

2.5. ELECTRON DIFFRACTION AND ELECTRON MICROSCOPY IN STRUCTURE DETERMINATION

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	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 ($0k'l' \perp [0kl]$, $h'k'0 \perp [hk0]$, ...). 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 6H-SiC and succeeded in observing the fringes with a shift of half a period due to a glide plane. Tsuda *et al.*'s method

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Table 2.5.3.9. Dynamical extinction lines appearing in ZOLZ reflections for all crystal space groups except Nos. 1 and 2

Point groups 2, *m*, 2/*m* (second setting, unique axis *b*)

Space group	Incident-beam direction		
	[<i>h0l</i>]		
3 <i>P2</i>			
4 <i>P2</i> ₁	0 <i>k</i> 0 2 ₁	<i>A</i> ₂	<i>B</i> ₂ <i>B</i> ₃
5 <i>C2</i>			
6 <i>Pm</i>			
7 <i>Pc</i>	<i>h0l</i> ₀ <i>c</i>	<i>A</i> ₂ <i>A</i> ₃	<i>B</i> ₂
8 <i>Cm</i>			
9 <i>Cc</i>	<i>h_c0l</i> ₀ <i>c</i>	<i>A</i> ₂ <i>A</i> ₃	<i>B</i> ₂
10 <i>P2/m</i>			
11 <i>P2</i> ₁ / <i>m</i>	0 <i>k</i> 0 2 ₁	<i>A</i> ₂	<i>B</i> ₂ <i>B</i> ₃
12 <i>C2/m</i>			
13 <i>P2/c</i>	<i>h0l</i> ₀ <i>c</i>	<i>A</i> ₂ <i>A</i> ₃	<i>B</i> ₂
14 <i>P2</i> ₁ / <i>c</i>	0 <i>k</i> 0 2 ₁	<i>A</i> ₂	<i>B</i> ₂ <i>B</i> ₃
	<i>h0l</i> ₀ <i>c</i>	<i>A</i> ₂ <i>A</i> ₃	<i>B</i> ₂
15 <i>C2/c</i>	<i>h_c0l</i> ₀ <i>c</i>	<i>A</i> ₂ <i>A</i> ₃	<i>B</i> ₂

Point group 222

Space group	Incident-beam direction					
	[100]	[010]	[001]	[<i>hk</i> 0]	[0 <i>kl</i>]	[<i>h0l</i>]
16 <i>P222</i>						
17 <i>P222</i> ₁	00 <i>l</i> 2 ₁	00 <i>l</i> 2 ₁		00 <i>l</i> 2 ₁		
18 <i>P2</i> ₁ 2 ₁ 2	0 <i>k</i> 0 2 ₁₂	<i>h</i> 00 2 ₁₁	<i>h</i> 00 2 ₁₁ 0 <i>k</i> 0 2 ₁₂		<i>h</i> 00 2 ₁₁	0 <i>k</i> 0 2 ₁₂
19 <i>P2</i> ₁ 2 ₁ 2 ₁	0 <i>k</i> 0 2 ₁₂ 00 <i>l</i> 2 ₁₃	<i>h</i> 00 2 ₁₁ 00 <i>l</i> 2 ₁₃	<i>h</i> 00 2 ₁₁ 0 <i>k</i> 0 2 ₁₂	00 <i>l</i> 2 ₁₃	<i>h</i> 00 2 ₁₁	0 <i>k</i> 0 2 ₁₂
20 <i>C222</i> ₁	00 <i>l</i> 2 ₁	00 <i>l</i> 2 ₁		00 <i>l</i> 2 ₁		
21 <i>C222</i>						
22 <i>F222</i>						
23 <i>I222</i>						
24 <i>I2</i> ₁ 2 ₁ 2 ₁						

Point group *mm*2

Space group	Incident-beam direction					
	[100]	[010]	[001]	[<i>hk</i> 0]	[0 <i>kl</i>]	[<i>h0l</i>]
25 <i>Pmm</i> 2						
26 <i>Pmc</i> 2 ₁	00 <i>l</i> <i>c</i> , 2 ₁	00 <i>l</i> 2 ₁		00 <i>l</i> 2 ₁		<i>h0l</i> ₀ <i>c</i>
27 <i>Pcc</i> 2	00 <i>l</i> <i>c</i> ₂	00 <i>l</i> <i>c</i> ₁			0 <i>kl</i> ₀ <i>c</i> ₁	<i>h0l</i> ₀ <i>c</i> ₂
28 <i>Pma</i> 2			<i>h</i> 00 <i>a</i>	<i>A</i> ₂ <i>A</i> ₃		<i>h</i> ₀ 0 <i>l</i> <i>a</i>
29 <i>Pca</i> 2 ₁	00 <i>l</i> 2 ₁	00 <i>l</i> <i>c</i> , 2 ₁	<i>h</i> 00 <i>a</i>	<i>A</i> ₂ <i>A</i> ₃	00 <i>l</i> 2 ₁	0 <i>kl</i> ₀ <i>c</i>

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Table 2.5.3.9 (cont.)

