

Scanning of two-dimensional space groups

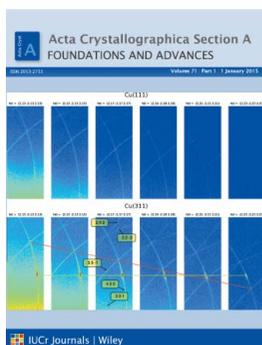
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Tables of the scanning of two-dimensional space groups are presented to determine the frieze-group symmetry of lines that transect two-dimensional crystals. It is shown how these tables can be used to predict the (001) projection symmetries of migration-related segments of coincidence site lattice tilt boundaries with [001] tilt axis.

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1. Introduction

The term *scanning* was introduced by Kopský (1990) for the process of determining the spatial distribution of local symmetries in a crystal. Using this terminology, the description of site point-group symmetries of points by Wyckoff positions in *International Tables for Crystallography*, Volume A, *Space-Group Symmetry* (ITA; Hahn, 2005) and Volume E, *Subperiodic Groups* (ITE; Kopský & Litvin, 2010) is the result of the *scanning* of three-dimensional space groups and subperiodic groups for point-group symmetries of points in a crystal. The description of the symmetries of planes that transect three-dimensional crystals by layer groups in Volume E, *Subperiodic Groups* (ITE; Kopský & Litvin, 2010) is the result of the *scanning* of three-dimensional space groups for the layer-group symmetries of the planes.

In §2 we give tables of the results of the scanning of two-dimensional space groups for the frieze-group symmetries of lines that transect two-dimensional crystals. In §3, it is shown how these tables can be used to predict the (001) projection symmetries of migration-related segments of coincidence site lattice tilt boundaries with [001] tilt axis.

2. Scanning of two-dimensional space groups

The conventional coordinate system of a two-dimensional space group consists of an origin, denoted by P , and two vectors \mathbf{a} and \mathbf{b} , the conventional basis (see Fig. 1). The two-dimensional space can be transected by a straight line in a crystallographic direction given by Miller directional indices $[n, m]$ where n and m are integers. That is, there are pairs of points on this line separated by a vector $n\mathbf{a} + m\mathbf{b}$.

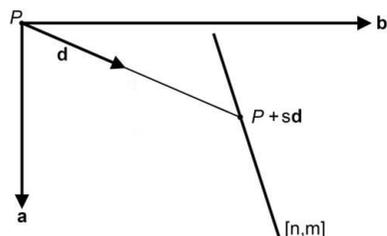


Figure 1

Position and direction of a line: P and \mathbf{a} , \mathbf{b} denote, respectively, the origin and conventional basis of the conventional coordinate system of a two-dimensional space group. The direction of a line transecting a crystal of this two-dimensional space-group symmetry is denoted by Miller directional indices $[n, m]$. The position of the line is given by a vector \mathbf{d} and a real number s , the vector $s\mathbf{d}$ going from the origin to a point $P + s\mathbf{d}$ on the line.

This guarantees that the subgroup of the two-dimensional space group that leaves the line invariant contains a one-dimensional translational subgroup, *i.e.* that the subgroup is a frieze group. The position of the line in the two-dimensional space is specified by a vector \mathbf{d} and real number 's', $P + s\mathbf{d}$ being a point on the line.

The scanning tables of the scanning of two-dimensional space groups to determine the frieze-group symmetry of lines that transect two-dimensional crystals consist of six columns (see Table 1¹):

(i) *Two-dimensional space group*. Following ITA (Hahn, 2005), the sequential numbering, Hermann–Mauguin symbol and symmetry diagram of each two-dimensional space group are given.

(ii) *Direction*. The direction of the line transecting a two-dimensional crystal of the given two-dimensional space group is specified by Miller directional indices $[n, m]$. For *specific directions*, n and m are fixed integers. For *general directions*, n and m are integer variables. When a two-dimensional space group contains both specific and general directions, the general directions $[n, m]$ do not include the given specific directions. For example, in the case of $p4mm$ (see Table 1), the general directions $[n, m]$ do not include $[1, 0]$, $[0, 1]$, $[1, 1]$ or $[1, -1]$.

