

Index

- α - MoO_3 , 130, 491
- α -quartz, 312, 489
- A15 structure, 154, 156
- absorption correction, 241
- AgI, 411
- Al, 21, 407
- AlAs, 414
- $\text{Al}_2\text{Ca}_3(\text{SiO}_4)_3$, 499
- AlN, 414
- Al_2O_3 , 129, 497
- AlO(OH), boehmite, 501
- AlO(OH), diaspore, 500
- AlP, 411
- alkali metal, 345
 - hydrides, 177
- Allen, 315
- allotropes, 21
- Allred, 313
- Allred and Rochow, 315, 317
- aluminum oxyhydroxide, 500, 501
- aluminum sesquioxide, *see* Al_2O_3
- amorphous materials, 196
- anatase, 260, 511
- antibonding state, 370
- anti-fluorite, 312
- anti-structures, 451
- As, 10
- atomic form factor, 219
- atomic mass, 2
- atomic scattering factor, 235, 515–17
- atomic size, 3, 20, 455
- atomic term values, 532
- AuCd, 131
- AuCu_3 , 150
- Aurivillius phases, 64
- axial glide, 108
- axis–angle pair, 71, 74

- β -aluminas, 66
- β -AuCd, 510
- β -copper mercury tetraiodide, 506
- β - Cu_2HgI_4 , 201
- β - $\text{Li}_2\text{BeSiO}_4$, 184
- β - LiGaO_2 , 184
- $\beta\text{II-Li}_3\text{PO}_4$, 184
- $\beta\text{II-Li}_3\text{ZnSiO}_4$, 184
- B1 structure, 160
- B2 structure, 147, 148
- B3 structure, 171, 184
- B4 structure, 172
- B8, structure, 161
- B27 structure, 495
- B31 structure, 494
- BN, 411
- backscatter Kikuchi diffraction pattern, 247
- band gap, 11, 354, 357, 366, 374, 390, 396, 412, 414, 527, 528
- band structure, 352
 - diagram, 351
- basis, 31, 44, 45, 46
 - vectors, 42
- bcc alkali metals, 343
- BeO, 411
- BiF_3 , 151
- binding energy, 346
- bixbyite, 312, 503
- Bloch, 363
 - theorem, 377
- body centered cubic (bcc), 12
- boehmite, 199, 501
- Bohr radius, 329
- bond valence
 - method, 443
 - parameters, 445
- bonding state, 370
- Born–Haber cycle, 290, 292
- Born–Mayer–Huggins, 320
 - potential energy parameters, 320
- Born–von Karman boundary conditions, 332

INDEX

- Br, 10
 Bragg, 205
 condition, 212, 215, 352
 law, 206
 bra-ket notation, 330
 Brandon criterion, 80
 Bravais lattice, 28, 30, 31, 37, 38, 39, 44, 45,
 50, 56, 81, 92
 vector, 46
 Brillouin zone, 53, 338, *see also* first
 Brillouin zone
 brookite, 260
 Brown and Altermatt, 444
 bulk modulus, 272, 345
- C, 10, 21, 22, 407, 411, 414, 495, 506
 C1 structure, 173
 C4 structure, 163
 C6 structure, 164
 C14 structure, 179, 507
 C15 structure, 180
 C16 structure, 498
 C19 structure, 165
 C36 structure, 179
 C₆₀, 22, 191, 198
 CO₂, 11, 21
 CaF₂, 173
 CaTiO₃, 174
 CaWO₄, 129, 490
 carbon, *see* C
 cassiterite, 11
 cation eutaxy, 450
 ccp structure, 139
 CdCl₂ structure, 162, 165
 CdI₂ structure, 162, 164
 CdS, 414
 CdSe, 414
 CdTe, 414
 chalcogenides, 521–5
 chalcopyrite, 183, 200, 505
 charge transfer energy, 472
 chromium boride, 501
 clay minerals, 64
 close packed crystal structures, 20, 135, 136
 coefficients of location, 46
 cohesion, 42
 cohesive energy, 264, 271, 309, 326, 346,
 357, 366, 402, 410, 459, 460, 527
 coincident site lattice, 76, 78
 compressibility, 272, 300
 conventional cell, 41, 42
 conventional vectors, 43
 coordination number, 12, 14, 135, 136
 corundum, 312
 structure, 199, 497
 Coulomb
 law, 7
 potential, 294
 Coulombic bonding force, 294
 Coulombic energy, 339
 covalent bonding, 10, 17
 model for, 7
 covalent bonds, 5, 9, 23, 363
 covalent energy, 372, 406, 413
 covalent network, 7, 10
 covalently bonded
 networks, 8
 solids, 18
 Cr, 44
 Cr₂Al, 201, 505
 CrB, 131, 501
 CrCuS₂, 184
 crystal-field stabilization energy, 303, 305
 crystallographic point groups, 96
 crystallographic shear, 190
 CsCl, 44, 131, 148
 Cu, 140
 CuAl₂, 498
 Cu₃AsS₄, 184
 CuAu, 131, 148
 CuBr, 11, 411
 CuFeS₂, 183, 184, 505
 Cu₂HgI₄, 506
 Cu₂Mg, 180
 Cu₃SbS₄, 184
 cubic
 F lattice, 32, 33, 42, 43, 44, 53
 I lattice, 31, 33, 35, 43, 44, 53, 55
 P lattice, 31, 32, 40, 42, 45
 space groups, 487
 cyclic boundary conditions, 332
- D₀₃ structure, 147, 151
 D₀₉ structure, 496
 D₀₁₉ structure, 154, 155
 D₀₂₂ structure, 158