Space group	Incident-beam direction					
	[100]	[010]	[001]	[hk0]	[0kl]	[h0l]
30 <i>Pnc2</i>	00l c A ₃	00l n A ₃	0k0 n A ₂ B ₂ A ₃		0kl: k + l = 2n + 1 n A ₂ B ₂ A ₃	h0l _o c A ₂ B ₂ A ₃
31 <i>Pmn2</i> ₁	00l n, 2 ₁ A ₂ B ₂ A ₃ B ₃	00l 2 ₁ B ₃	h00 n A ₂ B ₂ A ₃	00l 2 ₁ A ₂ B ₂ B ₃		h0l: h + l = 2n + 1 n A ₂ B ₂ A ₃
32 <i>Pba2</i>			h00 a 0k0 b A ₂ B ₂ A ₃		0k _o l b A ₂ B ₂ A ₃	h _o 0l a A ₂ B ₂ A ₃
33 <i>Pna2</i> ₁	00l 2 ₁ B ₃	00l n, 2 ₁ A ₂ B ₂ A ₃ B ₃	h00 a 0k0 n A ₂ B ₂ A ₃	00l 2 ₁ A ₂ B ₂ B ₃	0kl: k + l = 2n + 1 n A ₂ B ₂ A ₃	h _o 0l a A ₂ B ₂ A ₃
34 <i>Pnn2</i>	00l n ₂ A ₃	00l n ₁ A ₃	h00 n ₂ 0k0 n ₁ A ₂ B ₂ A ₃		0kl: k + l = 2n + 1 n ₁ A ₂ B ₂ A ₃	h0l: h + l = 2n + 1 n ₂ A ₂ B ₂ A ₃
35 <i>Cmm2</i> <i>ba2</i>						
36 <i>Cmc2</i> ₁ <i>bn2</i> ₁	00l c, 2 ₁ A ₂ B ₂ A ₃ B ₃	00l 2 ₁ B ₃		00l 2 ₁ A ₂ B ₂ B ₃		h _e 0l _o c A ₂ B ₂ A ₃
37 <i>Ccc2</i> <i>nn2</i>	00l c ₂ A ₃	00l c ₁ A ₃			0k _e l _o c ₁ A ₂ B ₂ A ₃	h _e 0l _o c ₂ A ₂ B ₂ A ₃
38 <i>Amm2</i> <i>nc2</i> ₁						
39 <i>Abm2</i> <i>cc2</i> ₁					0k _o l _o b A ₂ B ₂ A ₃	
40 <i>Ama2</i> <i>nn2</i> ₁			h00 a A ₂ B ₂ A ₃			h _o 0l _e a A ₂ B ₂ A ₃
41 <i>Aba2</i> <i>cn2</i> ₁			h00 a A ₂ B ₂ A ₃		0k _o l _o b A ₂ B ₂ A ₃	h _o 0l _e a A ₂ B ₂ A ₃
42 <i>Fmm2</i>						
43 <i>Fdd2</i> <i>dd2</i> ₁	00l: l = 4n + 2 d ₂ A ₃	00l: l = 4n + 2 d ₁ A ₃	h00: h = 4n + 2 d ₂ 0k0: k = 4n + 2 d ₁ A ₂ B ₂ A ₃		0k _e l _e : k _e + l _e = 4n + 2 d ₁ A ₂ B ₂ A ₃	h _e 0l _e : h _e + l _e = 4n + 2 d ₂ A ₂ B ₂ A ₃
44 <i>Imm2</i> <i>nn2</i> ₁						
45 <i>Iba2</i> <i>cc2</i> ₁					0k _o l _o b A ₂ B ₂ A ₃	h _o 0l _o a A ₂ B ₂ A ₃
46 <i>Ima2</i> <i>nc2</i> ₁						h _o 0l _o a A ₂ B ₂ A ₃

Point group *mmm*

Space group	Incident-beam direction					
	[100]	[010]	[001]	[hk0]	[0kl]	[h0l]
47 <i>P2/m2/m2/m</i>						
48 <i>P2/n2/n2/n</i>	00l n ₂ 0k0 n ₃ A ₃	00l n ₁ h00 n ₃ A ₃	0k0 n ₁ h00 n ₂ A ₃	hk0: h + k = 2n + 1 n ₃ A ₂ B ₂ A ₃	0kl: k + l = 2n + 1 n ₁ A ₂ B ₂ A ₃	h0l: h + l = 2n + 1 n ₂ A ₂ B ₂ A ₃
49 <i>P2/c2/c2/m</i>	00l c ₂ A ₃	00l c ₁ A ₃			0kl _o c ₁ A ₂ B ₂ A ₃	h0l _o c ₂ A ₂ B ₂ A ₃
50 <i>P2/b2/a2/n</i>	0k0 n A ₃	h00 n A ₃	0k0 b h00 a A ₃	hk0: h + k = 2n + 1 n A ₂ B ₂ A ₃	0k _o l b A ₂ B ₂ A ₃	h _o 0l a A ₂ B ₂ A ₃
51 <i>P2₁/m2/m2/a</i>		h00 2 ₁ , a A ₂ B ₂ A ₃ B ₃	h00 2 ₁ B ₃	h _o k0 a A ₂ B ₂ A ₃	h00 2 ₁ A ₂ B ₂ B ₃	

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Table 2.5.3.9 (cont.)

