

2.5. ELECTRON DIFFRACTION AND ELECTRON MICROSCOPY IN STRUCTURE DETERMINATION

Table 2.5.3.4. Diffraction groups expected at various crystal orientations for 32 point groups

This table is adapted from Buxton *et al.* (1976).

Point group	Zone-axis symmetries					
	$\langle 111 \rangle$	$\langle 100 \rangle$	$\langle 110 \rangle$	$\langle uv0 \rangle$	$\langle uuv \rangle$	$[uvw]$
$m\bar{3}m$	$6_Rmm_R$	$4mm1_R$	$2mm1_R$	$2_Rmm_R$	$2_Rmm_R$	$2_R$
$\bar{4}3m$	$3m$	$4_Rmm_R$	$m1_R$	$m_R$	$m$	1
432	$3m_R$	$4m_Rm_R$	$2m_Rm_R$	$m_R$	$m_R$	1

Point group	Zone-axis symmetries			
	$\langle 111 \rangle$	$\langle 100 \rangle$	$\langle uv0 \rangle$	$[uvw]$
$m\bar{3}$	$6_R$	$2mm1_R$	$2_Rmm_R$	$2_R$
23	3	$2m_Rm_R$	$m_R$	1

Point group	Zone-axis symmetries						
	$[0001]$	$\langle 11\bar{2}0 \rangle$	$\langle 1\bar{1}00 \rangle$	$[uv.0]$	$[uu.w]$	$[u\bar{u}.w]$	$[uv.w]$
$6/mmm$	$6mm1_R$	$2mm1_R$	$2mm1_R$	$2_Rmm_R$	$2_Rmm$	$2_Rmm_R$	$2_R$
$\bar{6}m2$	$3m1_R$	$m1_R$	$2mm$	$m$	$m_R$	$m$	1
$6mm$	$6mm$	$m1_R$	$m1_R$	$m_R$	$m$	$m$	1
622	$6m_Rm_R$	$2m_Rm_R$	$2m_Rm_R$	$m_R$	$m_R$	$m_R$	1

Point group	Zone-axis symmetries		
	$[0001]$	$[uv.0]$	$[uv.w]$
$6/m$	$61_R$	$2_Rmm_R$	$2_R$
$\bar{6}$	$31_R$	$m$	1
6	6	$m_R$	1

Point group	Zone-axis symmetries			
	$[0001]$	$\langle 11\bar{2}0 \rangle$	$[u\bar{u}.w]$	$[uv.w]$
$\bar{3}m$	$6_Rmm_R$	$21_R$	$2_Rmm_R$	$2_R$
$3m$	$3m$	$1_R$	$m$	1
32	$3m_R$	2	$m_R$	1

Point group	Zone-axis symmetries	
	$[0001]$	$[uv.w]$
$\bar{3}$	$6_R$	$2_R$
3	3	1

Point group	Zone-axis symmetries						
	$[001]$	$\langle 100 \rangle$	$\langle 110 \rangle$	$[u0w]$	$[uv0]$	$[uuv]$	$[uvw]$
$4/mmm$	$4mm1_R$	$2mm1_R$	$2mm1_R$	$2_Rmm_R$	$2_Rmm_R$	$2_Rmm_R$	$2_R$
$\bar{4}2m$	$4_Rmm_R$	$2m_Rm_R$	$m1_R$	$m_R$	$m_R$	$m$	1
$4mm$	$4mm$	$m1_R$	$m1_R$	$m$	$m_R$	$m$	1
422	$4m_Rm_R$	$2m_Rm_R$	$2m_Rm_R$	$m_R$	$m_R$	$m_R$	1

Point group	Zone-axis symmetries		
	$[001]$	$[uv0]$	$[uvw]$
$4/m$	$41_R$	$2_Rmm_R$	$2_R$
$\bar{4}$	$4_R$	$m_R$	1
4	4	$m_R$	1

Point group	Zone-axis symmetries				
	$[001]$	$\langle 100 \rangle$	$[u0w]$	$[uv0]$	$[uvw]$
$mmm$	$2mm1_R$	$2mm1_R$	$2_Rmm_R$	$2_Rmm_R$	$2_R$
$mm2$	$2mm$	$m1_R$	$m$	$m_R$	1
222	$2m_Rm_R$	$2m_Rm_R$	$m_R$	$m_R$	1

## 2. RECIPROCAL SPACE IN CRYSTAL-STRUCTURE DETERMINATION

Table 2.5.3.4 (cont.)

Point group	Zone-axis symmetries		
	[010]	[u0w]	[uvw]
$2/m$	$21_R$	$2_Rmm_R$	$2_R$
$m$	$1_R$	$m$	1
2	2	$m_R$	1

Point group	Zone-axis symmetry
	[uvw]
$\bar{1}$	$2_R$
1	1

the CBED symmetries for the two crystal (or incident-beam) settings which excite respectively the  $+G$  and  $-G$  reflections are drawn because the vertical rotation axes create the SMB patterns at different incident-beam orientations. [This had already been experienced for the case of symmetry  $2_R$  (Goodman, 1975; Buxton *et al.*, 1976).] In the rectangular four-beam case, the symmetries for four settings which excite the  $+G$ ,  $+H$ ,  $-G$  and  $-H$  reflections are shown. For the diffraction groups  $3m$ ,  $3m_R$ ,

$3m1_R$  and  $6_Rmm_R$ , two different patterns are shown for the two crystal settings, which differ by  $\pi/6$  rad from each other about the zone axis. Similarly, for the diffraction group  $4_Rmm_R$ , two different patterns are shown for the two crystal settings, which differ by  $\pi/4$  rad. Illustrations of these different symmetries are given in Fig. 2.5.3.7. The combination of the vertical threefold axis and a horizontal mirror plane introduces a new CBED symmetry  $3_R$ . Similarly, the combination of the vertical sixfold rotation axis and an inversion centre introduces a new CBED symmetry  $6_R$ .

