$p_{2a^*}12_11$ $p_{2a^*}11b$ $p_{2a^*}1$	$^{\beta}p12_111'\ (a^*/2)$ $^{\beta}p11n1'$ $^{\beta}p1'$	$^{\beta}p12_111'$ $^{\beta}p11n1'$ $^{\beta}p1'$	$^{\beta}p12_111'(a^*/2)$ $^{\beta}p11b1'$ $^{\beta}p1'$	$^{\beta}p12_111'$ $^{\beta}p11b1'$ $^{\beta}p1'$
	od	$p1a11'(b^*/4)$	$p2_1ab1'$	p11b1'	$p2_1111'$
$p2_1a'b'$ p1a'1	1/2 **d**	$p2_1ab1'$ $p1a11'(b^*/4)$	$p1a11'(b^*/4)$ $p1a11'(b^*/4)$	$p2_1111'$ p1'	p11b1' p1'

$^{\alpha}p \equiv p(a^*, 2b^*)$, $^{\beta}p \equiv p(2a^*, b^*)$

TABLE IV Domain Twin Symmetry of $Pca2_11' = Pc'a2_1' + (1|000)'Pc'a2_1'$

Orientation orbit (hkl)	***a****	***b****	***d***	*Translation orbit* ***sd***	*Domain twin symmetry*
(001)	**a**	**b**	**c**	[s**d**, (s+1/2)**d**]	p1a1
(100)	**b**	**c**	**a**	[0**d**, 1/2**d**]	$p12_11$
				[1/4**d**, 3/4**d**]	p11b'
				[±s**d**, (±s+1/2)**d**]	p1
(010)	**c**	**a**	**b**	0**d**,1/2**d**	$p2_1a'b'$
				[s**d**, −s**d**]	p1a'1(**b***/4)
(mn0)	**c**	n**a**−m**b**	p**a**+q**b**		
				0**d**,1/2**d**	$p2_111$
				[s**d**, −s**d**]	p1
($\bar{m}$n0)	**c**	n**a**+m**b**	−p**a**+q**b**		
(0mn)	**a**	n**b**−m**c**	p**b**+q**c**		
				[s**d**,(s+1/2)**d**]	¶p1(**a***/4)
				s**d**	§pb'11(**a***/4)
(0mn)	**a**	n**b**+m**c**	−p**b**+q**c**		
(n0m)	**b**	n**c**−m**a**	p**c**+q**a**		
				[s**d**,(s+1/2)**d**]	¶p1
				s**d**	§pb11
(n0m)	**b**	n**c**+m**a**	−p**c**+q**a**		

¶n odd, § n even

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