Space group	Incident-beam direction					
	[100]	[010]	[001]	[hk0]	[0kl]	[h0l]
52 $P2_1/n2_1/n2_1/a$	00l n_2 A_3	00l n_1 A_3 h00 a	0k0 A_2 B_2 $n_1, 2_1$ A_3 B_3	h_0k0 A_2 B_2 a A_3	0kl: $k+l=$ $2n+1$ n_1 A_3 B_2	h0l: $h+l=$ $2n+1$ n_2 A_2 B_2 A_3
	0k0 2_1 B_3		h00 n_2 A_3			0k0 A_2 B_2 2_1 B_3
53 $P2_1/m2_1/n2_1/a$	00l A_2 B_2 $n, 2_1$ A_3 B_3	h00 a A_3	h00 n A_3	h_0k0 A_2 B_2 a A_3		h0l: $h+l=$ $2n+1$ n A_2 B_2 A_3
		00l 2_1 B_3		00l 2_1 A_2 B_2 B_3		
54 $P2_1/c2_1/c2_1/a$	00l c_2 A_3	00l c_1 A_3	h00 2_1 B_3	h_0k0 A_2 B_2 a A_3	0kl ₀ A_2 B_2 c_1 A_3	h0l ₀ A_2 B_2 c_2 A_3
		h00 A_2 B_2 $a, 2_1$ A_3 B_3			h00 A_2 B_2 2_1 B_3	
55 $P2_1/b2_1/a2_1/m$	0k0 2_{12} B_3	h00 2_{11} B_3	0k0 A_2 B_2 $b, 2_{12}$ A_3 B_3		0k ₀ l A_2 B_2 b A_3	h ₀ 0l A_2 B_2 a A_3
			h00 $a, 2_{11}$		h00 A_2 B_2 2_{11} B_3	0k0 A_2 B_2 2_{12} B_3
56 $P2_1/c2_1/c2_1/n$	00l c_2 A_3	00l c_1 A_3	0k0 2_{12} B_3 h00 2_{11}	hk0: $h+k=$ $2n+1$ n A_2 B_2 A_3	0kl ₀ A_2 B_2 c_1 A_3	h0l ₀ A_2 B_2 c_2 A_3
	0k0 A_2 B_2 $2_{12}, n$ A_3 B_3	h00 A_2 B_2 $2_{11}, n$ A_3 B_3			h00 A_2 B_2 2_{11} B_3	0k0 A_2 B_2 2_{12} B_3
57 $P2_1/b2_1/c2_1/m$	00l A_2 B_2 $c, 2_{12}$ A_3 B_3	00l 2_{12} B_3	0k0 A_2 B_2 $b, 2_{11}$ A_3 B_3	00l A_2 B_2 2_{12} B_3	0k ₀ l A_2 B_2 b A_3	h0l ₀ A_2 B_2 c A_3
	0k0 2_{11} B_3					0k0 A_2 B_2 2_{11} B_3
58 $P2_1/n2_1/n2_1/m$	00l n_2 A_3	00l n_1 A_3	0k0 A_2 B_2 $n_1, 2_{12}$ A_3 B_3		0kl: $k+l=$ $2n+1$ n_1 A_2 B_2 A_3	h0l: $h+l=$ $2n+1$ n_2 A_2 B_2 A_3
	0k0 2_{12} B_3	h00 2_{11} B_3	h00 $n_2, 2_{11}$		h00 A_2 B_2 2_{11} B_3	0k0 A_2 B_2 2_{12} B_3
59 $P2_1/m2_1/m2_1/n$	0k0 A_2 B_2 $n, 2_{12}$ A_3 B_3	h00 A_2 B_2 $n, 2_{11}$ A_3 B_3	0k0 2_{12} B_3 h00 2_{11}	hk0: $h+k=$ $2n+1$ n A_2 B_2 A_3	h00 A_2 B_2 2_{11} B_3	0k0 A_2 B_2 2_{12} A_3
60 $P2_1/b2_1/c2_1/n$	00l A_2 B_2 $c, 2_{12}$ A_3 B_3	h00 A_2 B_2 $n, 2_{11}$ A_3 B_3	0k0 b A_3	hk0: $h+k=$ $2n+1$ n A_2 B_2 A_3	0k ₀ l A_2 B_2 b A_3	h0l ₀ A_2 B_2 c A_3
	0k0 n A_3	00l 2_{12} B_3	h00 2_{11} B_3	00l A_2 B_2 2_{12} B_3	h00 A_2 B_2 2_{11} B_3	
61 $P2_1/b2_1/c2_1/a$	00l A_2 B_2 $c, 2_{13}$ A_3 B_3	00l 2_{13} B_3	0k0 A_2 B_2 $b, 2_{12}$ A_3 B_3	h_0k0 A_2 B_2 a A_3	0k ₀ l A_2 B_2 b A_3	h0l ₀ A_2 B_2 c A_3
	0k0 2_{12} B_3	h00 A_2 B_2 $a, 2_{11}$ A_3 B_3	h00 2_{11} B_3	00l A_2 B_2 2_{13} B_3	h00 A_2 B_2 2_{11} B_3	0k0 A_2 B_2 2_{12} B_3
62 $P2_1/n2_1/m2_1/a$	00l 2_{13} B_3 0k0 2_{12}	00l A_2 B_2 $n, 2_{13}$ A_3 B_3 h00 $a, 2_{11}$	0k0 A_2 B_2 $n, 2_{12}$ A_3 B_3	h_0k0 A_2 B_2 a A_3	0kl: $k+l=$ $2n+1$ n A_2 B_2 A_3	0k0 A_2 B_2 2_{12} B_3
			h00 2_{11} B_3	00l A_2 B_2 2_{13} B_3	h00 A_2 B_2 2_{11} B_3	
63 $C2/m2_1/c2_1/m$	00l A_2 B_2 $c, 2_1$ A_3 B_3	00l 2_1 B_3		00l A_2 B_2 2_1 B_3		h ₀ 0l ₀ A_2 B_2 c A_3
64 $C2/m2_1/c2_1/a$	00l A_2 B_2 $c, 2_1$ A_3 B_3	00l 2_1 B_3		h_0k_00 A_2 B_2 a A_3		h ₀ 0l ₀ A_2 B_2 c A_3
				00l A_2 B_2 2_1 B_3		
65 $C2/m2_1/m2_1/m$						
66 $C2/c2_1/c2_1/m$	00l c_2 A_3	00l c_1 A_3			0k ₀ l ₀ A_2 B_2 c_1 A_3	h ₀ 0l ₀ A_2 B_2 c_2 A_3
67 $C2/m2_1/m2_1/a$				h_0k_00 A_2 B_2 a A_3		

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Table 2.5.3.9 (cont.)