INDEX

- $D0_{24}$ structure, 154, 156
 $D5_1$ structure, 497
 $D5_3$ structure, 503
 d_{hkl} , 483
 d-spacing, 206, 244
 Debye–Scherrer technique, 244
 defects, 357
 defect-spinels, 169
 degeneracy, 334, 529
 degrees of freedom, 77
 density of levels, 334
 density of states, 396, 403
 diagonal glide, 108
 diamond, 10, 22, 44, 366, 495, 527
 glide, 108
 diaspore, 199, 500
 diffraction, 50, 59, 145, 182, 205
 dipolar bonding, 7, 278
 dipole moment, 267, 269
 direct lattice/reciprocal lattice relationship, 53
 directions in the unit cell, 46
 disorientation, 76
 dispersion, 350, 384, 388, 394, 429
 relationship, 348
 distinction
 between a lattice and a basis, 45
 between a lattice and a crystal structure,
 32, 44
 between proper and improper operations,
 92
 dry ice, 11
- $E1_1$ structure, 184
 $E2_1$ structure, 174
 elastic scattering, 209
 condition, 215
 electron
 affinities, 290, 292, 317
 backscattered diffraction, 248
 compounds, 425, 426
 diffraction, 247
 electronegativity, 3, 4, 17, 20, 278, 286, 292,
 312, 313, 314, 316, 317, 365, 367, 413,
 426, 455, 461, 526
 equalization, 456
 embedded atom method, 358
 energy density of states, 337
 energy level diagram, 347
- equal area projection, 69
 equilibrium separation, 269, 300
 equilibrium spacing, 344
 ErAl, 131
 Euler angles, 71, 72
 eutactic, 449
 arrangement, 145
 Ewald
 construction, 216
 method, 518
 exchange
 energy, 342
 interaction, 342
 expectation value, 329, 330, 370
 extinction correction, 241
- face centered cubic (fcc), 12
 family of directions, 46
 faujasite, 66
 Fermi
 energy, 335
 level, 396
 wave vector, 334, 335
 FeB, 131, 495
 $(\text{FeMn})_2\text{O}_3$, 503
 FeSi, 131
 FeTiO_3 , 498
 Finnis–Sinclair, 358
 first Brillouin zone, 53, 350, 355
 fluorides, 288
 fluorite, 82
 structure, 170, 172
 Fourier series, 207, 512
 free electron
 energy, 338
 model, 337
 theory, 326, 328, 331, 341, 348
 Friedel
 law, 246
 model, 402
 Froyen and Harrison, 382
- γ -LaOF, 200, 505
 γ' -MoC, 131
 γ -TiCu, 131
 Ga, 10
 GaAs, 11, 366, 411, 414
 GaN, 414

