SCANNING OF SPACE GROUPS

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ABSTRACT

Given a crystal whose symmetry group is a three-dimensional space group. We set out a procedure, called scanning, by which one can determine the layer group symmetry of all planes in the crystal which are invariant under a two-dimensional subgroup of the translational subgroup of the space group. An example of scanning is given of a crystal with space group symmetry Cmcm (D_{4h}^{17}).

Given a three-dimensional Euclidean point space and a three-dimensional space group \(G\) defined in this space in a natural coordinate system \((O; T_1, T_2, T_3)\) where \(O\) is the origin of the coordinate system and \(T_1, T_2, T_3\) are a set of generators of the translational subgroup \(T\) of \(G\). We set out a procedure to determine all planes in this space which are invariant under a two-dimensional subgroup \(T_1\) of \(T\) and the subgroups \(G_3\) of all elements of \(G\) which leave each of the planes invariant. \(G_3\) will be called the symmetry group of the plane and a set of generators of the translational subgroup \(T_1\) of \(G_3\) will be denoted by \(T_{13}\) and \(T_{15}\).

We denote an element of \(G\) by \((R \mid t(R) + T)\) where \(R\) is an element of the point group \(R\) of \(G\), \(t(R)\) is the non-primitive translation associated with \(R\), and \(T\) is a translation of the translational subgroup \(T\) of \(G\).

Sets of parallel planes are defined by a vector \(u\), a vector perpendicular to the planes. Specific planes are defined by vectors \(d = au\) where \(a\) is a real number. The vector \(d\) is a vector from the
origin to a point on the plane.

A necessary, but not sufficient, condition that a plane defined by a vector \( d \) is invariant under an element \( (R | t(R)+T) \) of \( G \) is that \( Rd = td \). Since \( d = au \), \( Ru = tu \) for such elements of \( G \). Consequently, this condition determines the maximal possible point group of planes in the set of planes defined by \( u \), i.e. the maximal possible point group \( R_{\text{max}} \) of \( G \). For a given \( u \) and rotation \( R \) of the maximal possible point group \( R_{\text{max}} \) we shall determine if there exists planes defined by \( d = au \) which are invariant under an element \( (R | t(R)+T) \) of \( G \).

We first change the origin of the coordinate system from 0 to \( 0+d \), a point on the plane defined by \( d = au \). In the natural coordinate system \((0+d; T_1, T_2, T_3)\) an element \( G \) of \( G \) has the form \((R | t(R)+d-Rd)\). We now introduce a new basis for the natural coordinate system: We define a new set of generators \( T_1, T_2, \) and \( T_3' \) of the translational subgroup \( T \) of \( G \). \( T_1 \) and \( T_2 \) are the generators of \( T \), the translational subgroup of \( G \). Using

\[
T = m_1 T_1 + m_2 T_2 + m_3 T_3' 
\]

where \( m_1, m_2, \) and \( m_3 \) are integers, and

\[
t(R) = t(R)_{11} T_1 + t(R)_{12} T_2 + t(R)_{13}' T_3' 
\]

\[
d-Rd = (d-Rd)_{11} T_1 + (d-Rd)_{12} T_2 + (d-Rd)_{13}' T_3' 
\]

we have that the element \((R | t(R)+d-Rd)\) in the natural coordinate system \((0+d; T_1, T_2, T_3')\) is written in component form as:

\[
(R | t(R)_{11} + m_1 + (d-Rd)_{11}, t(R)_{12} + m_2 + (d-Rd)_{12}, t(R)_{13}' + m_3 + (d-Rd)_{13}') 
\]

A necessary and sufficient condition that \((R | t(R)+d-Rd)\) is a symmetry element of the plane defined by \( d = au \) and is an element of
the group $G_4$ is $t(R)_1', m_3 + (d-Rd)_1', 0$ which can be written as

$$t(R)_1' + (d-Rd)_1' = 0$$

where " $\equiv 0$ " means equal to zero modulo one. This condition is used to determine which are the values of $a$, if any exist, such that $(R | t(R)+T+d-Rd)$ is an element of the symmetry group $G_4$ of the plane specified by the vector $d = au$.

As an example we consider the orthorhombic space group $G = Cmcm (D_{4h}^+)$ (see Table 1). We choose the natural coordinate system $(O, T_1, T_2, T_3)$ where the generators of the translational subgroup $T$ of $G$ are

$$T_1 = (1/2, 1/2, 0) \quad T_2 = (1/2, -1/2, 0) \quad T_3 = (0, 0, 1)$$

and the origin $O$ is chosen such that coset representatives $(R | t(R))$ of the coset decomposition of $G$ with respect to $T$ can be taken as:

$$(E | 0, 0, 0) \quad (C_{4z} | 0, 0, 1/2) \quad (C_{4y} | 0, 0, 1/2) \quad (C_{4x} | 0, 0, 0)$$

$$(I | 0, 0, 0) \quad (m_x | 0, 0, 1/2) \quad (m_y | 0, 0, 1/2) \quad (m_z | 0, 0, 0)$$

We scan along the z-direction by taking $u = (0, 0, 1)$ and consequently $d = a(0, 0, 1)$. The maximal possible point group $R_{max} = mmm (D_{4h})$. In the coordinate system $(O+d; T_1', T_2', T_3')$ where $T_1' = T_1$, $T_2' = T_2$, and $T_3' = T_3$, the coset representatives take the form $(R | t(R)+d-Rd)$:

$$(E | 0, 0, 0) \quad (C_{4z} | 0, 0, 1/2) \quad (C_{4y} | 0, 0, 1/2 + 2a) \quad (C_{4x} | 0, 0, 2a)$$

$$(I | 0, 0, 2a) \quad (m_x | 0, 0, 1/2 + 2a) \quad (m_y | 0, 0, 1/2) \quad (m_z | 0, 0, 0)$$
Applying condition (1), we have three cases:

1) For an arbitrary value of \( a \), there are two elements which satisfy this condition: \( (E | 0,0,0) \) and \( (m_{1} | 0,0,0) \).

2) For \( a = \frac{P}{2} \), where \( P \) is an arbitrary integer, i.e. \( 2a \neq 0 \), we have four elements which satisfy this condition: \( (E | 0,0,0) \), \( (C_{2} | 0,0,0) \), \( (1 | 0,0,0) \), and \( (m_{1} | 0,0,0) \).

3) For \( a = (P+1/2)/2 \), i.e. \( 2a + 1/2 \neq 0 \), we have four elements which satisfy this condition: \( (E | 0,0,0) \), \( (C_{2} | 0,0,0) \), \( (m_{1} | 0,0,0) \), and \( (m_{1} | 0,0,0) \).

The symmetry group \( G_{a} \) of a plane \( d = a(0,0,1) \) is one of the eighty Layer Groups. The standard symbols for the Layer Group symmetry of the planes, in the coordinate system \( (O;x_{1},T_{2},T_{3}) \), for the above three cases are, respectively:

1) \( c11m \) in the coordinate system with the \( x \) and \( y \) coordinates interexchanged.

2) \( c112/m \) in the coordinate system with the \( x \) and \( y \) coordinates interexchanged.

3) \( cmm2 \).

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