Space group	Incident-beam direction					
	[100]	[010]	[001]	[hk0]	[0kl]	[h0l]
68 $C2/c2/c2/a$	00l c_2 A_3	00l c_1 A_3		h_0k_00 a A_2 B_2 A_3	$0k_0l_0$ c_1 A_2 B_2 A_3	h_0l_0 c_2 A_2 B_2 A_3
69 $F2/m2/m2/m$						
70 $F2/d2/d2/d$	00l: $l = A_3$ $4n + 2$ d_2 0k0: $k =$ $4n + 2$ d_3	h00: $h = A_3$ $4n + 2$ d_3 00l: $l =$ $4n + 2$ d_1	0k0: $k = A_3$ $4n + 2$ d_1 h00: $h =$ $4n + 2$ d_2	h_0k_00 : $h_0 + k_0 =$ $4n + 2$ d_3 A_2 B_2 A_3	$0k_0l_0$: $k_0 + l_0 =$ $4n + 2$ d_1 A_2 B_2 A_3	h_0l_0 : $h_0 + l_0 =$ $4n + 2$ d_2 A_2 B_2 A_3
71 $I2/m2/m2/m$						
72 $I2/b2/a2/m$					$0k_0l_0$ b A_2 B_2 A_3	h_0l_0 a A_2 B_2 A_3
73 $I2_1/b2_1/c2_1/a$				h_0k_00 a A_2 B_2 A_3	$0k_0l_0$ b A_2 B_2 A_3	h_0l_0 c A_2 B_2 A_3
74 $I2_1/m2_1/m2_1/a$				h_0k_00 a A_2 B_2 A_3		

 Point groups 4, $\bar{4}$, 4/m

Space group	Incident-beam direction	
	[hk0]	[0kl]
75 $P4$		
76 $P4_1$	00l 4_1	A_2 B_2 B_3
77 $P4_2$		
78 $P4_3$	00l 4_3	A_2 B_2 B_3
79 $I4$		
80 $I4_1$		
81 $P\bar{4}$		
82 $I\bar{4}$		
83 $P4/m$		
84 $P4_2/m$		
85 $P4/n$	$hk0: h + k = 2n + 1$ n	A_2 B_2 A_3
86 $P4_2/n$	$hk0: h + k = 2n + 1$ n	A_2 B_2 A_3
87 $I4/m$		
88 $I4_1/a$	h_0k_00 a	A_2 B_2 A_3

Point group 422

Space group	Incident-beam direction	
	[hk0]	[0kl]
89 $P422$		
90 $P42_12$		$h00$ A_2 B_2 2_1 B_3
91 $P4_122$	00l A_2 B_2 4_1 B_3	
92 $P4_12_12$	00l A_2 B_2 4_1 B_3	$h00$ A_2 B_2 2_1 B_3
93 $P4_222$		
94 $P4_22_12$		$h00$ A_2 B_2 2_1 B_3
95 $P4_322$	00l A_2 B_2 4_3 B_3	
96 $P4_32_12$	00l A_2 B_2 4_3 B_3	$h00$ A_2 B_2 2_1 B_3
97 $I422$		
98 $I4_122$		

2. RECIPROCAL SPACE IN CRYSTAL-STRUCTURE DETERMINATION

Table 2.5.3.9 (cont.)

Point group $4mm$. The symbol a in the column $[h0l]$ is equivalent to the symbol b in the space groups of the first column.

Space group	Incident-beam direction				
	[100]	[001]	[110]	$[h0l]$	$[hhl]$
99 $P4mm$					
100 $P4bm$		$h00$ A_2 B_2 a_2 A_3 $0k0$ b_1		h_00l A_2 B_2 a A_3	
101 $P4_2cm$	$00l$ c_2 A_3			$h0l_0$ A_2 B_2 c A_3	
102 $P4_2nm$	$00l$ n_2 A_3	$h00$ A_2 B_2 n_2 A_3 $0k0$ n_1		$h0l: h + l = 2n + 1$ A_2 B_2 n A_3	
103 $P4cc$	$00l$ c_{12} A_3		$00l$ c_2 A_3	$h0l_0$ A_2 B_2 c_1 A_3	hhl_0 A_2 B_2 c_2 A_3
104 $P4nc$	$00l$ n_2 A_3	$h00$ A_2 B_2 n_2 A_3 $0k0$ n_1	$00l$ c A_3	$h0l: h + l = 2n + 1$ A_2 B_2 n A_3	hhl_0 A_2 B_2 c A_3
105 $P4_2mc$			$00l$ c A_3		hhl_0 A_2 B_2 c A_3
106 $P4_2bc$		$h00$ A_2 B_2 a_2 A_3 $0k0$ b_1	$00l$ c A_3	h_00l A_2 B_2 a A_3	hhl_0 A_2 B_2 c A_3
107 $I4mm$					
108 $I4cm$				h_00l_0 A_2 B_2 c A_3	
109 $I4_1md$		$hh0, \bar{h}h0$ A_2 B_2 d A_3	$00l: l = 4n + 2$ d A_3		$hhl_c: 2h + l_c = 4n + 2$ A_2 B_2 d A_3
110 $I4_1cd$		$hh0, \bar{h}h0$ A_2 B_2 d A_3	$00l: l = 4n + 2$ d A_3	h_00l_0 A_2 B_2 c A_3	$hhl_c: 2h + l_c = 4n + 2$ A_2 B_2 d A_3

Point group $\bar{4}2m$. The symbol a in the column $[h0l]$ is equivalent to the symbol b in the space groups of the first column.

