SPATIAL DISTRIBUTION OF LAYER AND ROD SYMMETRIES IN A CRYSTAL

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A method is established for determining the spatial distribution of layer and rod group symmetries in a crystal. This method is based on the use of the so-called *scanning theorem* and *scanning groups* - equitranslational subgroups of the space group of the crystal, each of them uniquely being defined by a chosen set of parallel planes or lines. Classifying directions of planes and lines into orbits under the action of the point group of the space group in question, one applies the scanning theorem only to a chosen representative from each orbit.
In analogy with Wyckoff positions, planes and lines which transect a crystal are classified into *orbits* under the action of the crystal's space group; the layer and rod groups corresponding to each such orbit are conjugate subgroups of the space group.

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Given a crystal of a specific space group symmetry we pose the following problem: Determine the layer group and rod group symmetries of, respectively, all planes and lines which transect the crystal. This problem is of interest in the consideration of domain walls, twin boundaries [1–3], and dislocations [4], and in general, in the study of planar and linear defects. Hermann [5] has considered a more general problem of determining all subgroups of a given space group. More recently, Wondratschek [6] and Kopský and Litvin [7] have dealt with this problem. We shall sketch here a systematic group theoretical approach to this problem using so-called *scanning groups* and the *scanning theorem* [8]. An example is given for a crystal with space group symmetry $P4_2/mbc(D_{4h}^{13})$. A complete tabular solution for all space groups is to be given elsewhere [9].

Let $\mathcal{G} = \{\mathbf{G}, \mathbf{T_G}, P, \mathbf{u_G}\}$ denote a space group, where $\mathbf{G}$ is the point group, $\mathbf{T_G}$ the translational subgroup, P the origin, and a mapping $\mathbf{u_G} : \mathbf{G} \longrightarrow V(3)$ defines the set $\{\mathbf{u_G}(g), g \in \mathbf{G}\}$ of non-primmitive translations associated with the elements g of $\mathbf{G}$. Consider a crystal of space group symmetry $\mathcal{G}$ and a set of parallel planes $(P+\tau_2, V_1)$ and a set of parallel lines $(P+\tau_1, V_2)$ where V_1 and V_2 are respectively a two-dimensional and one-dimensional subspace of $V(3)$ spanning both together just $V(3)$. Under the *scanning of layer groups* with a plane orientation V_1 along the line (P, V_2) we will understand the determination of the manner in which the layer group changes as we shift the plane along the line (P, V_2). Similarly, the term of the *scanning of rod groups* with a line orientation V_2 along the plane (P, V_1) will stand for the determination of the manner in which the rod group changes as we shift the line on the plane (P, V_1).

Let $\mathbf{H}_1$ be the largest subgroup of $\mathbf{G}$ which leaves V_1 invariant. The *scanning group* for the space group $\mathcal{G}$ and planes of orientation V_1 is the equitranslational subgroup $\mathcal{H}_l$ of $\mathcal{G}$: $\mathcal{H}_l = \{\mathbf{H}_1, \mathbf{T_G}, P, \mathbf{u}_{\mathbf{G}\downarrow\mathbf{H}_1}\}$, where a mapping $\mathbf{u}_{\mathbf{G}\downarrow\mathbf{H}_1}$ is the restriction of the mapping $\mathbf{u_G}$ to the subgroup $\mathbf{H}_1$ of $\mathbf{G}$. The *scanning theorem* states that the scanning of layer groups with the plane orientation V_1 is identical for the space group $\mathcal{G}$ and for the scanning group $\mathcal{H}_l$[8].

For $\mathcal{G} = P4_2/mbc(D_{4h}^{13})$ and $V_1 = V(\mathbf{b},\mathbf{c})$ and $V_2 = V(\mathbf{a})$, the scanning group is $\mathcal{H}_l = Pbam(D_{2h}^{9})$. Scanning the layer groups with this planar orientation, perpendicular to the **a** axis, one determines:

Shift x: $\tau_2 = x\mathbf{a}$	Layer Group		
x	(L11)pm11	$p_{z,y}m_z11$	
0 , 1/2	(L14)p2/m11	$p_{z,y}2_z/m_z11$	(T1)
1/4, 3/4	(L28)pm2$_1$b	$p_{z,y}m_z2_{1y}b_x$	

where in the first column is the position of the plane along the scanning direction, the x-axis of the space group $\mathcal{G}$. The second column gives the layer group in the numbering and notation of reference (9), and the third column gives the layer group with subindices indicating the corresponding axes in the space group $\mathcal{G}$. Scanning for rod groups of the lines of orientation V(**a**) one determines:

