

2. RECIPROCAL SPACE IN CRYSTAL-STRUCTURE DETERMINATION

Table 2.5.3.5. Symmetries of hexagonal six-beam CBED patterns for diffraction groups

		Projection diffraction group											
		31 _R		3m1 _R					61 _R				
Diffraction group		3	31 _R	3m _R		3m		3m1 _R		6	6 _R	61 _R	
Two-dimensional symmetry		3	3	3		3m		3m		6	3	6	
Three-dimensional symmetry			m'	2'				m', (2')			i	m', (i)	
Zone-axis pattern	Bright-field pattern	3	6	3m		3m		6mm		6	3	6	
	Whole-field pattern	3	3	3		3m		3m		6	3	6	
Hexagonal six-beam pattern	O	1	1	1	m ₂	1	m _v	m ₂	m _v	1	1	1	
	G	1	1 _R	m ₂	1	1	m _v	1 _R	1 _R m _v (m ₂)	1	1	1 _R	
	F	1	1	m ₂	1	1	1	1	m ₂	1	1	1	
	S	1	1	1	m ₂	1	1	m ₂	1	1	1	1	
	FF'	1	3 _R	1	1	1	m _v	3 _R	3 _R m _v	1	1	3 _R	
	SS'	1	1	1	1	1	m _v	1	m _v	1	6 _R	6 _R	
A pair of symmetrical six-beam patterns 	±O	1	1 _R	m ₂	1	m _v	1	m _v 1 _R	1 _R m ₂	2	1	2(1 _R)	
	±G	1	1	1	m _R	m _v	1	m _v m _R	1	2	2 _R	21 _R	
	±F	1	1	1	1	m _v	1	m _v	1	1	6 _R	6 _R	
	±S	1	3 _R	1	1	m _v	1	3 _R m _v	3 _R	1	1	3 _R	
	F'F'	1	1	1	m _R	1	1	m _R	1	2	1	2	
	S'S'	1	1	m _R	1	1	1	1	m _R	2	1	2	
	Point group		23, 3	6̄	432, 32		4̄3m, 3m		6̄m2		6	m3, 3	6/m

		Projection diffraction group						
		6mm1 _R						
Diffraction group		6m _R m _R		6mm	6 _R mm _R	6mm1 _R		
Two-dimensional symmetry		6		6mm	3m	6mm		
Three-dimensional symmetry		2'			i, (2')	m', (i, 2')		
Zone-axis pattern	Bright-field pattern	6mm		6mm	3m	6mm		
	Whole-field pattern	6		6mm	3m	6mm		
Hexagonal six-beam pattern	O	m ₂		m _v	1	m _v (m ₂)	m _v (m ₂)	
	G	m ₂		m _v	m ₂	m _v	1 _R m _v (m ₂)	
	F	m ₂		1	m ₂	1	m ₂	
	S	m ₂		1	1	m ₂	m ₂	
	FF'	1		m _v	1	m _v	3 _R m _v	
	SS'	1		m _v	6 _R	6 _R m _v	6 _R m _v	
A pair of symmetrical six-beam patterns 	±O	2m ₂		2m _v	m _v (m ₂)	1	2(1 _R)m _v (m ₂)	
	±G	2m _R		2m _v	2 _R m _v	2 _R m _R	21 _R m _v (m _R)	
	±F	1		m _v	6 _R m _v	6 _R	6 _R m _v	
	±S	1		m _v	m _v	1	3 _R m _v	
	F'F'	2m _R		2	1	m _R	2m _R	
	S'S'	2m _R		2	m _R	1	2m _R	
	Point group		622		6mm	m3m, 3̄m		6/mmm

SMB pattern, and two-dimensional symmetry elements from a pair of SMB patterns, as shown in Tables 2.5.3.5, 2.5.3.6 and 2.5.3.7. Therefore, the use of a ZAP and SMB patterns is the most efficient way to find as many crystal symmetry elements in a specimen as possible.

2.5.3.3. Space-group determination

2.5.3.3.1. Lattice-type determination

When the point group of a specimen crystal is determined, the crystal axes may be found from a spot diffraction pattern recorded at a high-symmetry zone axis, using the orientations of the symmetry elements determined in the course of point-group determination. Integral-number indices are assigned to the spots of the diffraction patterns. The systematic absence of reflections indicates the lattice type of the crystal. It should be noted that

reflections forbidden by the lattice type are always absent, even if dynamical diffraction takes place. (This is true for all sample thicknesses and accelerating voltages.) By comparing the experimentally obtained absences and the extinction rules known for the lattice types [P, C (A, B), I, F and R], a lattice type may be identified for the crystal concerned.

2.5.3.3.2. Identification of screw axes and glide planes

There are three space-group symmetry elements of dipericodic plane figures: (1) a horizontal screw axis 2'₁, (2) a vertical glide plane g with a horizontal glide vector and (3) a horizontal glide plane g'. These are related to the point-group symmetry elements 2', m and m' of dipericodic plane figures, respectively. (It is noted that these symmetry elements and ten point-group symmetry elements form 80 space groups.)