

Index

a

absorption spectroscopy 62, 327, 694, 696, 778, 789, 805, 931
 – ultraviolet–visible (UV–vis) 343–348
 – X-ray absorption 358, 360
 acoustic phonons 777
 adatom 670, 750–754, 828, 851, 853, 857, 861, 862
 – and rest atom model 847–849
 adsorbate-induced reconstruction 493, 550.
 See also adsorbate-induced relaxation
 adsorbate-induced relaxation
 – surface relaxation change 550–551
 – surface restructuring 551
 – – reconstruction creation 551–552
 – – reconstruction lifting and reconstruction switch 552–555
 adsorbate states 660–661
 adsorption 9–10
 agreement factor 406
 American Vacuum Society (AVS) 243
 angle-resolved photoemission spectroscopy (ARPES) 63, 152, 186, 208, 605, 607, 627, 631
 – for band mapping and Fermi surface mapping on surfaces 190–199
 anisotropy 55–57
 – magnetic, and magnetization distribution 724–726
 – – dipolar/shape anisotropy and magnetocrystalline anisotropy 726–729
 – – magnetization distribution imaging and magnetic domains at surfaces 734–737
 – – magnetization distribution, magnetic domains, and domain walls at surfaces 732–733

– – thin films and surface magnetic determination and experimental determination 730–732
 – Néel-type 728
 – uniaxial 710, 724
 annealing 89
 antiphase domains 517
 antisymmetry, of wave function 21
 asymmetric dimer model (ADM) 45–46
 asymmetric environment 4, 6
 atomic basis 502
 atomic force microscopy, (AFM). *See* scanning force microscopy (SFM)
 attempt frequency 746
 Auger electron spectroscopy 177–179
 Auger electron spectroscopy (AES) 154, 215–217. *See also* National Institute of Standards and Technology (NIST), US and AES and XPS
 Auger yield 361
 average t-matrix approximation (ATA) 135
 Azimuthal angle scan 156, 165, 168, 284, 285, 405, 420, 562
 – recoils and 291–295
 – using shadow cone 290–291

b

backscattering correction factors (BCFs) 247–248
 bake-out procedure 81
 ballistic electron emission microscopy (BEEM) 436
 band gap 819
 band narrowing 61
 band structures and Bloch functions 561–565
 basis sets and electron–ion interactions 25–26

- Bessel function 112
- Bethe–Salpeter (BS) equation 643
- bias enhanced nucleation (BEN) 900
- biomolecules, at metal surfaces 334–343
- Bloch's theorem 24
- Bloch equations, optical 265 266
- Bloch law 721
- Bloch walls 733, 734
- blocking 300
- body-centered cubic 14–15
- Boltzmann equation 219
- bond-breaking reconstructions 490, 527, 534, 536–543
- bond counting picture 823, 825, 827
- bond-creating reconstructions 490, 534, 536–543
- Born–Oppenheimer approximation 18, 21
- boundary value analysis method 320
- Bragg component 414, 416, 418, 421
- Bragg condition 109
- Bragg peaks 109, 187
- Bravais lattice 14, 497, 498, 499–500
 - real space and 105
- Bravais–Miller indices 495
- bridge bond 45, 857
- Brillouin light scattering 716
- bulk phonon dispersion 790
- bulk states 648–649
- bulk X-ray crystallography 376–378, 410
- c**
- calcite 463–464
- Cartesian components 104
- characteristic frequencies. *See* group frequencies
- charge-coupled devices (CCDs) 345
- charge density wave (CDW) 624, 629, 630
- chemically disordered metallic compounds 528–530
- chemically ordered metallic compounds 527–528
- chemical ordering 492
- chemical reconstruction 492
- chemical shift 169–171
- chemical superstructure 492
- chemical tensor LEED 134–135
- chemical vapor deposition (CVD) 893, 897, 898, 899, 901, 902, 906
- closed-loop refrigerators 90
- cohesive energies 15–16
- coincidence lattice 116, 518–519
- cold-cathode gauges 86
- commensurate superlattice. *See* coincidence lattice
- Common Data Processing System 243
- complex molecule adsorption, at surfaces 330–331
- complex molecules, RAS of 355–357
- compound semiconductors 530–532
- compression pumps. *See* gas transfer pumps
- condensed phase DFT calculations 24–26
- conductance 78, 79
- conduction band minimum (CBM) 906
- confined electron spectroscopy 668
- Connes advantage 323
- constant-current mode 428
- constant-height mode 428, 450
- contact potential difference (CPD) 452
- conversion electron Mössbauer spectroscopy – CEMS 698–699, 704, 713
- coordination-number-bond-strength relationship 55
- correlation energy, of system 619
- Coulomb repulsion 683
- covalent bonding 17
 - and semiconductors 33–35
- cryogenic pumps 84
- cryosorption pump 83, 84
- cryostats 90
- crystal, schematic 3
- crystalline solids 13–15
 - bonding and
 - – elemental covalent solid cohesive properties 35–37
 - – metal cohesive properties 31–33
 - – metals 26–27
 - – semiconductors and covalent bonding 33–35
 - – simple metals and jellium 28–29
 - – transition metals and tight binding 29–31
 - bond types 16–18
 - cohesive energies 15–16
 - density functional theory (DFT)
 - – approximations for exchange and correlation 21–24
 - – condensed phase calculations 24–26
 - – theoretical framework 18–21
 - surface electronic structure 57, 67
 - – jellium surfaces 57–61
 - – surface states 63–65
 - – transition metal surfaces 61–63
 - surface energies 66
 - – anisotropy 55–57
 - – cohesive energies and 53–55
 - – experimental considerations 49–52
 - – theoretical considerations 52–53
 - surface structure 37–39, 66

