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	$2_R mm_R$	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 $6_R mm_R$, 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 $4_R mm_R$, 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 $\bar{S}$.

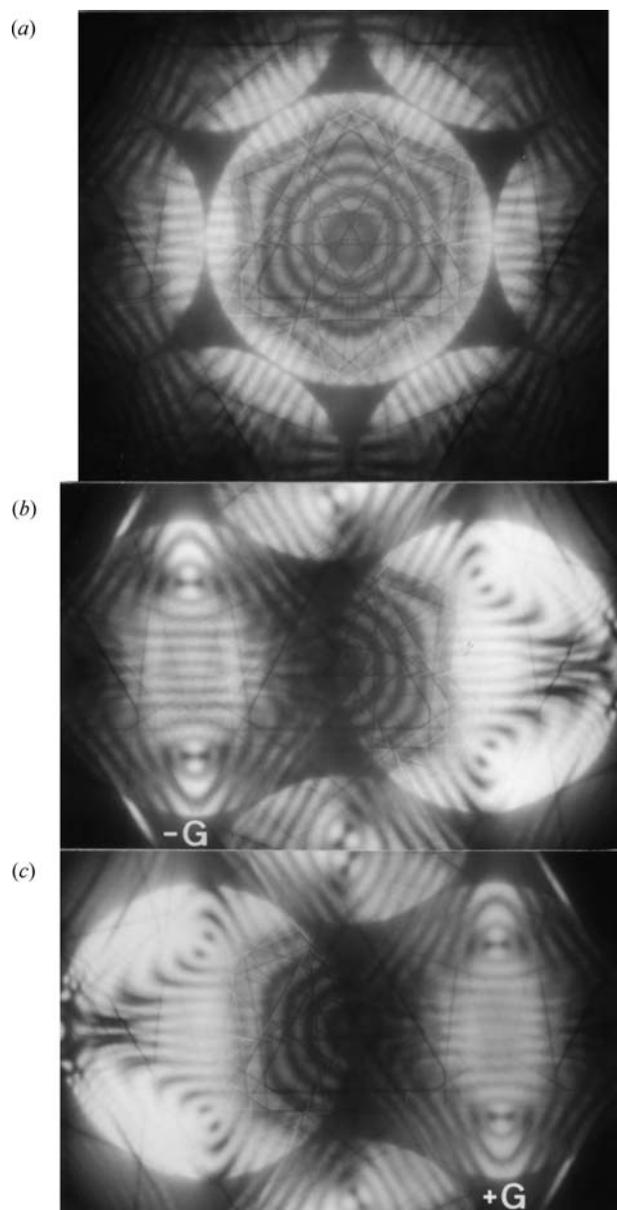Fig. 2.5.3.5. CBED patterns of Si taken with the [111] incidence. (*a*) BP and WP show symmetry $3m_v$. (*b*) and (*c*) DPs show symmetry m_2 and DP symmetry $2_R m_{v'}$.
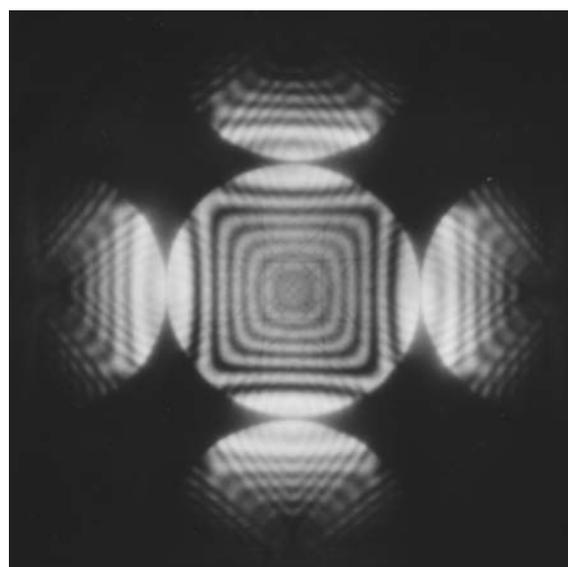
Fig. 2.5.3.6. CBED pattern of Si taken with the [100] incidence. The BP and WP show symmetry $4mm$.

references