

## Index

( $2 \times 2$ ) matrix notation 181, 277  
 2-, 3-, 4-, 6-fold rotation 88  
 4-index notation 79, 275  
 5-fold symmetry 56, 59

### **a**

A-centered lattices 29  
 achiral 158  
 achiral surface 160, 277  
 – bcc crystal 164  
 – fcc crystal 163  
 – hexagonal crystal 165  
 acute representation (hexagonal) 18, 40, 80, 273, 277  
 additivity theorem 146, 147, 149, 150, 277  
 adsorbate islands 192  
 adsorbate layer 191  
 – coverage 191  
 – overlayer warping 195  
 – partially disordered 192  
 – periodic overlayer 192  
 -- coincidence lattice 193  
 -- commensurate 192  
 -- incommensurate 196  
 -- rotational 197  
 Al<sub>65</sub>Cu<sub>20</sub>Fe<sub>15</sub> quasicrystal 58  
 alternative lattice description 10, 12, 24  
 anti-ferromagnetic ordering 22

### **b**

Bain path 32, 273  
 Balsac software 267  
 basis 8, 9, 273, 277  
 bcc 13, 273, *See* body centered cubic (bcc)  
 B-centered lattices 26  
 body centered cubic (bcc) lattice 13, 39, 48, 69, 75  
 body centered lattices 28

Bravais lattices (2-dimensional) 277  
 – centered rectangular 96, 98, 100, 107, 109, 117  
 – hexagonal 100, 101, 116  
 – oblique 115  
 – overview 117  
 – primitive rectangular 95, 97, 98, 107, 109, 123  
 – square 99, 116  
 Bravais lattices (3-dimensional) 35, 37, 273  
 – cubic-F 39, 70  
 – cubic-I 39, 70  
 – cubic-P 43, 70  
 – hexagonal-P 40, 70  
 – monoclinic-B 37, 70  
 – monoclinic-C 37  
 – monoclinic-P 37, 70  
 – orthorhombic-C 38, 70  
 – orthorhombic-F 38, 70  
 – orthorhombic-I 38, 70  
 – orthorhombic-P 38, 70  
 – overview 41  
 – tetragonal-I 39, 70  
 – tetragonal-P 38, 70  
 – triclinic-P 35, 70  
 – trigonal-R (rhombohedral) 41, 70  
 BrClFCH 156  
 Brillouin zone 273  
 bulk crystals 5  
 bulk truncation 139  
 BZ. *See* Brillouin zone

### **c**

Carbon nanotube 227  
 – armchair tube 228  
 – chiral pairs 229  
 – zigzag tube 228