INDEX

- GaP, 414
 GaSb, 414
 Ga₂Zr, 201, 506
 gamma lanthanum oxyfluoride, *see* γ -LaOF
 garnet structure, 199, 499
 Ge, 2, 10, 11, 25, 366, 407, 411, 414
 GeO₂, 11, 21
 GeS, 131
 general positions, 102
 germanium, *see* Ge
 glass, 197
 glide, 88
 operator, 106
 Goodenough, 405
 grain boundary, 69, 76
 graphite, 22, 64, 132, 506
 grossularite, 499
- H₂ structure, 184
 H₂_a structure, 184
 H-bonding, 280
 H₂S, 279
 Hägg, 179
 halides, 521–5
 Hamiltonian, 331
 hcp, *see* hexagonal close packed
 heat of formation, 433
 of binary alloys, 434
 Heusler alloy, 151
 hexagonal
 close packed (hcp), 12, 138
 groups, 116
 lattice, 36
 space groups, 486
 tungsten bronze structure, 496
 HgS, 131
 HI, structure, 166
 homologous temperature, 13, 26
 homopolar energy, 472
 HTB structure, 496
 Hume-Rothery rules, 425
 Hund's rules, 529
 hybrid bond orbital model, 408
 hybridization, 18
 hydrogen bonds, 7, 279
- ilmenite, 498
 improper operators, 95
- InAs, 414
 InGaAs₂, 183, 184
 InN, 414
 InP, 414
 InSb, 411, 414
 incommensurate structures, 192
 indices for planes, 47
 inert gases, 265, 275, 297
 insulators, 355
 intensity, 212, 232
 intercalation, 190
 reactions, 64
 intergrowth tungsten bronzes, 64
 interstitial compounds, 177
 interstitial positions, 140
 inverse-spinels, 165, 168
 inversion, 88, 91, 97
 ionic bonding, 10
 model, 286, 306
 ionic bonds, 5, 9, 20, 289
 model for, 6, 14
 ionic compounds, 25
 ionic pair potential, 294
 ionic radii, 310, 521–5
 ionic size, 20
 ionicity, 26, 472
 fraction, 5, 11, 26, 27
 ionization
 energies, 290, 291, 346
 potential, 317
 iron titanate, 498
- Jackson and Catlow, 518
 JCPDS-ICDD file, 245
- KAlF₄, 507
 KGe, 131
 K₂MgF₄, 508
k-space, 333, 349
 Kapustinskii's equation, 320
 Kepler conjecture, 136
 Ketelaar's triangle, 8, 26
 khatyrkite, 498
 kinetic energy operator, 331
- L1₀ structure, 147, 148, 184
 L1₁ structure, 184
 L1₂ structure, 147, 150

INDEX

- $L2_1$ structure, 147, 151
 La_2CuO_4 , 63, 121, 124, 125
 $LaOF$, 505
 lattice
 constants, 141
 energy, 286, 287, 300, 307
 Laue back-reflection, 242
 Laves phases, 179, 181
 layered compounds, 263
 LCAO, 363, 367, 376, 529
 model, 411
 Lennard-Jones
 energy, 300
 model, 268, 281, 357
 parameters, 296
 potential, 294
 $LiAs$, 131
 $LiFeO_2$, 200, 501
 $LiGaO_2$, 183, 495
 linear combination of atomic orbitals, *see*
 LCAO
 linear elasticity theory, 425
 liquid crystalline structures, 195
 lithium
 ferrite, *see* $LiFeO_2$
 metagallate, *see* $LiGaO_2$
 long range interactions, 273
 Lorentz-polarization factor, 236

 Madelung constant, 298, 317, 322, 518
 Magnéli phases, 190
 magnetism, 23
 magnetoplumbites, 66
 manganese phosphide, 494
 Martynov–Batsanov electronegativity, 467
 matrix elements, 370
 maximum volume principle, 449
 melting point, 264, 357, 366
 melting temperature, 11, 326
 Mendeleev, 2
 law of periods, 425
 numbers, 433
 metal–nonmetal, 326
 boundary, 9, 10, 20
 metallic bond, 9
 metallic bonding, 12
 model, 6
 metallic energy, 406, 413