Only directions are listed that are directions of lines with frieze-group symmetry having, for some position of the line, non-translational symmetry operations in addition to the identity symmetry operation. To have such additional symmetry operations, a line must pass through a twofold rotation point, overlap or be perpendicular to a mirror line, or overlap a glide line in the symmetry diagram. Consequently, no directions are listed for the two two-dimensional space group Nos. 1 $p1$ and 13 $p3$.

(iii) \mathbf{a}_F . The translation \mathbf{a}_F denotes the generator of the translational subgroup of the frieze-group symmetry of the line whose direction is given in the second column. For general directions $[n, m]$ $\mathbf{a}_F = n\mathbf{a} + m\mathbf{b}$.

(iv) \mathbf{d} . The vector \mathbf{d} , a translational vector of the two-dimensional space group, along with a real number s , specifies a vector $s\mathbf{d}$ which is used to determine the position of the line whose direction is given in the second column. The position of the line is specified by a point $P + s\mathbf{d}$ on the line (see Fig. 1). For general directions $[n, m]$, n and m are mutually prime integers and $\mathbf{d} = p\mathbf{a} - q\mathbf{b}$ where $nq + mp = 1$.

(v) *Linear orbit* $s\mathbf{d}$. The infinite set of all parallel lines of a specific direction which transect a crystal can be subdivided into subsets called *linear orbits*. All parallel lines obtained by applying all

¹ The complete two-dimensional space-group scanning tables are available from the IUCr electronic archives (Reference: TD5021) and at <http://www.bk.psu.edu/faculty/litvin/Cv.html>.

Table 1

Scanning of two-dimensional space group $p4mm$ giving the frieze-group symmetry of lines of a given direction and position $P + s\mathbf{d}$.

The origin P is taken to be in the upper left-hand corner of the group symmetry diagram.

Two-dimensional space group	Direction	\mathbf{a}_F	\mathbf{d}	Linear orbit $s\mathbf{d}$	Frieze group	
No. 11 $p4mm$	[1, 0]	\mathbf{a}	\mathbf{b}	$0\mathbf{d}, \frac{1}{2}\mathbf{d}$ [$s\mathbf{d}, -s\mathbf{d}$]	$\rho 2mm$ $\rho 1m1$	F6 F3
	[0, 1]	\mathbf{b}	\mathbf{a}	$0\mathbf{d}, \frac{1}{2}\mathbf{d}$ [$s\mathbf{d}, -s\mathbf{d}$]	$\rho 2mm$ $\rho 1m1$	F6 F3
	[1, 1]	$\mathbf{a} + \mathbf{b}$	$\mathbf{a} - \mathbf{b}$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$ $[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$ [$\pm s\mathbf{d}, (\pm s + \frac{1}{2})\mathbf{d}$]	$\rho 2mg (\mathbf{a}_F/4)$ $\rho 1m1$	F7 F3
	[1, -1]	$\mathbf{a} - \mathbf{b}$	$\mathbf{a} + \mathbf{b}$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$ $[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$ [$\pm s\mathbf{d}, (\pm s + \frac{1}{2})\mathbf{d}$]	$\rho 2mm$ $\rho 2mg (\mathbf{a}_F/4)$ $\rho 1m1$	F6 F7 F3
	[n, m]	$n\mathbf{a} + m\mathbf{b}$	$p\mathbf{a} - q\mathbf{b}$	$0\mathbf{d}, \frac{1}{2}\mathbf{d}$ [$s\mathbf{d}, -s\mathbf{d}$]	$\rho 211$ $\rho 1$	F2 F1

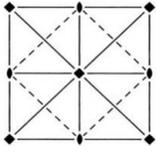
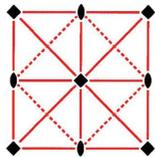


Table 2

Scanning of two-dimensional magnetic space group $p4m'm'$ giving the magnetic frieze-group symmetry of lines of a given direction and position $P + s\mathbf{d}$.

The magnetic frieze-group numbering is that of Litvin (2013).