Space group	Incident-beam direction				
	[100]	[001]	[110]	$[h0l]$	$[hhl]$
111 $P\bar{4}2m$					
112 $P\bar{4}2c$			$00l$ c A_3		hhl_0 A_2 B_2 c A_3
113 $P\bar{4}2_1m$	$0k0$ A_2 B_2 2_{12} B_3	$h00$ A_2 B_2 2_{11} B_3 $0k0$ 2_{12}		$0k0$ A_2 B_2 2_1 B_3	
114 $P\bar{4}2_1c$	$0k0$ A_2 B_2 2_{12} B_3	$h00$ A_2 B_2 2_{11} B_3 $0k0$ 2_{12}	$00l$ c A_3	$0k0$ A_2 B_2 2_1 B_3	hhl_0 A_2 B_2 c A_3
115 $P\bar{4}m2$					
116 $P\bar{4}c2$	$00l$ c_2 A_3			$h0l_0$ A_2 B_2 c A_3	
117 $P\bar{4}b2$		$h00$ A_2 B_2 a_2 A_3 $0k0$ b_1		h_00l A_2 B_2 a A_3	
118 $P\bar{4}n2$	$00l$ n_2 A_3	$h00$ A_2 B_2 n_2 A_3 $0k0$ n_1		$h0l: h + l = 2n + 1$ A_2 B_2 n A_3	
119 $I\bar{4}m2$					
120 $I\bar{4}c2$				h_00l_0 A_2 B_2 c A_3	
121 $I\bar{4}2m$					
122 $I\bar{4}2d$		$hh0, \bar{h}h0$ A_2 B_2 d A_3	$00l: l = 4n + 2$ d A_3		$hhl_c: 2h + l_c = 4n + 2$ A_2 B_2 d A_3

2.5. ELECTRON DIFFRACTION AND ELECTRON MICROSCOPY IN STRUCTURE DETERMINATION

Table 2.5.3.9 (cont.)

 Point group $4/mmm$. The symbol a in the column $[h0l]$ is equivalent to the symbol b in the space groups of the first column.

