International Tables for Crystallography (2010). Vol. B, Table 2.5.3.1, p. 309.

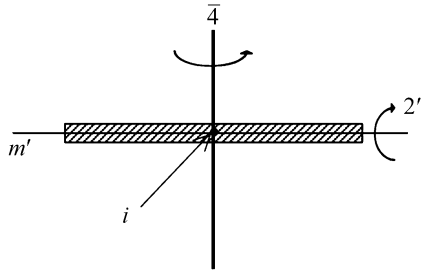

Fig. 2.5.3.1. Four symmetry elements m', i, $2'$ and $\bar{4}$ of an infinitely extended parallel-sided specimen.

Table 2.5.3.1. *Two- and three-dimensional symmetry elements of an infinitely extended parallel-sided specimen*

Symbols in parentheses show CBED symmetries appearing in dark-field patterns.

Two-dimensional symmetry elements	Three-dimensional symmetry elements
1	m' (1_R)
2	i (2_R)
3	$2'$ (m_2, m_R)
4	$\bar{4}$ (4_R)
5	
6	
m	

dimensional symmetry elements. A horizontal mirror plane m', an inversion centre i, a horizontal twofold rotation axis $2'$ and a fourfold rotary inversion $\bar{4}$ are the three-dimensional symmetry elements, and are shown in Fig. 2.5.3.1. The fourfold rotary inversion was not recognized as a symmetry element until the point groups of the diperiodic plane figures were considered (Buxton *et al.*, 1976). Table 2.5.3.1 lists these symmetry elements, where the symbols in parentheses express symmetries of CBED patterns expected from three-dimensional symmetry elements.

The diffraction groups are constructed by combining these symmetry elements (Table 2.5.3.2). Two-dimensional symmetry elements and their combinations are given in the top row of the table. The third symmetry m in parentheses is introduced automatically when the first two symmetry elements are combined. Three-dimensional symmetry elements are given in the first column. The equations given below the table indicate that no additional three-dimensional symmetry elements can appear by combination of two symmetry elements in the first column. As a result, 31 diffraction groups are produced by combining the elements in the first column with those in the top row. Diffraction groups in square brackets have already appeared ealier in the table. In the fourth row, three columns have two diffraction groups, which are produced when symmetry elements are combined at different orientations. In the last row, five columns are empty because a fourfold rotary inversion cannot coexist with threefold and sixfold rotation axes. In the last column, the number of independent diffraction groups in each row is given, the sum of the numbers being 31.

2.5.3.2.2. Identification of three-dimensional symmetry elements

It is difficult to imagine the symmetries in CBED patterns generated by the three-dimensional symmetry elements of the sample. The reason is that if a three-dimensional symmetry element is applied to a specimen, it turns it upside down, which is impractical in most experiments. The reciprocity theorem of scattering theory (Pogany & Turner, 1968) enables us to clarify the symmetries of CBED patterns expected from these three-dimensional symmetry elements. A graphical method for obtaining CBED symmetries due to sample symmetry elements is described in the papers of Goodman (1975), Buxton *et al.* (1976) and Tanaka (1989). The CBED symmetries of the three-dimensional symmetries do not appear in the zone-axis patterns, but do in a diffraction disc set at the Bragg condition, each of which we call a dark-field pattern (DP). The CBED symmetries obtained are illustrated in Fig. 2.5.3.2. A horizontal twofold rotation axis $2'$, a horizontal mirror plane m', an inversion centre i and a fourfold rotary inversion $\bar{4}$ produce symmetries m_R (m_2), 1_R, 2_R and 4_R in DPs, respectively.

Next we explain the symbols of the CBED symmetries. (1) Operation m_R is shown in the left-hand part of Fig. 2.5.3.2(*a*), which implies successive operations of (*a*) a mirror m with respect to a twofold rotation axis, transforming an open circle beam (○) in reflection G into a beam (+) in reflection G' and (*b*) rotation R of this beam by π about the centre point of disc G' (or the exact Bragg position of reflection G'), resulting in position ○ in reflection G'. The combination of the two operations is written as m_R. When the twofold rotation axis is parallel to the diffraction vector **G**, two beams (○) in the left-hand part of the figure become one reflection G, and a mirror symmetry, whose mirror line is perpendicular to vector **G** and passes through the centre of disc G, appears between the two beams (the right-hand side figure of Fig. 2.5.3.2*a*). The mirror symmetry is labelled m_2 after the twofold rotation axis. (2) Operation 1_R (Fig. 2.5.3.2*b*) for a horizontal mirror plane is a combination of a rotation by 2π of a beam (○) about a zone axis O (symbol 1), which is equivalent to no rotation, and a rotation by π of the beam about the exact Bragg position or the centre of disc G. (3) Operation 2_R is a rotation by π of a beam (○) in reflection G about a zone axis (symbol 2), which transforms the beam into a beam (+) in reflection $-G$, followed by a rotation by π of the beam (+) about the centre of disc $-G$, resulting in the beam (○) in disc $-G$ (Fig. 2.5.3.2*c*). The symmetry is called translational symmetry after Goodman (1975) because the pattern of disc $+G$ coincides with that of disc $-G$ by a translation. It is emphasized that an inversion centre is identified by the test of translational symmetry about a pair of $\pm G$ dark-field patterns – if one disc can be translated into coincidence with the other, an inversion centre exists. We call the pair $\pm$DP. (4) Operation 4_R (Fig. 2.5.3.2*d*) can be understood in a similar manner. It is noted that regular letters are symmetries about a zone axis, while subscripts R represent symmetries about the exact Bragg position. We call a pattern that contains an exact Bragg position (if possible at the disc centre) a dark-field pattern. As far as CBED symmetries are concerned, we

Table 2.5.3.2. *Symmetry elements of an infinitely extended parallel-sided specimen and diffraction groups*

	1	2	3	4	6	m	$2m(m)$	$3m$	$4m(m)$	$6m(m)$	
1	1	2	3	4	6	m	$2m(m)$	$3m$	$4m(m)$	$6m(m)$	10
(m') 1_R	1_R	21_R	31_R	41_R	61_R	$m1_R$	$2m(m)1_R$	$3m1_R$	$4m(m)1_R$	$6m(m)1_R$	10
(i) 2_R	2_R	[21_R]	6_R	[41_R]	[61_R]	$2_Rm(m_R)$ [$2_Rm(m_R)$]	[$2m(m)1_R$] [$2m(m)1_R$]	$6_Rm(m_R)$ [$3m1_R$]	[$4m(m)1_R$]	[$6m(m)1_R$]	4
($2'$) m_R	m_R	$2m_R(m_R)$	$3m_R$	$4m_R(m_R)$	$6m_R(m_R)$	[$m1_R$]	[$4_R(m)m_R$]	[$6_Rm(m_R)$]	[$4m(m)1_R$]	[$6_Rm(m_R)$]	5
($\bar{4}$) 4_R		4_R		[41_R]		$4_Rm(m_R)$	[$4_Rm(m_R)$]		[$4m(m)1_R$]		2

$1_R \times 2_R = 2$, $2_R \times 2_R = 1$, $m_R \times 2_R = m$, $4_R \times 2_R = 4$, $1_R \times m_R = m \times m_R$, $1_R \times 4_R = 4 \times 1_R$, $m_R \times 4_R = m \times 4_R$.

references