- Cartesian coordinates 12  
 C-centered lattices 29  
 centered lattices 26  
 centered netplanes 81  
 centering 26, 273, 277  
 Cesium chloride 10, 49  
 chiral 158  
 – partner 159  
 – surface 156, 277  
 chirality 156, 274  
 classification scheme (crystals) 35  
 – overview 41  
 classification scheme (netplanes) 115, 121  
 – overview 134  
 coincidence (super)lattice 277  
 compatibility constraints (2-dimensional) 81,  
     87, 94, 98, 104  
 compatibility constraints (3-dimensional)  
     34  
 coverage 191  
 crystal 7, 9, 274  
 crystal decompositions 10  
 crystal parameters 265  
 crystal systems (2-dimensional) 115, 277  
 – hexagonal 116  
 – oblique 115  
 – overview 121  
 – rectangular 115  
 – square 116  
 crystal systems (3-dimensional) 35, 274  
 – cubic 39  
 – hexagonal 39  
 – monoclinic 37  
 – orthorhombic 37  
 – rhombohedral 41  
 – tetragonal 38  
 – triclinic 36  
 – trigonal 41  
 crystallographic plane 66  
 Crystmet 220  
 CsCl 10, 49, 163  
 CSD 220  
 ct lattice 274
- d**  
 DAS model 173, 174  
 density-functional theory 195  
 DFT. *See* density-functional theory  
 diamond 11  
 Diophantine equations 255  
 – linear 25, 72, 73, 146, 161, 251  
 – linear (in)homogeneous 252  
 – quadratic 46, 49, 51, 254  
 –  $m^2 + 2 n^2 = N^2$  258
- $m^2 + m n + n^2 = N^2$  257  
 –  $n_1^2 + n_2^2 + n_3^2 = N$  255  
 –  $n_1^2 + n_2^2 = N$  256  
 Domain formation. *See* surface domain
- e**  
 enantiomer 156  
 Euclid formula 256  
 Euclid's algorithm 250–253
- f**  
 face centered cubic (fcc) lattice 15, 39, 50, 69,  
     75  
 face centered lattices 29  
 facet 181–185  
 – angle 184  
 – edge vector 183  
 – negative 182  
 – positive 182  
 facetting 181  
 fcc. *See* face centered cubic (fcc)  
 F-centered lattices 29  
 ferromagnetic ordering 22  
 Fibonacci numbers 57  
 – definition 281  
 Fourier expansion 173
- g**  
 GaAs 63, 142  
 Gallium arsenite 63, 142  
 general lattice vector 65, 183, 229, 274  
 geometric constraints (lattices) 23  
 glossary, abbreviations 273–277  
 Golden mean. *See* Golden ratio  
 Golden ratio 55  
 Graphene 274  
 Graphite 61
- h**  
 handedness 25, 156, 274  
 hcp. *See* hexagonal close-packed (hcp) crystal  
 Hermann-Mauguin notation 35, 87, 121,  
     274  
 hex (hcp). *See* hexagonal close-packed (hcp)  
 hexagonal close-packed (hcp) crystal 18, 53,  
     136  
 hexagonal graphite 61  
 hexagonal lattice 18  
 hexagonal sublattice (rhombohedral) 20
- i**  
 i-AlCuFe 58  
 I-centered lattices 28  
 ICSD 220

intercept factors 77  
 international notation 35  
 International Tables of Crystallography 34  
 inversion symmetry 142, 158  
 IS 224  
 ITC 121, *See* International Tables of Crystallography  
 IUCr 55  
 IUPAC 182

***I***

label 8  
 lattice 274  
 – classification 33  
 – definition 7, 9  
 – lattice basis vectors 8, 67, 275  
 – lattice constant 7, 275  
 – lattice points 7  
 – lattice vectors 7, 275  
 – symmetrically appropriate vectors 74  
 – symmetry 33  
 lattice gas 191  
 LEED 59, 219  
 LEEDpat software 207, 267  
 linear algebra 261  
 – linear transformation 261  
 linear transformations (lattices) 23

***m***

MgO 67, 140, 153, 182  
 microfacet notation 151, 152  
 Miller indices 65, 275  
 – additivity theorem  
 -- kinked surface 149, 151  
 -- stepped surface 146, 147  
 – alternative definition 77  
 – cubic lattices 76  
 – decomposition 146, 154  
 – large 145  
 Miller-Bravais indices 77, 79, 275  
 Minkowski reduction 74, 243  
 – iterative algorithm 244  
 – mathematics 243  
 mirror plane 158  
 modulation function 173, 176, 178  
 Moiré pattern 176, 177, 197  
 monoatomic crystal 186  
 monolayer 65  
 – definition 66  
 morphological unit cell 8, 29, 67, 82, 275  
 motif 122, 275  
 multiple atom height  
 – kinks 152

– steps 145, 152  
 multiplicity 275

***n***

NaCl 52, 140, 163, 182  
 NAD 220  
 nanotube 225, 227  
 – basic definition 225  
 – chiral pairs 230  
 – complex nanotubes 233  
 – coordinate transformation 227  
 – rolling indices (m, n) 226  
 – rolling vector 226  
 – symmetry 229  
 – translational periodicity 231  
 neighbor shells 44, 275  
 – complete set 45  
 – evaluation 53  
 – shell center 45  
 – shell multiplicity 44, 45  
 -- accidental 46  
 -- symmetry related 46, 49, 51  
 -- total 46, 49, 51  
 – shell radius 44, 45  
 – shell range 45  
 – shell thickness 45  
 netplane 65, 274  
 – atom density 70  
 – definition 66  
 – directions 77  
 – distances 70  
 netplane symmetry 80  
 – centered rectangular 127  
 – classification 117  
 – hexagonal 130  
 – oblique 122  
 – primitive rectangular 123  
 – square 128  
 netplane-adapted  
 – lattice vectors 7, 13, 71, 275  
 – matrix 67  
 n-fold rotation 35, 275  
 non-primitive lattice vectors 8, 26  
 non-primitive unit cell 8  
 non-symmorphic space group 276  
 number theory 72, 250  
 – basic definitions 247  
 – composite function 249  
 – coprime 248  
 – greatest common divisor 73, 248, 250  
 – least common multiple 249  
 – modulo function 247  
 – nearest integer function 247  
 – truncation function 247