Two-dimensional magnetic space group	Direction	\mathbf{a}_F	\mathbf{d}	Linear orbit $s\mathbf{d}$	Magnetic frieze group	
$p4m'm'$	[1, 0]	\mathbf{a}	\mathbf{b}	$0\mathbf{d}, \frac{1}{2}\mathbf{d}$ [$s\mathbf{d}, -s\mathbf{d}$]	$\rho 2m'm'$ $\rho 1m'1$	6.3.22 3.3.10
	[0, 1]	\mathbf{b}	\mathbf{a}	$0\mathbf{d}, \frac{1}{2}\mathbf{d}$ [$s\mathbf{d}, -s\mathbf{d}$]	$\rho 2m'm'$ $\rho 1m'1$	6.3.22 3.3.10
	[1, 1]	$\mathbf{a} + \mathbf{b}$	$\mathbf{a} - \mathbf{b}$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$ $[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$ [$\pm s\mathbf{d}, (\pm s + \frac{1}{2})\mathbf{d}$]	$\rho 2m'g' (\mathbf{a}_F/4)$ $\rho 1m'1$	7.3.29 3.3.10
	[1, -1]	$\mathbf{a} - \mathbf{b}$	$\mathbf{a} + \mathbf{b}$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$ $[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$ [$\pm s\mathbf{d}, (\pm s + \frac{1}{2})\mathbf{d}$]	$\rho 2m'm'$ $\rho 2m'g' (\mathbf{a}_F/4)$ $\rho 1m'1$	6.3.22 7.3.29 3.3.10
	[n, m]	$n\mathbf{a} + m\mathbf{b}$	$p\mathbf{a} - q\mathbf{b}$	$0\mathbf{d}, \frac{1}{2}\mathbf{d}$ [$s\mathbf{d}, -s\mathbf{d}$]	$\rho 211$ $\rho 1$	2.1.4 1.1.1



elements of the two-dimensional space group to any one line of a specified orientation constitute a single linear orbit. The linear orbit of parallel lines which contain the line at the position $P + s_1\mathbf{d}$ is denoted by

$$[s_1\mathbf{d} + n\mathbf{d}, s_2\mathbf{d} + n\mathbf{d}, \dots, s_q\mathbf{d} + n\mathbf{d}]$$

where $n \in \mathbb{Z}$ and $s_i\mathbf{d}, i = 2, 3, \dots, q$ are a set of position vectors related to $s_1\mathbf{d}$ by non-translational symmetry elements. For typographical simplicity, only these later position vectors are explicitly listed in the tables, *i.e.* a linear orbit is denoted by $[s_1\mathbf{d}, s_2\mathbf{d}, \dots, s_q\mathbf{d}]$. If this set of vectors contains a single vector $[s\mathbf{d}]$ then it is written without the brackets. The *linear orbit or orbits* $s\mathbf{d}$ of lines of the direction in column two and vector \mathbf{d} of column four are given in column five.

(vi) *Frieze group.* The frieze group of lines of direction given in column two and orientation orbit $s\mathbf{d}$ of column five is given in column six in both Hermann–Mauguin notation and the sequential numbering of ITE (Kopský & Litvin, 2010). If the origin of the frieze group at $P + s\mathbf{d}$ is not the same as the choice of the origin in the representative frieze group given in ITE (Kopský & Litvin, 2010), then the origin is translated to $P + s\mathbf{d} + \boldsymbol{\tau}$ where $\boldsymbol{\tau}$ is given in parentheses after the Hermann–Mauguin frieze-group symbol. For example (see Table 1), for the direction [1, 1] and linear orbit $[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$ the frieze group is given as $\rho 2mg (\mathbf{a}_F/4)$ where $\mathbf{a}_F = \mathbf{a} + \mathbf{b}$.

3. Symmetry of coincidence site lattice boundaries

Moeck *et al.* (2014) have derived a two-step method to predict the (001) projection symmetries of migration-related segments of coincidence site lattice tilt boundaries with a [001] tilt axis for all holohedral cubic materials. Their method, in the terminology of bicystallography, is the sectioning of a black–white plane group of a dichromatic pattern, and is analogous to the scanning of magnetic space groups in the analysis of non-magnetic domain walls (Janovec & Litvin, 2007). As we now show, these two steps are easily performed with the tabular information provided here.

