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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) ±dark-field patterns (±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	1	1	1	$m1_R$
	(m_2)			m_R	
			m_2	1	
m	m_v	m_v	1	1	
				m_v	
			m_v	1	
$m1_R$	$2mm$	m_v	2	1	
	$[m_v + m_2 + (1_R)]$			m_v1_R	
			$2m_vm_2$	1	
$2m_Rm_R$	$2mm$	2	1	2	$2mm1_R$
	$(2 + m_2)$		m_2	$2m_R(m_2)$	
$2mm$	$2m_vm_{v'}$	$2m_vm_{v'}$	1	2	
			m_v	$2m_{v'}(m_v)$	
2_Rmm_R	m_v	m_v	1	2_R	
			m_2	$2_Rm_{v'}(m_2)$	
			m_v	$2_Rm_R(m_v)$	
$2mm1_R$	$2m_vm_{v'}$	$2m_vm_{v'}$	2	21_R	
			$2m_vm_2$	$21_Rm_{v'}(m_v)$	
4	4	4	1	2	41_R
4_R	4	2	1	2	
41_R	4	4	2	21_R	
$4m_Rm_R$	$4mm$	4	1	2	$4mm1_R$
	$(4 + m_2)$		m_2	$2m_R(m_2)$	
$4mm$	$4m_vm_{v'}$	$4m_vm_{v'}$	1	2	
			m_v	$2m_{v'}(m_v)$	
4_Rmm_R	$4mm$	$2m_vm_{v'}$	1	2	
	$(2m_vm_{v'} + m_2)$		m_2	$2m_R(m_2)$	
			m_v	$2m_{v'}(m_v)$	
$4mm1_R$	$4m_vm_{v'}$	$4m_vm_{v'}$	2	21_R	
			$2m_vm_2$	$21_Rm_{v'}(m_v)$	
3	3	3	1	1	31_R
31_R	6 $(3 + 1_R)$	3	2	1	
$3m_R$	$3m$	3	1	1	$3m1_R$
	$(3 + m_2)$			m_R	
			m_2	1	
$3m$	$3m_v$	$3m_v$	1	1	
				m_v	
			m_v	1	
$3m1_R$	$6mm$	$3m_v$	2	1	
	$[3m_v + m_2 + (1_R)]$			m_v1_R	
			$2m_vm_2$	1	
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
$6m_Rm_R$	$6mm$	6	1	2	$6mm1_R$
	$(6 + m_2)$		m_2	$2m_R(m_2)$	
$6mm$	$6m_vm_{v'}$	$6m_vm_{v'}$	1	2	
			m_v	$2m_{v'}(m_v)$	
6_Rmm_R	$3m_v$	$3m_v$	1	2_R	
			m_2	$2_Rm_{v'}(m_2)$	
			m_v	$2_Rm_R(m_v)$	
$6mm1_R$	$6m_vm_{v'}$	$6m_vm_{v'}$	2	21_R	
			$2m_vm_2$	$21_Rm_{v'}(m_v)$	

however, noted that many diffraction groups are determined from a WP and BP pair without using a DP or ±DP (or from one photograph) or from a set of a WP, a BP and a DP without using a ±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 $2\bar{2}0$ and $\bar{2}20$ 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_Rmm_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_Rmm_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