Space group	Incident-beam direction					
	[100]	[001]	[110]	$[h0l]$	$[hhl]$	$[hk0]$
123 $P4/mmm$ $P4/m2/m2/m$						
124 $P4/mcc$ $P4/m2/c2/c$	$00l$ $c_{12} \quad A_3$		$00l$ $c_2 \quad A_3$	$h0l_0$ A_2 B_2 $c_1 \quad A_3$	hhl_0 A_2 B_2 $c_2 \quad A_3$	
125 $P4/nbm$ $P4/n2/b2/m$	$0k0$ $n \quad A_3$	$h00$ $a_2 \quad A_3$ $0k0$ b_1		h_00l A_2 B_2 $a \quad A_3$		$hk0:$ A_2 B_2 $h + k =$ A_3 $2n + 1$ n
126 $P4/nnc$ $P4/n2/n2/c$	$0k0$ $n_1 \quad A_3$ $00l$ n_{22}	$h00$ $n_{22} \quad A_3$ $0k0$ n_{21}	$00l$ $c \quad A_3$	$h0l:$ A_2 B_2 $h + l =$ A_3 $2n + 1$ n_2	hhl_0 A_2 B_2 $c \quad A_3$	$hk0:$ A_2 B_2 $h + k =$ A_3 $2n + 1$ n_1
127 $P4/mbm$ $P4/m2_1/b2/m$	$0k0$ $2_{12} \quad B_3$	$h00$ A_2 B_2 $a_2, 2_{11}$ A_3 B_3 $0k0$ $b_1, 2_{12}$		h_00l A_2 B_2 $a \quad A_3$ $0k0$ A_2 B_2 $2_1 \quad B_3$		
128 $P4/mnc$ $P4/m2_1/n2/c$	$00l$ A_3 n_2 $0k0$ B_3 2_{12}	$h00$ A_2 B_2 $n_2, 2_{11}$ A_3 B_3 $0k0$ $n_1, 2_{12}$	$00l$ A_3 c	$h0l:$ A_2 B_2 $h + l =$ A_3 $2n + 1$ n $0k0$ A_2 B_2 $2_1 \quad B_3$	hhl_0 A_2 B_2 $c \quad A_3$	
129 $P4/nmm$ $P4/n2_1/m2/m$	$0k0$ A_2 B_2 $n, 2_{12}$ A_3 B_3	$h00$ B_3 2_{11} $0k0$ 2_{12}		$0k0$ A_2 B_2 $2_1 \quad B_3$		$hk0:$ A_2 B_2 $h + k =$ A_3 $2n + 1$ n
130 $P4/ncc$ $P4/n2_1/c2/c$	$0k0$ A_2 B_2 $n, 2_{12}$ A_3 B_3 $00l$ A_3 c_{12}	$h00$ B_3 2_{11} $0k0$ 2_{12}	$00l$ A_3 c_2	$h0l_0$ A_2 B_2 $c_1 \quad A_3$ $0k0$ A_2 B_2 $2_1 \quad B_3$	hhl_0 A_2 B_2 $c_2 \quad A_3$	$hk0:$ A_2 B_2 $h + k =$ A_3 $2n + 1$ n
131 $P4_2/mmc$ $P4_2/m2/m2/c$			$00l$ A_3 c		hhl_0 A_2 B_2 $c \quad A_3$	
132 $P4_2/mcm$ $P4_2/m2/c2/m$	$00l$ A_3 c_2			$h0l_0$ A_2 B_2 $c \quad A_3$		
133 $P4_2/nbc$ $P4_2/n2/b2/c$	$0k0$ A_3 n	$h00$ A_3 a_2 $0k0$ b_1	$00l$ A_3 c	h_00l A_2 B_2 $a \quad A_3$	hhl_0 A_2 B_2 $c \quad A_3$	$hk0:$ A_2 B_2 $h + k =$ A_3 $2n + 1$ n
134 $P4_2/nnm$ $P4_2/n2/n2/m$	$0k0$ A_3 n_1 $00l$ n_{22}	$h00$ A_3 n_{22} $0k0$ n_{21}		$h0l:$ A_2 B_2 $h + l =$ A_3 $2n + 1$ n_2		$hk0:$ A_2 B_2 $h + k =$ A_3 $2n + 1$ n_1
135 $P4_2/mbc$ $P4_2/m2_1/b2/c$	$0k0$ B_3 2_{12}	$h00$ A_2 B_2 $a_2, 2_{11}$ A_3 B_3 $0k0$ $b_1, 2_{12}$	$00l$ A_3 c	h_00l A_2 B_2 $a \quad A_3$ $0k0$ A_2 B_2 $2_1 \quad B_3$	hhl_0 A_2 B_2 $c \quad A_3$	
136 $P4_2/mnm$ $P4_2/m2_1/n2/m$	$00l$ A_3 n_2 $0k0$ B_3 2_{12}	$h00$ A_2 B_2 $n_2, 2_{11}$ A_3 B_3 $0k0$ $n_1, 2_{12}$		$h0l:$ A_2 B_2 $h + l =$ A_3 $2n + 1$ n $0k0$ A_2 B_2 $2_1 \quad B_3$		
137 $P4_2/nmc$ $P4_2/n2_1/m2/c$	$0k0$ A_2 B_2 $n, 2_{12}$ A_3 B_3	$h00$ B_3 2_{11} $0k0$ 2_{12}	$00l$ A_3 c	$0k0$ A_2 B_2 $2_1 \quad B_3$	hhl_0 A_2 B_2 $c \quad A_3$	$hk0:$ A_2 B_2 $h + k =$ A_3 $2n + 1$ n
138 $P4_2/ncm$ $P4_2/n2_1/c2/m$	$0k0$ A_2 B_2 $n, 2_{12}$ A_3 B_3 $00l$ A_3 c_2	$h00$ B_3 2_{11} $0k0$ 2_{12}		$h0l_0$ A_2 B_2 $c \quad A_3$ $0k0$ A_2 B_2 $2_1 \quad B_3$		$hk0:$ A_2 B_2 $h + k =$ A_3 $2n + 1$ n
139 $I4/mmm$ $I4/m2/m2/m$						

2. RECIPROCAL SPACE IN CRYSTAL-STRUCTURE DETERMINATION

Table 2.5.3.9 (cont.)

Space group	Incident-beam direction					
	[100]	[001]	[110]	[h0l]	[hhl]	[hk0]
140 $I4/mcm$ $I4/m2/c2/m$				h_0l_0 A_2 B_2 c A_3		
141 $I4_1/amd$ $I4_1/a2/m2/d$		$hh0, \bar{h}h0$ d A_3	$00l$: $l =$ A_3 $4n + 2$ d $\bar{h}h0$ a		hhl_c : A_2 B_2 $2h + l_c =$ A_3 $4n + 2$ d	h_0k0 A_2 B_2 a A_3
142 $I4_1/acd$ $I4_1/a2/c2/d$		$hh0, \bar{h}h0$ d A_3	$00l$: $l =$ A_3 $4n + 2$ d $\bar{h}h0$ a	h_0l_0 A_2 B_2 c A_3	hhl_c : A_2 B_2 $2h + l_c =$ A_3 $4n + 2$ d	h_0k0 A_2 B_2 a A_3

Point groups $3, \bar{3}, 32, 3m, \bar{3}m$

Space group	Incident-beam direction	
	[11 $\bar{2}$ 0]	[1 $\bar{1}$ 00]
Nos. 143–155: no GM line		
156 $P3m1$		
157 $P31m$		
158 $P3c1$		$00l$ A_2 B_2 c A_3
159 $P31c$	$00l$ A_2 B_2 c A_3	
160 $R3m$		
161 $R3c$		$00l$: $l = 6n + 3$ A_2 B_2 c A_3
162 $P\bar{3}1m$		
163 $P\bar{3}1c$	$00l$ A_2 B_2 c A_3	
164 $P\bar{3}m1$		
165 $P\bar{3}c1$		$00l$ A_2 B_2 c A_3
166 $R\bar{3}m$		
167 $R\bar{3}c$		$00l$: $l = 6n + 3$ A_2 B_2 c A_3