***o***

obtuse representation (hexagonal) 18, 40, 78, 276

***p***

PDB 220

PED 219, 224

Penrose tiling 55

periodicity cells 29

plane group 115

point symmetry group 113, 276,

- associativity 113

- highest 121

- inverse element 113

- list of groups 113

- product 113

- unit element 113

point symmetry operations (2-dimensional)

81

point symmetry operations (3-dimensional)

34

polyatomic crystal 153, 276

primitive lattice vectors 8

prototiles 55

Pythagorean equation 180, 256

Pythagorean triplets 256

***q***

quasicrystals 55, 56, 276

- icosahedral 57

- polygonal (dihedral) 58

quasiperiodic crystals. *See* quasicrystals

***r***

reciprocal lattice 68, 276

- Bravais lattices 69

- double reciprocal lattice 262

- lattice vectors 68

- orthogonality relations 68

reconstruction. *See* surface reconstruction

reconstruction matrix. *See* surface

- reconstruction

references, literature 269

relative coordinates 9, 276

repeated slab geometry 21

representation bulk crystals 9

rhombohedral graphite 61

rhombohedral lattice 18

***s***

sc. *See* simple cubic (sc)

sc notation. *See* simple cubic notation

Schönflies notation 34, 35, 87, 111, 121,

276

self-similarity 56

SEXAFS 219, 224

shell models 44

simple cubic (sc) lattice 13, 45, 50, 75

simple cubic notation 75, 76, 139, 276

single crystal 276

Sodium chloride 52, 140

space groups (2-dimensional) 121, 276

- non-symmorphic 115, 121

- simple 115

- symmorphic 115, 121

space groups (3-dimensional) 43, 276

SSD. *See* Surface Structure Database (SSD)

