SCANNING OF SPACE GROUPS

V. Kopsky
Institute of Physics, Czechoslovak Academy of Sciences
Na Slovance 2, POB 24,180 40 Prague, Czechoslovakia

and

D.B. Litvin
Department of Physics, The Pennsylvania State University
The Berks Campus, POB 7009, Reading, PA 19610-6009, U.S.A.

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_{2h}^{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, and 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_L of T and the subgroups G_L of all elements of G which leave each of the planes invariant. G_L will be called the symmetry group of the plane and a set of generators of the translational subgroup T_L of G_L will be denoted by T_{L1} and T_{L2}.

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 $(R \mid t(R)+T)$ of G is that $Rd = \pm d$. Since $d = au$, $Ru = \pm u$ 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_{Lmax} of G_L. For a given u and rotation R of the maximal possible point group R_{Lmax} we shall determine if there exists planes defined by $d = au$ which are invariant under an element $(R \mid t(R)+T)$ of G.

We first change the origin of the coordinate system from O to $O+d$, a point on the plane defined by $d = au$. In the natural coordinate system $(O+d; T_1, T_2, T_3)$ an element G of G has the form $(R \mid t(R)+d-Rd)$. We now introduce a new basis for the natural coordinate system: We define a new set of generators T_{L1}, T_{L2}, and $T_3{}'$ of the translational subgroup T of G. T_{L1} and T_{L2} are the generators of T_L, the translational subgroup of G_L. Using

$$T = m_1 T_{L1} + m_2 T_{L2} + m_3 T_3{}'$$

where m_1, m_2, and m_3 are integers, and

$$t(R) = t(R)_{L1} T_{L1} + t(R)_{L2} T_{L2} + t(R)_3{}' T_3{}'$$

$$d-Rd = (d-Rd)_{L1} T_{L1} + (d-Rd)_{L2} T_{L2} + (d-Rd)_3{}' T_3{}'$$

we have that the element $(R \mid t(R)+d-Rd)$ in the natural coordinate system $(O+d; T_{L1}, T_{L2}, T_3{}')$ is written in component form as:

$$(R \quad t(R)_{L1}+m_1+(d-Rd)_{L1},\ t(R)_{L2}+m_2+(d-Rd)_{L2},\ t(R)_3{}'+m_3+(d-Rd)_3{}'$$

A necessary and sufficient condition that $(R \mid t(R)+d-Rd)$ is a symmetry element of the plane defined by $d = au$ and is an element of the group G_L is $t(R)_3' + m_3 + (d-Rd)_3' = 0$ which can be written as

$$t(R)_3' + (d-Rd)_3' \doteq 0$$

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

As an example we consider the orthorhombic space group G = Cmcm (D_{2h}^{17}). 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 $(R \mid t(R))$ of the coset decomposition of G with respect to T can be taken as:

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

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

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_{Lmax} = mmm (D_{2h}). In the coordinate system $(O+d; T_{L1}, T_{L2}, T_3')$ where $T_{L1} = T_1$, $T_{L2} = T_2$, and $T_3' = T_3$, the coset representatives take the form $(R \mid t(R)+d-Rd)$:

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

$$(I \mid 0,0,2a) \quad (m_z \mid 0,0,1/2 +2a) \quad (m_y \mid 0,0,1/2) \quad (m_x \mid 0,0,0)$$

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 $(m_z|0,0,0)$.

2) For a = P/2, where P is an arbitrary integer, i.e. $2a \doteq 0$, we have four elements which satisfy this condition: $(E|0,0,0)$, $(C_{2x}|0,0,0)$, $(I|0,0,0)$, and $(m_x|0,0,0)$.

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

The symmetry group G_L of a plane d = a(0,0,1) is one of the eighty *Layer Groups*[1]. The standard symbols for the Layer Group symmetry of the planes, in the coordinate system $(O+d; T_{L1}, T_{L2}, T_3')$, 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.

ACKNOWLEGMENTS

One of us (DBL) gratefully acknowledges the financial support of The Pennsylvania State University through a 1987/1988 Research Development Grant and of the Institute of Physics of the Czechoslovak Academy of Sciences.

REFERENCES

1) E.A. Wood, Bell Telephone Tech. J. 43 541 (1964); Bell Telephone Tech. Publ. Monograph 4680 (1964).

XVIIth INTERNATIONAL COLLOQUIUM ON GROUP THEORETICAL METHODS IN PHYSICS

June 27 to July 2, 1988, Sainte-Adèle, Canada

Editors

Y. Saint-Aubin and L. Vinet

Université de Montréal

World Scientific

Singapore • New Jersey • London • Hong Kong