

## 2. RECIPROCAL SPACE IN CRYSTAL-STRUCTURE DETERMINATION

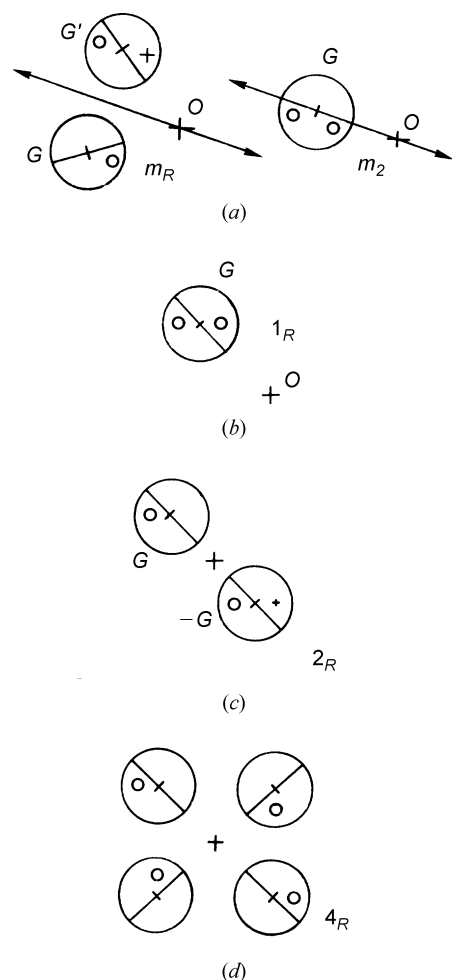


Fig. 2.5.3.2. Illustration of symmetries appearing in dark-field patterns (DPs). (a)  $m_R$  and  $m_2$ ; (b)  $1_R$ ; (c)  $2_R$ ; (d)  $4_R$ , originating from  $2'$ ,  $m'$ ,  $i$  and  $\bar{4}$ , respectively.

do not use the term dark-field pattern if a disc does not contain the exact Bragg position.

The four three-dimensional symmetry elements are found to produce different symmetries in the DPs. These facts imply that these symmetry elements can be identified unambiguously from the symmetries of CBED patterns.

### 2.5.3.2.3. Identification of two-dimensional symmetry elements

Two-dimensional symmetry elements that belong to a zone axis exhibit their symmetries in CBED patterns or zone-axis patterns (ZAPs) directly, even if dynamical diffraction takes place. A ZAP contains a bright-field pattern (BP) and a whole pattern (WP). The BP is the pattern appearing in the bright-field disc [the central or 'direct' (000) beam]. The WP is composed of the BP and the pattern formed by the surrounding diffraction discs, which are not exactly excited. The two-dimensional symmetry elements  $m$ , 1, 2, 3, 4 and 6 yield symmetry  $m_v$  and one-, two-, three-, four- and sixfold rotation symmetries, respectively, in WPs, where the suffix  $v$  for  $m_v$  is assigned to distinguish it from mirror symmetry  $m_2$  caused by a horizontal twofold rotation axis.

It should be noted that a BP shows not only the zone-axis symmetry but also three-dimensional symmetries, indicating that the BP can have a higher symmetry than the symmetry of the corresponding WP. The symmetries of the BP due to three-dimensional symmetry elements are obtained by moving the DPs to the zone axis. As a result, the three-dimensional symmetry elements  $m'$ ,  $i$ ,  $2'$  and  $\bar{4}$  produce, respectively, symmetries  $1_R$ , 1,  $m_2$  and 4 in the BP, instead of  $1_R$ ,  $2_R$ ,  $m_2$  and  $4_R$  in the DPs (Fig. 2.5.3.2). We mention that the BP cannot distinguish whether a

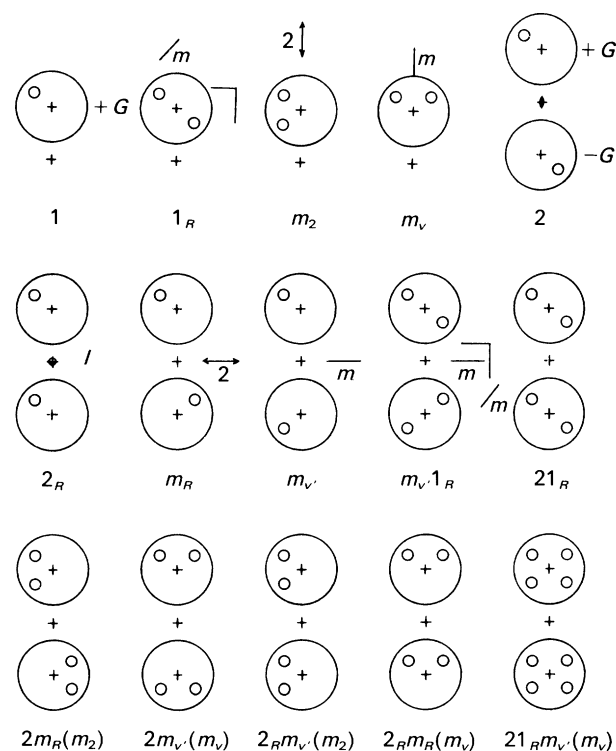


Fig. 2.5.3.3. Illustration of symmetries appearing in dark-field patterns (DPs) and a pair of dark-field patterns ( $\pm$ DP) for the combinations of symmetry elements.

specimen crystal has an inversion centre or not, because an inversion centre forms the lowest symmetry 1 in the BP.

In conclusion, all the two-dimensional symmetry elements can be identified from the WP symmetries.

### 2.5.3.2.4. Diffraction-group determination

All the symmetry elements of the diffraction groups can be identified from the symmetries of a WP and DPs. But it is practical and convenient to use just the four patterns WP, BP, DP and  $\pm$ DP to determine the diffraction group. The symmetries appearing in these four patterns are given for the 31 diffraction groups in Table 2.5.3.3 (Tanaka, Saito & Sekii, 1983), which is a detailed version of Table 2 of Buxton *et al.* (1976). All the possible symmetries of the DP and  $\pm$ DP appearing at different crystal orientations are given in the present table. When a BP has a higher symmetry than the corresponding WP, the symmetry elements that produce the BP are given in parentheses in column II except only for the case of  $4_R$ . When two types of vertical mirror planes exist, these are distinguished by symbols  $m_v$  and  $m'_v$ . Each of the two or three symmetries given in columns IV and V for many diffraction groups appears in a DP or  $\pm$ DP in different directions.

It is emphasized again that no two diffraction groups exhibit the same combination of BP, WP, DP and  $\pm$ DP, which implies that the diffraction groups are uniquely determined from an inspection of these pattern symmetries. Fig. 2.5.3.3 illustrates the symmetries of the DP and  $\pm$ DP appearing in Table 2.5.3.3, which greatly eases the cumbersome task of determining the symmetries. The first four patterns illustrate the symmetries appearing in a single DP and the others treat those in  $\pm$ DPs. The pattern symmetries are written beneath the figures. The other symbols are the symmetries of a specimen. The crosses outside the diffraction discs designate the zone axis. The crosses inside the diffraction discs indicate the exact Bragg position.

When the four patterns appearing in three photographs are taken and examined using Table 2.5.3.3 with the aid of Fig. 2.5.3.3, one diffraction group can be selected unambiguously. It is,