step notation 147, 148

structure 8

subterraces 149

supercell 21

superlattice 21, 171, 277

- methods 12

- rotational 177

surface

- achiral 160

- buckling 176

- bulk truncated 170

- chiral 156, 159

- ideal 139

- kinked 143

- microfaceted 184

- morphology 143

- orientation 139

- real 169

- reconstruction 170

- coincidence lattice 174

- commensurate 171

- disordered 170

- displacive 172

- high order commensurate 174

- incommensurate 177

- matrix 171, 174, 176

- scaled commensurate 174

- relaxation 169

- inwards 169

- outwards 169

- stepped 143

- termination 140

- terrace 144

- vicinal 144, 146, 149, 156

surface domain 205, 207

- anti-phase 213

- glide plane 212

- mirrored 208

- rotational 208

- translational 213

surface explorer 267

- surface structure  
 – Ag(1 1 0) + (2 × 1) – O 213  
 – Ag(1 1 1) + Xe hex disordered 175  
 – Al(1 1 1) + (1 × 1) – O 208  
 – Au(1 0 0) hex disordered 177  
 – Au(1 1 1) – ( $\sqrt{3} \times 22$ ) rect 175  
 – Co(1 0 -1 5) 166  
 – Cu(1 0 0) + ( $\sqrt{2} \times \sqrt{2}$ )R45° – Cl 200  
 – Cu(1 0 0) + c(2 × 2) – Cl 200  
 – Cu(1 1 1) + (1 × 1) – NH<sub>3</sub>(disordered) 191  
 – Cu(1 1 1) + (4 × 4) – C<sub>60</sub> 193  
 – fcc(11 13 19) 149  
 – fcc(15 15 23) 149  
 – fcc(3 3 1) 160  
 – fcc(3 3 5) 146  
 – fcc(37 25 17) 152  
 – fcc(5 6 8) 144  
 – fcc(6 1 1) 145  
 – fcc(7 1 1) facets 183  
 – fcc(7 7 9) 144  
 – fcc(*h k l*) crystal ball 186  
 – Fe(1 2 3) 164  
 – GaAs(1 1 1) 142  
 – GaAs(-1 -1 -1) 142  
 – MgO(1 1 1) facets 182  
 – MgO(15 11 9) 153  
 – NaCl(*h k l*) 140  
 – Ni(1 1 0) + c(2 × 2) – CN 208, 212  
 – Ni(1 1 0) + p2mg(2 × 1) – 2CO 193  
 – Ni(1 1 1) + (1 × 1)R3.5° – Ag 197  
 – Ni(*h k l*) 139  
 – Pd(1 1 0) – (2 × 1) missing row 171, 199  
 – Pt(1 1 1) + c(4 × 2) – 2CO 208  
 – Rh(1 1 0) + (1 × 3) – H 213  
 – Rh(1 1 0) + p2mg(2 × 1) – 2O 206  
 – Rh(1 1 1) + (13 × 13) – BN 195  
 – Ru(0 0 0 1) + (13 × 13) – C 196  
 – sc(0 0 1) – (1 × 1)R36.87° 178  
 – Si(1 0 0) – (2 × 1) symmetric dimer 173  
 – Si(1 0 0) – c(4 × 2) buckled dimer 173  
 – Si(1 1 1) – (7 × 7) DAS model 173  
 – SrTiO<sub>3</sub>(0 1 8) 153  
 – V<sub>2</sub>O<sub>3</sub>(0 0 0 1) 141  
 – V<sub>2</sub>O<sub>5</sub>(0 0 1) 141  
 – V<sub>2</sub>O<sub>5</sub>(0 1 0) 141  
 – W(1 0 0) – c(2 × 2) 171  
 – W(2 1 1) microfacetted 185  
 Surface Structure Database (SSD) 171, 200, 221, 267  
 – experimental methods 223  
 – statistical analysis 221  
 surface structure, experimental methods 219, 220
- surface symmetry 205  
 – allowed space groups 207  
 symmetry groups (2-dimensional) 111  
 symmetry operation (2-dimensional)  
 – glide reflection 81, 103  
 – conclusion 109  
 – identity 112  
 – inversion 81, 84  
 – conclusion 85  
 – mirroring (reflection) 81, 91, 111  
 – conclusion 102  
 – rotation 81, 86, 111  
 – conclusion 91  
 symmetry operation (3-dimensional)  
 – glide reflection 34  
 – inversion 34, 158  
 – mirroring (reflection) 34, 157  
 – rotation 34, 158  
 – rotoinversion 34  
 – rotoreflection 34  
 – rototranslation (screw operation) 34  
 symmorphic space group 277
- t**  
 table of contents, V  
 TiO<sub>2</sub> 63  
 Titanium dioxide 63  
 transformation matrix (supercell) 22  
 translation  
 – group 113  
 – operation 33  
 – symmetry 33  
 trigonal lattice 18
- u**  
 unit cell 8, 277  
 – origin 9  
 – primitive 8, 67
- v**  
 V<sub>2</sub>O<sub>3</sub> 140  
 V<sub>2</sub>O<sub>5</sub> 141  
 Vanadium pentoxide 141  
 Vanadium sesquioxide 140  
 vector calculus 261  
 – scalar product 261  
 – vector product 261  
 – volume product 261  
 Voronoi cells 31, 277
- w**  
 web sites 267  
 Wigner-Seitz cells (2-dimensional) 118, 277

- Wigner-Seitz cells (3-dimensional) 31, 277  
Wood notation 171, 199, 277  
– additional information 201  
– definition 200  
– examples 202, 239  
– mathematics 237  
– matrix transformation 201  
WSC. *See* Wigner-Seitz cells
- x**  
XSW 224
- y**  
 $\text{YBa}_2\text{Cu}_3\text{O}_7$  5, 10
- z**  
Zinc blende 63