

2.5. ELECTRON DIFFRACTION AND ELECTRON MICROSCOPY IN STRUCTURE DETERMINATION

Table 2.5.3.3. Symmetries of different patterns for diffraction and projection diffraction groups

(II) Bright-field patterns (BPs); (III) whole patterns (WPs); (IV) dark-field patterns (DPs); and (V) \pm dark-field patterns (\pm DPs) for diffraction groups (I) and projection diffraction groups (VI).

I	II	III	IV	V	VI
1	1	1	1	1	1_R
1_R	2 (1_R)	1	$2 = 1_R$	1	
2	2	2	1	2	21_R
2_R	1	1	1	2_R	
21_R	2	2	2	21_R	
m_R	m (m_2)	1	1	1 m_R	$m1_R$
m	m_v	m_v	1 m_v	1 m_v	
$m1_R$	$2mm$ [$m_v + m_2 + (1_R)$]	m_v	2 $2m_v m_2$	1 $m_v 1_R$	
$2m_R m_R$	$2mm$ ($2 + m_2$)	2	1 m_2	2 $2m_R(m_2)$	$2mm1_R$
$2mm$	$2m_v m_v$	$2m_v m_v$	1 m_v	2 $2m_v(m_v)$	
$2_R mm_R$	m_v	m_v	1 m_2 m_v	2_R $2_R m_v(m_2)$ $2_R m_R(m_v)$	
$2mm1_R$	$2m_v m_v$	$2m_v m_v$	2 $2m_v m_2$	21_R $21_R m_v(m_v)$	
4	4	4	1	2	41_R
4_R	4	2	1	2	
41_R	4	4	2	21_R	
$4m_R m_R$	$4mm$ ($4 + m_2$)	4	1 m_2	2 $2m_R(m_2)$	$4mm1_R$
$4mm$	$4m_v m_v$	$4m_v m_v$	1 m_v	2 $2m_v(m_v)$	
$4_R mm_R$	$4mm$ ($2m_v m_v + m_2$)	$2m_v m_v$	1 m_2 m_v	2 $2m_R(m_2)$ $2m_v(m_v)$	
$4mm1_R$	$4m_v m_v$	$4m_v m_v$	2 $2m_v m_2$	21_R $21_R m_v(m_v)$	
3	3	3	1	1	31_R
31_R	6 ($3 + 1_R$)	3	2	1	
$3m_R$	$3m$ ($3 + m_2$)	3	1 m_2	1 m_R	$3m1_R$
$3m$	$3m_v$	$3m_v$	1 m_v	1 m_v	
$3m1_R$	$6mm$ [$3m_v + m_2 + (1_R)$]	$3m_v$	2 $2m_v m_2$	1 $m_v 1_R$	
6	6	6	1	2	61_R
6_R	3	3	1	2_R	
61_R	6	6	2	21_R	

Table 2.5.3.3 (cont.)

I	II	III	IV	V	VI
$6m_R m_R$	$6mm$ ($6 + m_2$)	6	1 m_2	2 $2m_R(m_2)$	$6mm1_R$
$6mm$	$6m_v m_v$	$6m_v m_v$	1 m_v	2 $2m_v(m_v)$	
$6_R mm_R$	$3m_v$	$3m_v$	1 m_2 m_v	2_R $2_R m_v(m_2)$ $2_R m_R(m_v)$	
$6mm1_R$	$6m_v m_v$	$6m_v m_v$	2 $2m_v m_2$	21_R $21_R m_v(m_v)$	

however, noted that many diffraction groups are determined from a WP and BP pair without using a DP or \pm DP (or from one photograph) or from a set of a WP, a BP and a DP without using a \pm DP (or from two photographs).

2.5.3.2.5. Point-group determination

Fig. 2.5.3.4 provides the relationship between the 31 diffraction groups for slabs and the 32 point groups for infinite crystals given by Buxton *et al.* (1976). When a diffraction group is determined, possible point groups are selected by consulting this figure. Each of the 11 high-symmetry diffraction groups corresponds to only one crystal point group. In this case, the point group is uniquely determined from the diffraction group. When more than one point group falls under a diffraction group, a different diffraction group has to be obtained for another zone axis. A point group is identified by finding a common point group among the point groups obtained for different zone axes. It is clear from the figure that high-symmetry zones should be used for quick determination of point groups because low-symmetry zone axes exhibit only a small portion of crystal symmetries in the CBED patterns. Furthermore, it should be noted that CBED cannot observe crystal symmetries oblique to an incident beam or horizontal three-, four- or sixfold rotation axes. The diffraction groups to be expected for different zone axes are given for all the point groups in Table 2.5.3.4 (Buxton *et al.*, 1976). The table is useful for finding a suitable zone axis to distinguish candidate point groups expected in advance.

We shall explain the point-group determination procedure using an Si crystal. Fig. 2.5.3.5(a) shows a [111] ZAP of the Si specimen. The BP has threefold rotation symmetry and mirror symmetry or symmetry $3m_v$, which are caused by the threefold rotation axis along the [111] direction and a vertical mirror plane. The WP has the same symmetry. Figs. 2.5.3.5(b) and (c) are 220 and $2\bar{2}0$ DPs, respectively. Both show symmetry m_2 perpendicular to the reflection vector. This symmetry is caused by a twofold rotation axis parallel to the specimen surface. One DP coincides with the other upon translation. This translational or 2_R symmetry indicates the existence of an inversion centre. By consulting Table 2.5.3.3, the diffraction group giving rise to these pattern symmetries is found to be $6_R mm_R$. Fig. 2.5.3.4 shows that there are two point groups $\bar{3}m$ and $m\bar{3}m$ causing diffraction group $6_R mm_R$. Fig. 2.5.3.6 shows another ZAP, which shows symmetry $4mm$ in the BP and the WP. The point group which has fourfold rotation symmetry is not $\bar{3}m$ but $m\bar{3}m$. The point group of Si is thus determined to be $m\bar{3}m$.

2.5.3.2.6. Projection diffraction groups

HOLZ reflections appear as excess HOLZ rings far outside the ZOLZ reflection discs and as deficit lines in the ZOLZ discs. By ignoring these weak diffraction effects with components along the beam direction, we may obtain information about the symmetry of the sample as projected along the beam direction. Thus when HOLZ reflections are weak and no deficit HOLZ