There is an empirical and conventional technique for reproducing the symmetries of the SMB patterns which uses three operations of two-dimensional rotations, a vertical mirror at the centre of disc  $O$  and a rotation of  $\pi$  about the centre of a disc ( $1_R$ ) without involving the reciprocal process. For example, we may consider  $3_R$  between discs  $F$  and  $F'$  in Table 2.5.3.5 in the case of diffraction group  $31_R$ . Disc  $F'$  is rotated anticlockwise not about the zone axis but *about the centre of disc  $O$*  by  $2\pi/3$  rad (symbol  $3$ ) to coincide with disc  $F$ , and followed by a rotation of  $\pi$  rad (symbol  $R$ ) about the centre of disc  $F'$ , resulting in the correct symmetry seen in Fig. 2.5.3.7. When the symmetries appearing between different SMB patterns are considered, this technique assumes that the symmetry operations are conducted after discs  $O$  and  $\bar{O}$  are superposed. Another assumption is that the vertical mirror plane perpendicular to the line connecting discs  $O$  and  $\bar{O}$  acts at the centre of disc  $O$  when the symmetries between two SMB patterns are considered. As an example, symmetry  $3_R$  between discs  $S$  and  $\bar{S}$  appearing in the two SMB patterns is reproduced by a threefold anticlockwise rotation of disc  $S$  about the centre of disc  $O$  (or  $\bar{O}$ ) and followed by a rotation of  $\pi$  rad ( $R$ ) about the centre of disc  $\bar{S}$ .

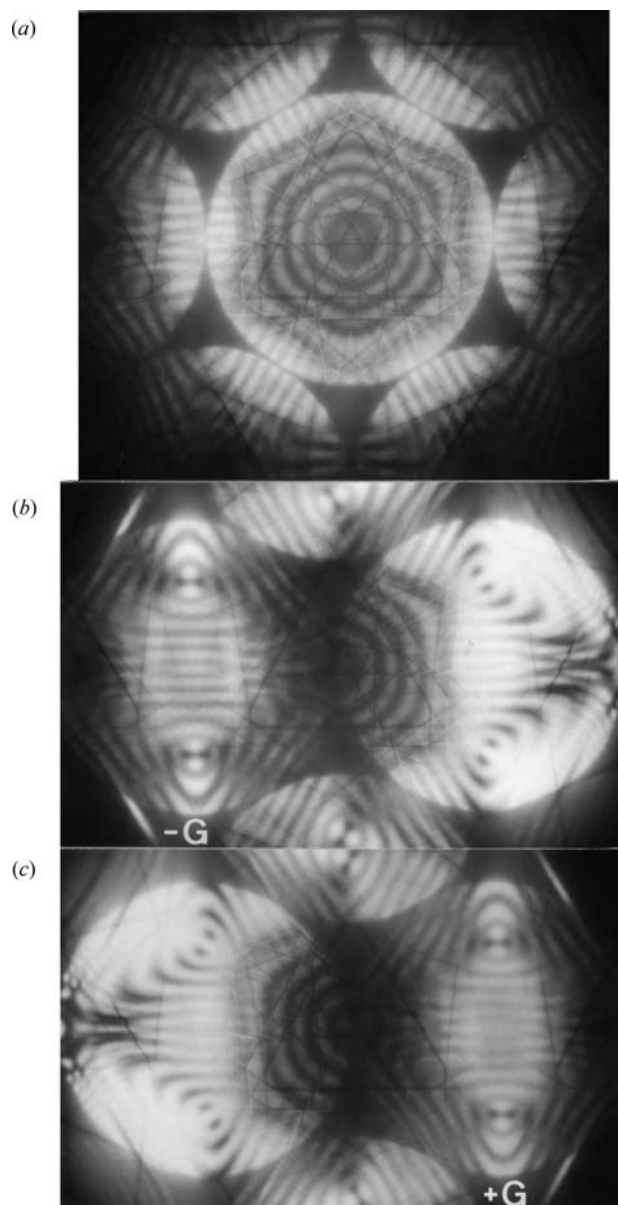


Fig. 2.5.3.5. CBED patterns of Si taken with the [111] incidence. (a) BP and WP show symmetry  $3m_v$ . (b) and (c) DPs show symmetry  $m_2$  and DP symmetry  $2_Rm_v$ .

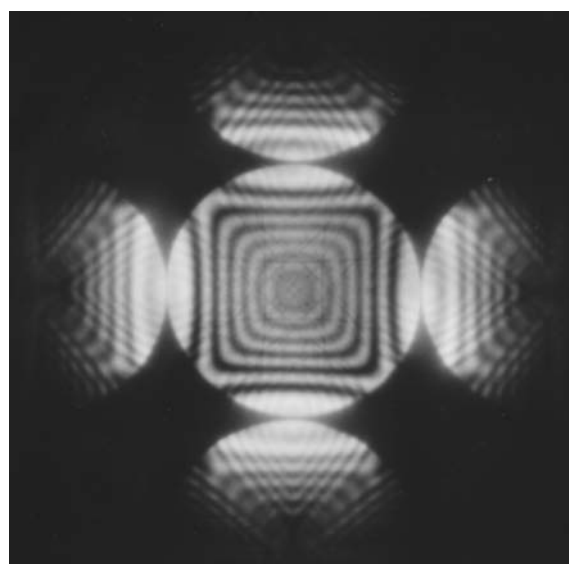


Fig. 2.5.3.6. CBED pattern of Si taken with the [100] incidence. The BP and WP show symmetry  $4mm$ .