 metallicity, 2, 20, 26, 406, 407
 metals, 4, 6, 25, 355, 406
 metric tensor, 57, 480
 Mg , 21, 140
 $MgNi_2$, 179
 MgO , 302
 Mg_2SiO_4 , 169
 $MgZn_2$, 179, 507
 microstructure, 69
 Miedema's model for alloy formation,
 429
 Miller indices, 47, 52, 71, 74, 84
 Millerite structure, 492
 misorientation, 70, 75
 axis–angle pair, 71
 MnP , 131, 494
 $MoCl_5$, 128
 Mo_2Cl_{10} , 129
 Mo_8O_{23} , 191
 $Mo_{18}O_{52}$, 191
 molecular covalent solid, 10
 molecular materials, 279, 280
 molecular solids, 7, 8, 190, 280
 molybdate bronzes, 66
 molybdenum trioxide, *see* α - MoO_3
 molybdate, *see* α - MoO_3
 monoclinic
 A lattice, 36
 C lattice, 36
 groups, 111
 lattice, 37
 P lattice, 36
 space groups, 485
 Mooser–Pearson plot, 461
 Mott–Littleton, 318
 Mulliken, 315
 multiplicity factor, 237

 Na - β -alumina, 188
 Na - β' -alumina, 446
 $NaCl$, 131, 160, 301
 structure, 198
 $NaPb$, 131
 $NaTl$, 131
 $NaVS_2$, 184
 $Na_{0.1}WO_3$, 496
 $Na_{0.8}WO_3$, 189, 240
 Na_xWO_3 , 405

INDEX

- nearest neighbour, 40, 84
 distances, 287
- nearly free electron theory, 352
- neutron diffraction, 250
- NiAl, 25
- NiAs, 83, 131, 161
 structure, 159, 161, 198
- NiO, 318, 404
- NiS, 130, 492
- Ni₃Sn, 155
- Ni₃Ti, 155
- nickel arsenide, *see* NiAs
- nickel sulfide, 492
- nonmetals, 4, 406
- non-primitive cell, 41, 42
- O'Keeffe and Brese, 444
- O'Keeffe and Hyde, 452
- olivine structure, 162, 169
- operator, 329
- orbital angular momentum, 529
- orbital hybridization, 17, 19
- orbital overlap, 383
- orientation, 71
 imaging microscopy, 249
 matrix, 73, 74
- orthorhombic, 35
 A lattice, 36
 B lattice, 36
 C lattice, 36
 F lattice, 36
 groups, 113
 I lattice, 36
 P lattice, 35
 space groups, 485
- oxide bronzes, 189
- oxides, 289, 312
- P_{black}, 21
- PH₃, 279
- P_{white}, 21
- packing fraction, 12, 13, 26, 135, 136
- palladous sulfide, 491
- Pantelides, 395
- partial charge, 456
- Pauli exclusion principle, 267, 331, 334, 342
- Pauling, 3, 5, 17, 60
- Pauling electronegativities, 526
- Pauling's empirical crystal radii, 478
- Pauling's rules, 440
- Pb, 10, 25, 407
- PdS, 129, 491
- Penrose tiling, 193, 194
- periodic boundary conditions, 378
- periodic chart, 4
- periodic trends, 2, 3, 4, 5, 312
- perovskite, 235
 structure, 170, 174
- Phillips ionicity, 471
- point group nomenclature, 95
- point symmetry groups, 92
- polar compounds, 528
- polar covalent bond, 372, 453
- polar energy, 374, 406, 413
- polarity, 376, 388, 412, 461
- polarization, 306, 312
- polyacetylene, 25
- polyethylene, 18
- polyhedral models, 60, 62
- polymeric solids, 7
- polymeric structures, 312
- polymorphic, 13
- polymorphs, 21
- polytypic disorder, 186
- polytypism, 23
- powder diffraction, 243
- preferred orientation, 240
- primitive cell, 41
- primitive lattice vectors, 31, 42, 43
- principal quantum number, 529
- promotion energy, 408
- pseudopotential model, 344
- pyrochlore, 502
- quartz, 11
- quasicrystals, 192
- radius ratio, 14, 15, 17, 20, 26, 288, 310, 312
 rules, 287
- Rb_{0.33}WO₃, 496
- ReO₃, 496
 structure, 188
- Read and Shockley, 80
- reciprocal lattice, 50, 52, 55, 208, 227
 vector, 51, 57, 333, 349
- reduced zone scheme, 350

