Table 2.5.3.8. *Dynamical extinction rules for an infinitely extended parallel-sided specimen*

Symmetry elements of plane-parallel specimen	Orientation to specimen surface	Dynamical extinction lines: Two-dimensional (zeroth Laue zone) interaction	Dynamical extinction lines: Three-dimensional (HOLZ) interaction
Glide planes	perpendicular: g	A_2 and B_2	A_3
	parallel: g'	—	intersection of A_3 and B_3
Twofold screw axis	perpendicular: 2_1	—	—
	parallel: $2'_1$	A_2 and B_2	B_3

beam. With reference to Fig. 2.5.3.10(*a*), extinction lines A_3 produced by a glide plane remain even when the crystal is rotated with respect to axis h but the lines are destroyed by a rotation of the crystal about axis k. Extinction lines B_3 originating from a 2_1 screw axis are not destroyed by a crystal rotation about axis k but the lines are destroyed by a rotation with respect to axis h.

2.5.3.3.3. *Space-group determination*

We now describe a space-group determination method which uses the dynamical extinction lines caused by the horizontal screw axis $2'_1$ and the vertical glide plane g of an infinitely extended parallel-sided specimen. We do not use the extinction due to the glide plane g' because observation of the extinction requires a laborious experiment. It should be noted that a vertical glide plane with a glide vector not parallel to the specimen surface cannot be a symmetry element of a specimen of finite thickness; however, the component of the glide vector perpendicular to the incident beam acts as a symmetry element g. (Which symmetry elements are observed by CBED is discussed in Section 2.5.3.3.5.) The 2_1, 4_1, 4_3, 6_1, 6_3 and 6_5 screw axes of crystal space groups that are set perpendicular to the incident beam act as a symmetry element $2'_1$ because two or three successive operations of 4_1, 4_3, 6_1, 6_3 and 6_5 screw axes make them equivalent to a 2_1 screw axis: $(4_1)^2 = (4_3)^2 = (6_1)^3 = (6_3)^3 = (6_5)^3 = 2_1$. The 4_2, 3_1, 3_2, 6_2 and 6_4 screw axes that are set perpendicular to the incident beam do not produce dynamical extinction lines because the 4_2 screw axis acts as a twofold rotation axis due to the relation $(4_2)^2 = 2$, the 3_1 and 3_2 screw axes give no specific symmetry in CBED patterns, and the 6_2 and 6_4 screw axes are equivalent to 3_1 and 3_2 screw axes due to the relations $(6_2)^2 = 3_2$ and $(6_4)^2 = 3_1$. Modifications of the dynamical extinction rules were investigated by Tanaka, Sekii & Nagasawa (1983) when more than one crystal symmetry element (that gives rise to dynamical extinction lines) coexists and when the symmetry elements are combined with various lattice types. Using these results, dynamical extinction lines A_2, A_3, B_2 and B_3 expected from all the possible crystal settings for all the space groups were tabulated.

Table 2.5.3.9 shows all the dynamical extinction lines appearing in the kinematically forbidden reflections for all the possible crystal settings of all the space groups. The first column gives space groups. In each of the following pairs of columns, the left-hand column of the pair gives the reflection indices and the symmetry elements causing the extinction lines and the right-hand column gives the types of the extinction lines. The (second) suffixes 1, 2 and 3 of a 2_1 screw axis in each column distinguish the first, the second and the third screw axis of the space group (as in the symbols 2_{11} and 2_{12} of space group $P2_12_12$). The glide symbols in the [001] column for space group $P4/nnc$ have two suffixes (n_{21} and n_{22}). The first suffix 2 denotes the second glide plane of the space group. The second suffixes 1 and 2, which appear in the tetragonal and cubic systems, distinguish two equivalent glide planes which lie in the x and y planes. The equivalent planes are distinguished only for the cases of [100], [010] and [001] electron-beam incidences, for convenience. The c-glide planes of space group $Pcc2$ are distinguished with symbols c_1 and c_2 (the first suffix only), because the equivalent planes do not exist. The glide symbol in the [001] column for space group $P4/mbm$ has only one suffix 1 or 2. The suffix distinguishes the equivalent glide planes lying in the x and y planes. The first suffix to distinguish the first and the second glide planes is not necessary because the space group has only one glide symbol b. When the index of the incident-beam direction is expressed with a symbol like [$h0l$] for point groups 2, m and $2/m$, the index h or l can take a value of zero. That is, the extinction rules are applicable to the [100] and [001] electron-beam incidences. However, if columns for [100], [010] and [001] incidences are present, as in the case of point group $mm2$, [$hk0$], [$0kl$] and [$h0l$] incidences are only for nonzero h, k and l. The reflections in which the extinction lines appear are always perpendicular to the corresponding incident-beam directions ($0k'l' \perp [0kl]$, $h'k'0 \perp [hk0], \ldots$). The indices of the reflections in which extinction lines appear are odd if no remark is given. For c-glide planes of space groups $R3c$ and $R\bar{3}c$ and for d-glide planes, the reflections in which extinction lines appear are specified as $6n + 3$ and $4n + 2$ orders, respectively.

The number of indistinguishable space groups was first counted by Tanaka, Sekii & Nagasawa (1983) but later corrections were made by Eades & Spence (1987). It was found that 177 space groups out of 230 can be identified using the extinction lines (Tanaka *et al.*, 2002). Another reference for space-group determination is due to Eades (1988). The indistinguishable space-group sets using the extinction lines are listed in Table 2.5.3.10. Most of the sets are caused by the fact that CBED cannot identify 4_2, 3_1 (3_2) and 6_2 (6_4) screw axes. However, these sets can be rather easily distinguished in the ordinary way, that is, by observing how the intensities of the reflections which may be kinematically forbidden change when the crystal orientation is varied. If the axis concerned is a screw axis, kinematically forbidden reflections show a sudden decrease in intensity when an orientation change causes the loss of *Umweganregung* paths. If the axis is a rotation axis, the intensities of the reflections do not change conspicuously for such an orientation change. Using this test, each space group in the 23 sets can be identified except the pairs in parentheses and pairs (16) and (17) in Table 2.5.3.10 (see Eades, 1988).

Tsuda *et al.* (2000) showed theoretically that the coherent CBED method can distinguish between space groups ($I23$ and $I2_13$) and between ($I222$ and $I2_12_12_1$), which are indistinguishable pairs (16) and (17), respectively, in Table 2.5.3.10. The coherent CBED pattern is obtained in such a way that the convergence angle of the incident beam is set to a larger value than usual to make adjacent CBED discs overlap (Dowell & Goodman, 1973). When the focus point is displaced from the specimen, or a certain area is illuminated, sinusoidal interference fringes of the lattice spacing corresponding to the adjacent discs are formed in the overlapping regions if the probe size of the incident beam is smaller than the lattice spacing. (If the focus point of the incident beam is on the specimen, each overlapping region of the CBED discs shows uniform intensity.) Formation of the interference fringes was explained in detail first by Spence & Cowley (1978). Vine *et al.* (1992) showed distortion-free interference fringes from 6*H*-SiC and succeeded in observing the fringes with a shift of half a period due to a glide plane. Tsuda *et al.*'s method