Point groups $6, \bar{6}, 6/m, 622, 6mm, \bar{6}m2, 6/mmm$

Space group	Incident-beam direction	
	[11 $\bar{2}$ 0]	[1 $\bar{1}$ 00]
168 $P6$		
169 $P6_1$	$00l$ A_2 B_2 6_1 B_3	$00l$ A_2 B_2 6_1 B_3
170 $P6_5$	$00l$ A_2 B_2 6_5 B_3	$00l$ A_2 B_2 6_5 B_3
171 $P6_2$		
172 $P6_4$		
173 $P6_3$	$00l$ A_2 B_2 6_3 B_3	$00l$ A_2 B_2 6_3 B_3
174 $P\bar{6}$		
175 $P6/m$		
176 $P6_3/m$	$00l$ A_2 B_2 6_3 B_3	$00l$ A_2 B_2 6_3 B_3

2.5. ELECTRON DIFFRACTION AND ELECTRON MICROSCOPY IN STRUCTURE DETERMINATION

Table 2.5.3.9 (cont.)

Space group	Incident-beam direction					
	[11 $\bar{2}$ 0]			[1 $\bar{1}$ 00]		
177 <i>P622</i>						
178 <i>P6₁22</i>	00 <i>l</i> 6 ₁	<i>A</i> ₂	<i>B</i> ₂ <i>B</i> ₃	00 <i>l</i> 6 ₁	<i>A</i> ₂	<i>B</i> ₂ <i>B</i> ₃
179 <i>P6₅22</i>	00 <i>l</i> 6 ₅	<i>A</i> ₂	<i>B</i> ₂ <i>B</i> ₃	00 <i>l</i> 6 ₅	<i>A</i> ₂	<i>B</i> ₂ <i>B</i> ₃
180 <i>P6₂22</i>						
181 <i>P6₄22</i>						
182 <i>P6₃22</i>	00 <i>l</i> 6 ₃	<i>A</i> ₂	<i>B</i> ₂ <i>B</i> ₃	00 <i>l</i> 6 ₃	<i>A</i> ₂	<i>B</i> ₂ <i>B</i> ₃
183 <i>P6mm</i>						
184 <i>P6cc</i>	00 <i>l</i> c ₂	<i>A</i> ₃		00 <i>l</i> c ₁	<i>A</i> ₃	
185 <i>P6₃cm</i>	00 <i>l</i> 6 ₃		<i>B</i> ₃	00 <i>l</i> 6 ₃ , c	<i>A</i> ₂ <i>A</i> ₃	<i>B</i> ₂ <i>B</i> ₃
186 <i>P6₃mc</i>	00 <i>l</i> 6 ₃ , c	<i>A</i> ₂ <i>A</i> ₃	<i>B</i> ₂ <i>B</i> ₃	00 <i>l</i> 6 ₃		<i>B</i> ₃
187 <i>P$\bar{6}$m2</i>						
188 <i>P$\bar{6}$c2</i>				00 <i>l</i> c	<i>A</i> ₂ <i>A</i> ₃	<i>B</i> ₂
189 <i>P$\bar{6}$2m</i>						
190 <i>P$\bar{6}$2c</i>	00 <i>l</i> c	<i>A</i> ₂ <i>A</i> ₃	<i>B</i> ₂			
191 <i>P6/mmm</i>						
192 <i>P6/mcc</i>	00 <i>l</i> c ₂	<i>A</i> ₃		00 <i>l</i> c ₁	<i>A</i> ₃	
193 <i>P6₃/mcm</i>	00 <i>l</i> 6 ₃		<i>B</i> ₃	00 <i>l</i> 6 ₃ , c	<i>A</i> ₂ <i>A</i> ₃	<i>B</i> ₂ <i>B</i> ₃
194 <i>P6₃/mmc</i>	00 <i>l</i> 6 ₃ , c	<i>A</i> ₂ <i>A</i> ₃	<i>B</i> ₂ <i>B</i> ₃	00 <i>l</i> 6 ₃		<i>B</i> ₃

Point groups 23, *m*3

Space group	Incident-beam direction					
	[100] (cyclic)		[110] (cyclic)		[<i>h</i> k0] (cyclic)	
195 <i>P23</i>						
196 <i>F23</i>						
197 <i>I23</i>						
198 <i>P2₁3</i>	00 <i>l</i> 2 ₁₃ 0 <i>k</i> 0 2 ₁₂	<i>A</i> ₂	<i>B</i> ₂ <i>B</i> ₃	00 <i>l</i> 2 ₁₃	<i>A</i> ₂ <i>B</i> ₂ <i>B</i> ₃	00 <i>l</i> 2 ₁
199 <i>I2₁3</i>						
200 <i>Pm3</i> <i>P2/m3</i>						
201 <i>Pn3</i> <i>P2/n3</i>	00 <i>l</i> n ₂ 0 <i>k</i> 0 n ₃	<i>A</i> ₃				$\bar{k}h0$ n
202 <i>Fm3</i> <i>F2/m3</i>						
203 <i>Fd3</i> <i>F2/d3</i>	00 <i>l</i> : <i>l</i> = 4 <i>n</i> + 2 d ₂ 0 <i>k</i> 0: <i>k</i> = 4 <i>n</i> + 2 d ₃	<i>A</i> ₃				$\bar{k}h0$: <i>h</i> + <i>k</i> = 4 <i>n</i> + 2 d
204 <i>Im3</i> <i>I2/m3</i>						
205 <i>Pa3</i> <i>P2₁/a3</i>	00 <i>l</i> c ₂ , 2 ₁₃ 0 <i>k</i> 0 2 ₁₂	<i>A</i> ₂ <i>A</i> ₃	<i>B</i> ₂ <i>B</i> ₃	00 <i>l</i> 2 ₁₃	<i>A</i> ₂ <i>B</i> ₂ <i>B</i> ₃	00 <i>l</i> 2 ₁
206 <i>Ia3</i> <i>I2₁/a3</i>				$\bar{h}h0$ a ₃	<i>A</i> ₂ <i>A</i> ₃	<i>B</i> ₂ <i>B</i> ₃
						$\bar{k}h0$ a

2. RECIPROCAL SPACE IN CRYSTAL-STRUCTURE DETERMINATION

Table 2.5.3.9 (cont.)