Shift (y,z): $\tau_1 = y\mathbf{b} + z\mathbf{c}$	Rod Group		
(y,z)	(R1)p111	p_x111	
(y,0),(y,1/2)	(R4)pm11	p_xm_z11	
(0,z),(1/2,z)	(R3)p211	p_x2_z11	
(1/4,z),(3/4,z)	(R5)pc11	p_xc_y11	(T2)
(0,0),(1/2,0), (0,1/2),(1/2,1/2)	(R6)p2/m11	p_x2_z/m_z11	
(1/4,0),(3/4,0), (1/4,1/2),(3/4,1/2)	(R17)$p$mc2$_1$	$p_xm_zc_y2_{1x}$	

In analogy with Wyckoff positions, the planes and lines which transect a crystal are classified into orbits, sets of equivalent planes and lines. We write the coset decomposition

$$\mathbf{G} = \mathbf{H}_1 + g_2\mathbf{H}_1 + ... + g_p\mathbf{H}_1.$$

For planes, for example, we have a set of planar orientations $V(\mathbf{a}_i, \mathbf{b}_i) = g_i\mathbf{H}_1 V(\mathbf{a}_1, \mathbf{b}_1)$ with scanning groups $\mathcal{H}_i = \{\mathbf{H}_i, \mathbf{T}_\mathbf{G}, P, \mathbf{u}_{\mathbf{G}\downarrow\mathbf{H}_i}\}$ conjugated to $\mathcal{H}_1$ in $\mathcal{G}$ where $\mathbf{H}_i = g_i\mathbf{H}_1 g_i^{-1}$. With the use of the above coset representatives the space group $\mathcal{G}$ can analogously be written as a union of the left cosets $\{g_i \mid \mathbf{u}_\mathbf{G}(g_i)\}\mathcal{H}_1$, i=1,...,p . Applying successively all the representatives $\{g_i \mid \mathbf{u}_\mathbf{G}(g_i)\}$ to all planes involved in the suborbit in $\mathcal{H}_1$ one easily obtains the whole orbit of planes in $\mathcal{G}$.

In the above example $\mathbf{G} = D_{4h}$, $\mathbf{H}_1 = D_{2h}$, $p = 2$, $g_2 = 4_z$, $\mathbf{u}_\mathbf{G}(g_2) = \mathbf{c}/2$, $\mathbf{H}_2 = D_{2h}$, and $\mathcal{H}_2 = \{\mathbf{H}_2, \mathbf{T}_\mathbf{G}, P, \mathbf{u}_{\mathbf{G}\downarrow\mathbf{H}_2}\} = D_{2h}^9$. Consequently, the plane orientations $V(\mathbf{b}, \mathbf{c})$ and $V(\mathbf{a}, \mathbf{c})$, perpendicular to the $\mathbf{a}$ and $\mathbf{b}$ axes, respectively, constitute a single orbit, and the results of scanninng of planes of orientation $V(\mathbf{a}, \mathbf{c})$ can be determined from Table 1 above by rotating (in this case) the shift vectors and conjugating the corresponding layer symmetry groups by the element $\{4_z \mid \mathbf{c}/2\}$. One has:

Shift y: $\tau_2 = y\mathbf{b}$	Layer Group		
y	(L11)pm11	$p_{z,x}m_z11$	
0 , 1/2	(L14)p2/m11	$p_{z,x}2_z/m_z11$	(T3)
1/4, 3/4	(L28)pm2$_1$b	$p_{z,x}m_z2_{1x}b_y$	

Analogously, line orientations $V(\mathbf{a})$ and $V(\mathbf{b})$ constitute an orbit, and the results of scanning of rod groups of lines of orientation $V(\mathbf{b})$ can be derived from Table 2. One obtains:

Shift (x,z): $\tau_1 = y\mathbf{a} + z\mathbf{c}$	Rod Group		
(x,z)	(R1)p111	p_y111	
(x,0),(x,1/2)	(R4)pm11	p_ym_z11	
(0,z),(1/2,z)	(R3)p211	p_y2_z11	
(1/4,z),(3/4,z)	(R5)pc11	p_yc_x11	(T4)
(0,0),(1/2,0), (0,1/2),(1/2,1/2)	(R6)p2/m11	p_y2_z/m_z11	
(1/4,0),(3/4,0), (1/4,1/2),(3/4,1/2)	(R17)$p$mc2$_1$	$p_ym_zc_x2_{1y}$	

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