

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 π 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 π 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 π rad (R) about the centre of disc \bar{S} .

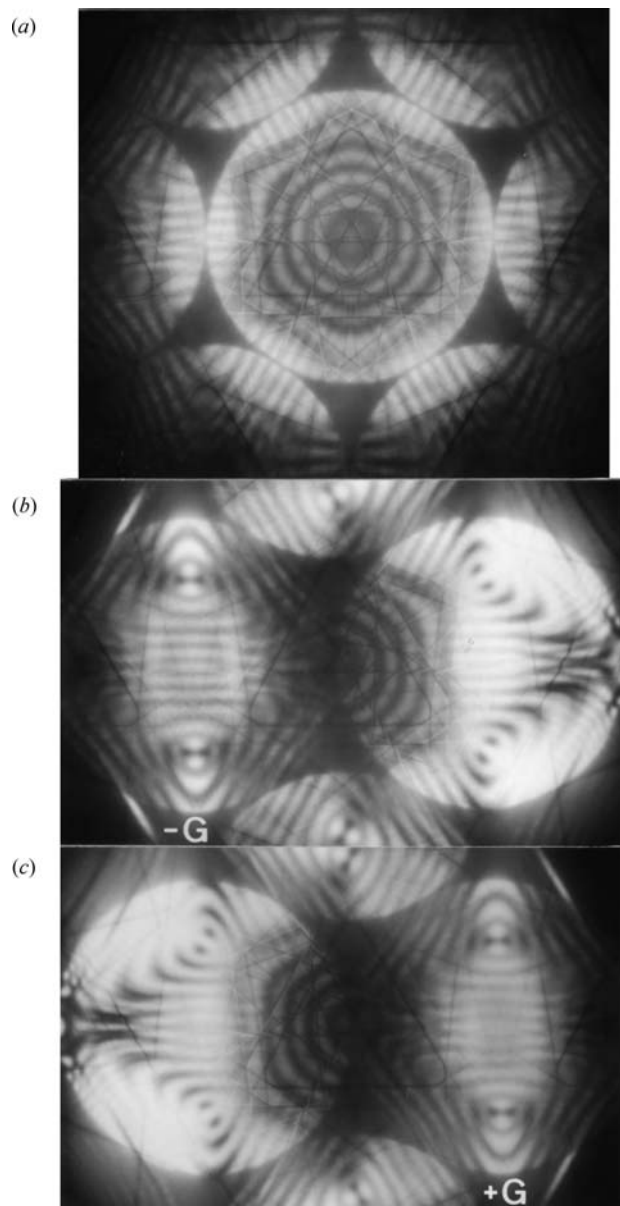


Fig. 2.5.3.5. CBED patterns of Si taken with the [111] incidence. (a) BP and WP show symmetry $3m_v$. (b) and (c) DPs show symmetry m_2 and DP symmetry 2_Rm_v .

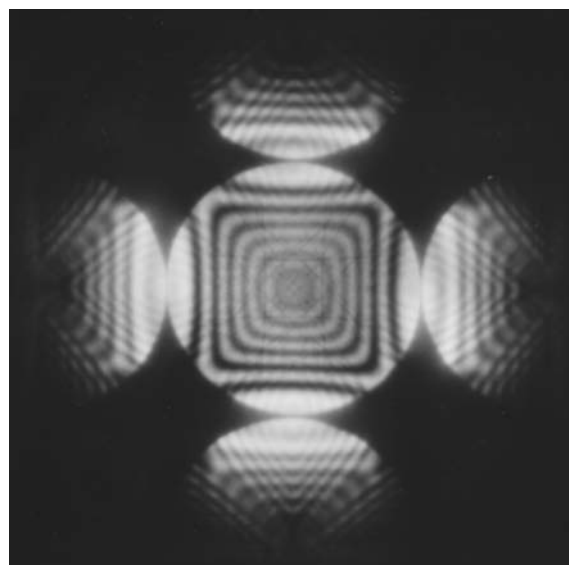


Fig. 2.5.3.6. CBED pattern of Si taken with the [100] incidence. The BP and WP show symmetry $4mm$.