Point group 432

Space group	Incident-beam direction		
	[hk0] (cyclic)		
207 $P432$			
208 $P4_232$			
209 $F432$			
210 $F4_132$			
211 $I432$			
212 $P4_332$	00l 4 ₃	A ₂	B ₂ B ₃
213 $P4_132$	00l 4 ₁	A ₂	B ₂ B ₃
214 $I4_132$			

 Point group $\bar{4}3m$

Space group	Incident-beam direction		
	[100] (cyclic)	[110] (cyclic)	[hhl] (cyclic)
215 $P\bar{4}3m$			
216 $F\bar{4}3m$			
217 $I\bar{4}3m$			
218 $P\bar{4}3n$		00l n A ₃	hhl _o n A ₂ B ₂ A ₃
219 $F\bar{4}3c$			h _o h _o l _o c A ₂ B ₂ A ₃
220 $I\bar{4}3d$	0kk, 0 \bar{k} k d A ₂ B ₂ A ₃	00l: l = 4n + 2 d A ₃	hhl _e : 2h + l _e = 4n + 2 d A ₂ B ₂ A ₃

Point group m3m

Space group	Incident-beam direction			
	[100] (cyclic)	[110] (cyclic)	[hk0] (cyclic)	[hhl] (cyclic)
221 $Pm\bar{3}m$ $P4/m\bar{3}2/m$				
222 $Pn\bar{3}n$ $P4/n\bar{3}2/n$	00l n ₁₂ 0k0 n ₁₃ A ₃	00l n ₂ A ₃	hk0: h + k = 2n + 1 n ₁ A ₂ B ₂ A ₃	hhl _o n ₂ A ₂ B ₂ A ₃
223 $Pm\bar{3}n$ $P4_2/m\bar{3}2/n$		00l n A ₃		hhl _o n A ₂ B ₂ A ₃
224 $Pn\bar{3}m$ $P4_2/n\bar{3}2/m$	00l n ₂ 0k0 n ₃ A ₃		hk0: h + k = 2n + 1 n A ₂ B ₂ A ₃	
225 $Fm\bar{3}m$ $F4/m\bar{3}2/m$				
226 $Fm\bar{3}c$ $F4/m\bar{3}2/c$				h _o h _o l _o c A ₂ B ₂ A ₃
227 $Fd\bar{3}m$ $F4_1/d\bar{3}2/m$	00l: l = 4n + 2 d ₂ 0k0: k = 4n + 2 d ₃ A ₃		h _e k _e 0: h _e + k _e = 4n + 2 d A ₂ B ₂ A ₃	
228 $Fd\bar{3}c$ $F4_1/d\bar{3}2/c$	00l: l = 4n + 2 d ₂ 0k0: k = 4n + 2 d ₃ A ₃		h _e k _e 0: h _e + k _e = 4n + 2 d A ₂ B ₂ A ₃	h _o h _o l _o c A ₂ B ₂ A ₃
229 $Im\bar{3}m$ $I4/m\bar{3}2/m$				
230 $Ia\bar{3}d$ $I4_1/a\bar{3}2/d$	0kk, 0 \bar{k} k d A ₃	00l: l = 4n + 2 d h \bar{h} 0 a ₃	h _o k _o 0 a A ₂ B ₂ A ₃	hhl _e : 2h + l _e = 4n + 2 d A ₂ B ₂ A ₃

2.5. ELECTRON DIFFRACTION AND ELECTRON MICROSCOPY IN STRUCTURE DETERMINATION

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) $P422$, $P4_22$
(13) $P4_212$, $P4_2212$	(14) $I4$, $I4_1$	(15) $I422$, $I4_122$
(16) $I23$, $I2_13$	(17) $I222$, $I2_1212_1$	(18) $P432$, $P4_232$
(19) ($P4_132$, $P4_332$)	(20) $I432$, $I4_132$	(21) $F432$, $F4_132$
(22) ($P4_122$, $P4_322$)	(23) ($P4_1212$, $P4_3212$)	

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.

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 diperic 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_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.

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) $P312$, ($P3_112$, $P3_212$)	[$\bar{1}\bar{1}01$]
(3) $P321$, ($P3_121$, $P3_221$)	[$\bar{1}\bar{1}\bar{2}3$]
(5) $P622$, ($P6_222$, $P6_422$)	[$\bar{1}\bar{1}\bar{2}3$]
(7) $P6_322$, ($P6_122$, $P6_522$)	[$\bar{1}\bar{1}\bar{2}3$]
(12) $P422$, $P4_222$	[321], [211], [112]*
(13) $P4_212$, $P4_2212$	[211]
(15) $I422$, $I4_122$	[111]
(16) $I23$, $I2_13$	[111]
(17) $I222$, $I2_1212_1$	[111]
(18) $P432$, $P4_232$	[321], [211]*
(20) $I432$, $I4_132$	[111]
(21) $F432$, $F4_132$	[432]