Table 2.5.3.10. *Space-group sets indistinguishable by dynamical extinction lines*

(1) $P3$, ($P3_1$, $P3_2$)	(2) $P312$, ($P3_112$, $P3_212$)	(3) $P321$, ($P3_121$, $P3_221$)
(4) $P6$, ($P6_2$, $P6_4$)	(5) $P622$, ($P6_222$, $P6_422$)	(6) $P6_3$, ($P6_1$, $P6_5$)
(7) $P6_322$, ($P6_122$, $P6_522$)	(8) $P4$, $P4_2$	(9) ($P4_1$, $P4_3$)
(10) $P4/m$, $P4_2/m$	(11) $P4/n$, $P4_2/n$	(12) $P422$, $P4_222$
(13) $P42_12$, $P4_22_12$	(14) $I4$, $I4_1$	(15) $I422$, $I4_122$
(16) $I23$, $I2_13$	(17) $I222$, $I2_12_12_1$	(18) $P432$, $P4_232$
(19) ($P4_132$, $P4_332$)	(20) $I432$, $I4_132$	(21) $F432$, $F4_132$
(22) ($P4_122$, $P4_322$)	(23) ($P4_12_12$, $P4_32_12$)	

distinguishes the difference in the relative arrangements of twofold rotation axes and 2_1 screw axes along the [111] direction between the two space groups by examining the symmetry of intensity pairs appearing in the overlapping discs of a coherent [111] ZOLZ pattern. Saitoh, Tsuda *et al.* (2001) extended the method to distinguish the other ten indistinguishable space-group pairs. The method can distinguish between a space group which is composed of a principal rotation axis and a twofold rotation axis like $P321$ and a space group which is composed of a principal screw axis and a twofold rotation axis like $P3_121$ (or $P3_221$) by investigating the difference in the relative arrangements of the twofold rotation axis with respect to the principal axis. Table 2.5.3.11 shows the 12 space-group pairs which are distinguishable by applying the coherent CBED method.

The pairs in parentheses form left- and right-handed space groups. Handedness or chirality may occur in space groups that do not possess mirror and/or inversion symmetry. The handedness of space groups is identified in such a way that the senses of two crystal axes are determined with the aid of kinematical structure-factor calculations and the sense of the third axis is determined with the aid of dynamical calculations. This method was used for quartz by Goodman & Secomb (1977) and Goodman & Johnson (1977) and for MnSi by Tanaka *et al.* (1985). We also mention that Taftø & Spence (1982) developed a simple but clever method without computation for determining the absolute polarity of the sphalerite structure utilizing multiple-scattering effects on weak beams, which are almost independent of thickness. Because of the importance of structure in the field of semiconductor science, this method is conveniently used nowadays to determine polarity.

It is worth mentioning that space groups that are indistinguishable by CBED (Table 2.5.3.10) do not appear frequently in real inorganic materials. The crystal data collected by Nowacki (1967) on 5572 different inorganic materials shows that the number of materials belonging to space groups among sets (2), (3), (5), (7) and (11) in Table 2.5.3.10 is more than 15 but the number belonging to space groups among the other sets is less than ten. This implies that the probability of finding indistinguishable space groups is very low.

Table 2.5.3.11. *Space-group sets distinguishable by coherent CBED*

The space-group pairs in parentheses can not be distinguished by coherent CBED but can be distinguished by a handedness test. An asterisk (*) indicates the incidence at which the distinction is carried out by many-beam interference (Saitoh, Tsuda *et al.*, 2001).

Space-group set	Incidence
(2) $P312$, ($P3_112$, $P3_212$)	$[1\bar{1}01]$
(3) $P321$, ($P3_121$, $P3_221$)	$[11\bar{2}3]$
(5) $P622$, ($P6_222$, $P6_422$)	$[11\bar{2}3]$
(7) $P6_322$, ($P6_122$, $P6_522$)	$[11\bar{2}3]$
(12) $P422$, $P4_222$	[321], [211], [112]*
(13) $P42_12$, $P4_22_12$	[211]
(15) $I422$, $I4_122$	[111]
(16) $I23$, $I2_13$	[111]
(17) $I222$, $I2_12_12_1$	[111]
(18) $P432$, $P4_232$	[321], [211]*
(20) $I432$, $I4_132$	[111]
(21) $F432$, $F4_132$	[432]

2.5.3.3.4. Dynamical extinction in HOLZ reflections

Space-group determination as described in the previous sections is carried out using the extinction lines appearing in ZOLZ reflections. Vertical glide planes whose translation vectors are perpendicular to the specimen surface do not cause extinction lines in ZOLZ reflections but cause them in HOLZ reflections. (It is noted that the vertical glide planes with glide translations not parallel to the surface are not the symmetry elements of diperiodic plane figures.) Vertical glide planes whose translation vectors are parallel to the surface cause extinction lines in both ZOLZ and HOLZ reflections. Vertical screw axes are expected to form extinction lines in HOLZ reflections whose vectors are parallel to the screw axes. These reflections, however, cannot be observed by ordinary CBED. Thus, the extinction lines appearing in observable HOLZ reflections are used to identify not screw axes but glide planes. Examination of HOLZ extinction lines together with ZOLZ extinction lines is an efficient way to characterize the glide vectors and determine the space group.

The dynamical extinction lines appearing in HOLZ reflections caused by the glide planes whose glide vectors are not only parallel but also not parallel to the specimen surface were tabulated by Nagasawa (1983) for various incident-beam orientations of all the space groups that have glide planes. The tabulated results appear on pages 214–225 of the book by Tanaka *et al.* (1988). Table 2.5.3.12 shows the results. The meanings of the letters used in the table are explained in Fig. 2.5.3.13. We consider a vertical glide plane with a glide vector perpendicular to the surface as is shown in Fig. 2.5.3.13(*a*). Letter A is given for cases in which the Ewald sphere intersects two circled-cross reflections in the first Laue zone as seen in Fig. 2.5.3.13(*b*), where black circles and circled crosses denote allowed reflections and kinematically forbidden but dynamically allowed reflections due to the glide plane, respectively. A^* denotes cases in which the Ewald sphere intersects a circled-cross reflection on one side of the incident beam and a black-circled reflection on the other, as seen in Fig. 2.5.3.13(*c*). This case occurs only in space group $P2_1/a\bar{3}$. $A_{\rm h}$ denotes cases in which the Ewald sphere intersects a circled-cross reflection on one side but does not intersect on the other, owing to the asymmetric arrangement of reflections with respect to the incident beam.

The first column of Table 2.5.3.12 list the space groups and the following columns show the type of the extinction lines for possible incident-beam directions. In each pair of columns, the left-hand column gives the reflection indices of the extinction line and the symmetry elements causing the extinction and the right-hand column gives the type of extinction. The first suffix 1, 2 or 3 of a glide symbol distinguishes the first, the second or the third glide plane of a 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 suffix o of a reflection index implies that the index is odd-order. Figs.

  references