- – surface reconstruction 40–49
- – surface relaxation 39–40
- crystallographic directions 495
- crystallographic two-dimensional point groups 500–502
- crystal truncation rods 379–382
- Curie temperature 681, 717, 723

d

- dangling bonds 5, 6, 44, 89, 534, 823, 837, 851
- Debye model 792
- Debye–Waller factor 112, 388
- delocalization, of electrons 26
- density functional theory (DFT)
 - approximations for exchange and correlation 21–24
 - condensed phase calculations 24–26
 - local density approximation (LDA) and 568–570
 - theoretical framework 18–21
- density matrix formalism 265
- density of states (DOS) 27, 433, 683, 684, 685, 700, 705, 711
- depth distribution function (DDF) 218–222
- detuning. *See* frequency shift
- Dewar–Chatt–Duncanson (DCD) model 331
- diamond surfaces 15
 - low index surface atomic and electronic structure 902
 - – diamond (100) surface 902–909
 - – diamond (110) surface 914–916
 - – diamond (111) surface 909–914
 - – hydrocarbon contaminants and surface core level shifts 916–917
 - reconstructions and surface states 917–918
 - from negative to positive electron affinity 918–927
 - preparation 901–902
 - properties 889–896
 - synthesis from gas phase 897–901
 - yield spectroscopy 927–936
- differential cross sections (DCSs) 239
- diffraction rods 379, 381, 387, 388, 389–392, 394, 396, 422
- dimer-adatom-stacking (DAS) 437, 758
- dimerisation 827, 829, 831, 832, 833–834, 837–844, 846, 853, 858, 859, 866, 869
- dipolar/shape anisotropy and magnetocrystalline anisotropy 726–729
- dipolar coupling 327
- dipole–dipole interaction 683
- dipole scattering 783