INDEX

- reflection, 88, 90
 Rh_2O_3 , 130, 492
 rhodium sesquioxide, 492
 rhombohedral lattice, 37
 Rietveld method, 245
 rigid band assumption, 428
 rock salt, 44, 312
 structure, 48, 159, 160, 390, 397, 404
 Rodrigues–Frank space, 76
 rotation, 88, 89, 93
 roto-inversion, 88, 91
 Ruddlesdon–Popper phases, 63
 rule of parsimony, 442
 rutile, 11, 312
 structure, 162, 163, 199

 6–12 potential, 276
 model, 268
 Sanderson, 453
 sapphire, 497
 scanning electron microscope, 247
 scattering factor, 230
 Schechtman, 193
 scheelite, 129
 structure, 175, 176, 490
 Scherrer formula, 213
 Schrödinger wave equation, 331
 screw, 88
 operator, 105
 Se, 10
 semiconductors, 411, 414
 Shannon, 311
 shear phases, 190
 shell model, 318
 Si, 10, 21, 363, 366, 407, 411, 414
 SiC, 23, 187
 SiC(3C), 414
 SiH_4 , 279
 SiO_2 , 11, 21, 129, 196, 489
 SiO_4 , 19
 silicon, *see* Si
 silicon carbide, *see* SiC
 simple metals, 345
 single crystal X-ray diffraction, 246
 Slater, 315
 Slater and Koster, 393
 Sn, 25, 407, 411, 366
 SnO_2 , 11, 21

 solubility, 425
 space group, 105, 108, 485–7
 symbols, 109
 special positions, 100
 sphalerite, 527
 structure, 170, 171, 184, 398
 spinel structure, 162, 166
 $\text{Sr}_3\text{Ti}_2\text{O}_7$, 64
 $\text{Sr}_4\text{Ti}_3\text{O}_{10}$, 64
 $\text{Sr}_{n+1}\text{Ti}_n\text{O}_{3n+1}$, 63
 stereographic projection, 66, 68
 steric factors, 265, 287
 structure
 factor, 218, 231, 234
 type, 143
 Structurebericht names, 143, 144
 superconducting oxides, 24
 superconductivity, 23
 superlattice structures, 145, 182, 183, 192
 symmetry
 elements, 88
 operator, 88
 systematic absences, 52, 222, 227

 temperature factor, 236
 tetragonal
 close packed arrangement, 497
 groups, 114
 I lattice, 34
 P lattice, 34
 space groups, 486
 tungsten bronze structure, 496
 tetrahedral covalent radii, 365
 texture, 240
 TiAl_2 , 508
 TiAl_3 , 84, 158
 TiAs, 131
 Ti_2CS , 199, 499
 TiO_2 , 11, 21, 23, 163, 504, 511
 $\text{Ti}_n\text{O}_{2n-1}$, 190
 tin, *see* Sn
 tilt boundary, 77
 titanium carbosulfide, 499
 transformation matrix, 71
 transition metal, 401
 carbides, 178
 nitrides, 178
 translation, 88, 89, 92

INDEX

- transmission electron microscopy, 249
 triclinic
 groups, 110
 lattice, 36
 space groups, 485
 tridymite, 129, 489
 trigonal
 groups, 116
 lattice, 36
 space groups, 486
 TTB structure, 496
 twist boundary, 77

 univalent radii, 479

 V_2MoO_8 , 191
 V_2O_5 , 131, 191, 493
 $VOMoO_4$, 125, 126, 127
 vacancy, 169
 van der Waals bonds, 7, 23, 263, 302
 vanadate bronzes, 66
 vanadium pentoxide, *see* V_2O_5
 Villars, 465
 method, 435

 W, 140
 WC, 131
 W_3O , 156

 W_nO_{3n-2} , 190
 wave
 function, 329, 368
 vector, 50
 Wigner–Seitz cell, 42, 44, 53
 wurtzite, 170, 172, 184, 451, 527
 Wyckoff letter, 120

 X-ray scattering, 206

 $YBaCuFeO_5$, 131, 493
 $YBa_2Cu_3O_7$, 23, 131, 494
 $Y_3Fe_5O_{12}$, 23

 zeolites, 66
 zero-point energy, 303
 zinc blende structure, 171
 zircon, 509
 zirconia, 11
 Zn, 10
 ZnO, 172, 184, 414
 ZnS, 131, 184, 414
 ZnSe, 11, 366, 411, 414
 ZnTe, 414
 zone, 58
 axis, 58
 ZrO_2 , 11, 21
 $ZrSiO_4$, 509