In the example given in Moeck *et al.* (2014), the first step is the sectioning of $p4m'm'$, a black–white plane group of the overlapping projections of two crystal structures, along lines in the [1, 1] direction. The color exchange operation is interpreted as the exchange of the two crystal structures (Janovec & Přívratská, 2003). This gave rise to three dichromatic frieze groups, $\rho 2m'm', \rho 2m'g'$ and $\rho 1m'1$, depending on the sectioning line's position. Black–white groups are isomorphic with magnetic groups (Litvin, 2013). Consequently, the sectioning of black–white plane groups is isomorphic with the scanning of two-dimensional magnetic space groups. The scanning table of the two-dimensional magnetic space group $p4m'm'$ can be derived from the scanning

table of the two-dimensional space group $p4mm$ (Table 1) (Litvin & Kopský, 1997; Janovec & Litvin, 2007) and is given in Table 2. The three magnetic frieze groups of lines of the direction [1, 1], *i.e.* the three dichromatic frieze groups $\rho 2m'm', \rho 2m'g'$ and $\rho 1m'1$ (Moeck *et al.*, 2014) can be read directly off Table 2 along with their positions.

Table 3

The reduction in frieze-group symmetry when one structure is removed from one side of the sectioning line and the second structure is removed from the other side of the sectioning line; structures on opposite sides now of opposite color.

Change in origin and convectional basis of frieze group, if any, is given after the reduced frieze-group symbol.

$\rho 1$	→	$\rho 1$	$\rho 11g$	→	$\rho 1$
$\rho 11'$	→	$\rho 1$	$\rho 11g1'$	→	$\rho 11g'$
$\rho 2a1$	→	$\rho 1(0, 0; 2a, b)$	$\rho 11g'$	→	$\rho 11g'$
$\rho 211$	→	$\rho 1$	$\rho 2mm$	→	$\rho 1m1$
$\rho 2111'$	→	$\rho 2'11$	$\rho 2mm1'$	→	$\rho 2'mm'$
$\rho 2'11$	→	$\rho 2'11$	$\rho 2m'm'$	→	$\rho 11m'$
$\rho 2a211$	→	$\rho 2'11(\frac{1}{2}, 0; 2a, b)$	$\rho 2'mm'$	→	$\rho 2'mm'$
$\rho 1m1$	→	$\rho 1m1$	$\rho 2'm'm$	→	$\rho 2'11$
$\rho 1m11'$	→	$\rho 1m1$	$\rho 2a2m'm'$	→	$\rho 2'mm'(\frac{1}{2}, 0; 2a, b)$
$\rho 1m'1$	→	$\rho 1$	$\rho 2a2mm$	→	$\rho 2'mg'(\frac{1}{2}, 0; 2a, b)$
$\rho 2a1m1$	→	$\rho 1m1(0, 0; 2a, b)$	$\rho 2mg$	→	$\rho 1m1$
$\rho 11m$	→	$\rho 1$	$\rho 2mg1'$	→	$\rho 2'mg'$
$\rho 11m1'$	→	$\rho 11m'$	$\rho 2m'g'$	→	$\rho 11g'$
$\rho 11m'$	→	$\rho 11m'$	$\rho 2'mg'$	→	$\rho 2'mg'$
$\rho 2a11m'$	→	$\rho 11m'(0, 0; 2a, b)$	$\rho 2'm'g$	→	$\rho 2'11$
$\rho 2a11m$	→	$\rho 11g'(0, 0; 2a, b)$			

The second step is to determine the reduction in frieze-group symmetry when in the overlapping projections of the two crystal structures, one structure is removed from one side of the sectioning line and the second structure is removed from the other side of the sectioning line. The structures on opposite sides of the sectioning line are now of opposite color and frieze-group symmetry elements are limited to (i) twofold rotation points and mirror and glide planes parallel to the sectioning line all coupled (primed) with a color exchange and (ii) mirror planes perpendicular to the sectioning line not coupled (not primed) with a color exchange. This reduction in all types of magnetic frieze groups is given in Table 3. From this table one immediately finds that the three dichromatic frieze groups $\#2m'm'$, $\#2m'g'$ and $\#1m'1$ are reduced, respectively, to the three groups $\#11m'$, $\#11g'$ and $\#1$ in agreement with Moeck *et al.* (2014).

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