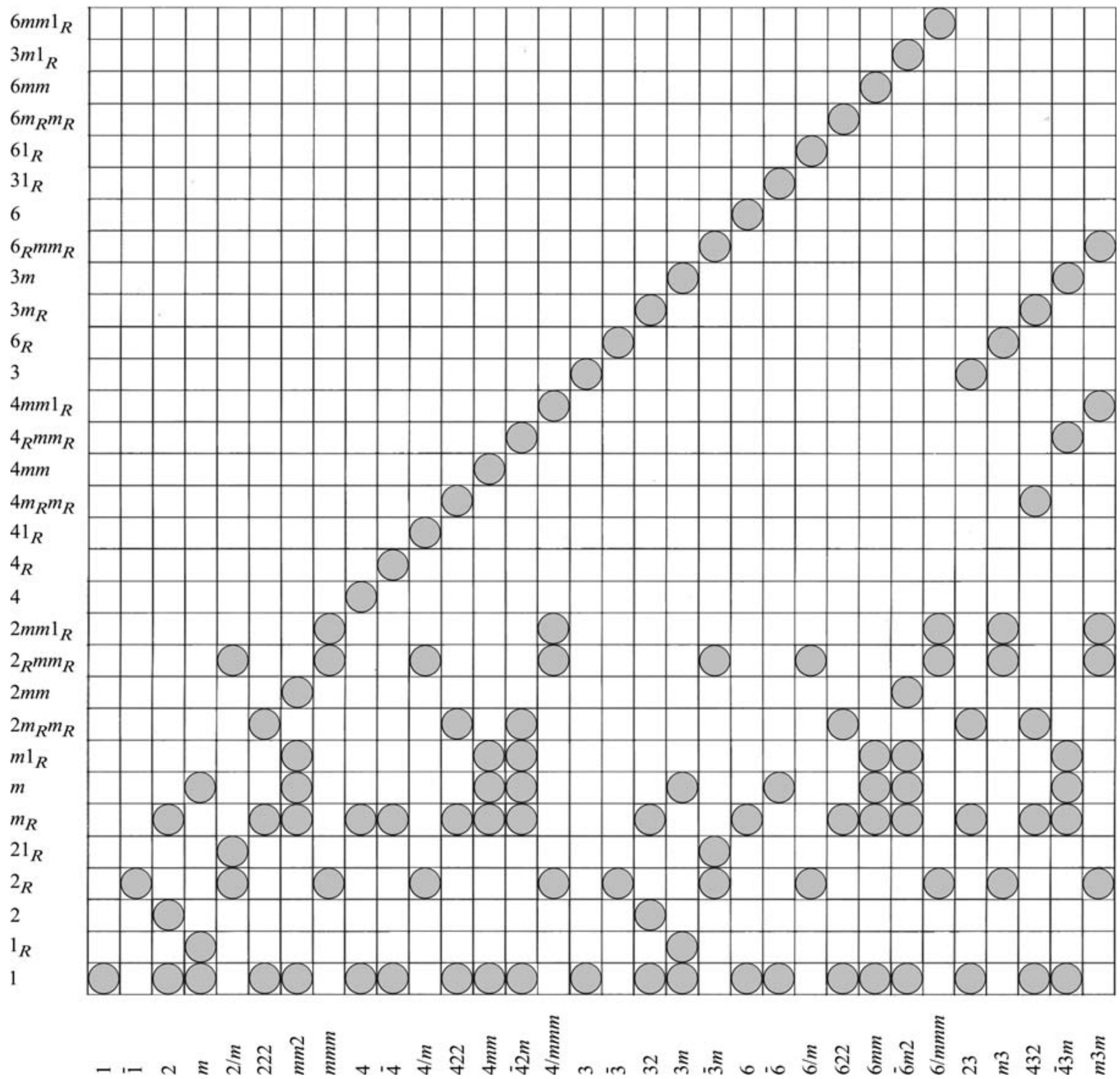

Fig. 2.5.3.4. Relation between diffraction groups and crystal point groups (after Buxton *et al.*, 1976).

lines are seen in the ZOLZ discs, the symmetry elements found from the CBED patterns are only those of the specimen projected along the zone axis. The projection of the specimen along the zone axis causes horizontal mirror symmetry m', the corresponding CBED symmetry being 1_R. When symmetry 1_R is added to the 31 diffraction groups, ten projection diffraction groups having symmetry symbol 1_R are derived as shown in column VI of Table 2.5.3.3. If only ZOLZ reflections are observed in CBED patterns, a projection diffraction group instead of a diffraction group is obtained, where only the pattern symmetries given in the rows of the diffraction groups having symmetry symbol 1_R in Table 2.5.3.3 should be consulted. Two projection diffraction groups obtained from two different zone axes are the minimum needed to determine a crystal point group, because it is constructed by the three-dimensional combination of symmetry elements. It should be noted that if a diffraction group is determined carelessly from CBED patterns with no HOLZ lines, the wrong crystal point group is obtained.

2.5.3.2.7. Symmetrical many-beam method

In the sections above, the point-group determination method established by Buxton *et al.* (1976) was described, where two- and three-dimensional symmetry elements were determined, respectively, from ZAPs and DPs.

The Laue circle is defined as the intersection of the Ewald sphere with the ZOLZ, and all reflections on this circle are simultaneously at the Bragg condition. If many such DPs are recorded (all simultaneously at the Bragg condition), many three-dimensional symmetry elements can be identified from one photograph. Using a group-theoretical method, Tinnappel (1975) studied the symmetries appearing in simultaneously excited DPs for various combinations of crystal symmetry elements. Based upon his treatment, Tanaka, Saito & Sekii (1983) developed a method for determining diffraction groups using simultaneously excited symmetrical hexagonal six-beam, square four-beam and rectangular four-beam CBED patterns. All the CBED symmetries appearing in the symmetrical many-beam (SMB) patterns were derived by the graphical method used in the paper of Buxton *et al.* (1976). From an experimental viewpoint, it is advantageous that symmetry elements can be identified from one photograph. It was found that twenty diffraction groups can be identified from one SMB pattern, whereas ten diffraction groups can be determined by Buxton *et al.*'s method. An experimental comparison between the two methods was performed by Howe *et al.* (1986).

SMB patterns are easily obtained by tilting a specimen crystal or the incident beam from a zone axis into an orientation to excite low-order reflections simultaneously. Fig. 2.5.3.7 illustrates the symmetries of the SMB patterns for all the diffraction groups except for the five groups 1, 1_R, 2, 2_R and 21_R. For these groups, the two-beam method for exciting one reflection is satisfactory because many-beam excitation gives no more information than the two-beam case. In the six-beam and square four-beam cases,

references