

2. RECIPROCAL SPACE IN CRYSTAL-STRUCTURE DETERMINATION

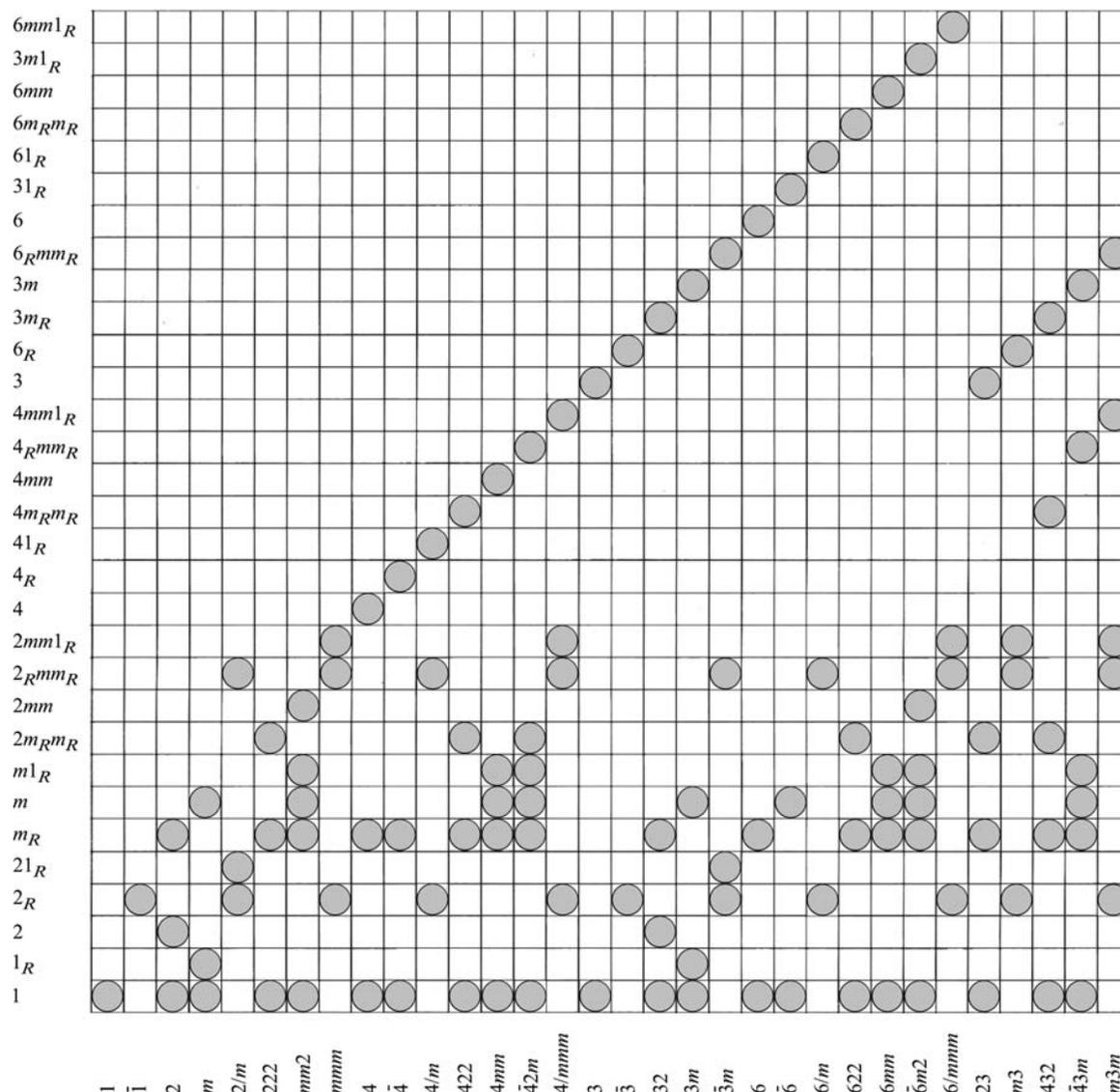


Fig. 2.5.3.4. Relation between diffraction groups and crystal point groups (after Buxton *et al.*, 1976).

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,