- dipole selection rules 158
- Dirac–Hartree–Fock (DHF) 239
- disordered magnetic moments 718
- displacive reconstruction 490
 - at constant layer density 41
- double diffraction spots 129
- double scattering 283, 284–286
- double toroidal analyzer 277
- down atom 837
- dynamical scattering 114–115
 - of atom 119–123

e

- effective attenuation length (EAL) 222, 223, 224, 233–238
- effective negative electron affinity 919
- elastic-backscattering probability 226
- elastic electron scattering 218–221, 222, 223, 224, 230, 231, 232, 234–235, 239, 240, 247
- elastic interband scattering 658–659
- elastic intraband scattering 659–660
- elastic-peak electron spectroscopy (EPES) experiments 226, 227, 228
- elastic scattering 105
- electric dipole 59
- electrochemical scanning tunneling microscope (ECSTM) 431, 443, 444
- electron attenuation 93
- electron capture spectroscopy (ECS) 693
- electron–defect interaction 653–655, 672–673
- electron–defect scattering 638
- electron-density difference map 410
- electron dynamics, at surfaces 637–640
 - electron–defect interaction 672–673
 - electron–electron interaction
 - – image-potential states 671
 - – Shockley surface states 670–671
 - electron–phonon interaction 671–672
- energy-resolved measurements
 - – photoemission lineshape analysis 663–667
 - – scanning tunneling spectroscopy 667–668
- spatially-resolved measurements 668–669
 - – scattering patterns at steps 669–670
 - – scattering patterns in adatom arrays 670
- theoretical description 641
 - – electron–defect interaction 653–655
 - – electron–electron interaction 641–649
 - – electron–phonon interaction 649–652

- electron dynamics, at surfaces (*contd.*)
 - time-resolved measurements
 - – adsorbate states 660–661
 - – hot electrons lifetimes 662–663
 - – image-potential states 655–660
 - – semiconductor surface states 661–662
 - – Shockley surface states 655
 - electron dynamics, of colloidal systems 347
 - Electron Effective-Attenuation-Length
 - Database 220, 235
 - Electron Elastic-Scattering Cross-Section
 - Database (SRD 64) 220, 239
 - electron–electron Coulomb repulsion 21
 - electron–electron interaction
 - bulk states 648–649
 - electron self-energy 646–647
 - GW method 642–643
 - GW + T method 643
 - homogeneous electron gas 647
 - image-potential states 671
 - screened interaction 643–646
 - Shockley surface states 670–671
 - surface states 647–648
 - electron–electron scattering 637–638
 - electron energy loss spectroscopy (EELS)
 - 753, 754
 - electron gas model (EGM) 648
 - electronic band structure 564
 - electronic structures, surface-specific 8
 - Electron Inelastic-Mean-Free-Path Database
 - 227
 - electron–nuclei interaction 20
 - electron–phonon coupling 666–667
 - electron–phonon interaction 649–652, 671–672
 - electron–phonon scattering 638
 - electron–phonon system 200
 - electron scattering 783. *See also* low-energy
 - electron diffraction (LEED)
 - electron self-energy 646–647
 - electron spectroscopy for chemical analysis (ESCA) 152
 - electron transfer 638
 - electron transport 220, 239, 248
 - elemental covalent solid cohesive properties
 - 35–37
 - elemental metals
 - multilayer relaxation 520–524
 - registry shifts 524–525
 - elemental semiconductor surfaces
 - 525–527, 815–816
 - bulk properties
 - – bulk electronic properties 818–823
 - – covalent bonding and crystal lattice 816–818
 - stepped surfaces 863–864
 - – Si(001) surface 864–873
 - surface phonons 873–877
 - surface photovoltage 883–884
 - surface states and band bending 879–883
 - surface structure
 - – basic considerations 823, 825–828
 - – Jahn–Teller instability 828–831
 - – Si(001) surface structure 831–844
 - – Si(001)-(2×1) surface electronic structure 857–859
 - – Si(111) and Ge(111) surface structure 844–855
 - – Si(111)-(2×1) surface electronic structure 859–860
 - – Si(111)-(7×7) surface electronic structure 860–863
 - work function 878
 - Eliashberg function 650, 651
 - empirical DFT functionals 22
 - energy band 563
 - energy-resolved spectroscopy 256–258
 - equation of state (EOS) 15–16
 - ethylene adsorption, low-temperature
 - 331–334
 - evanescent waves 127
 - even modes 811
 - Ewald-sphere construction
 - – for normal incidence of primary beam 106
 - – for two different electron energies 105
 - Ewald summation 457
 - exchange-correlational functional
 - 21–24
 - exchange splitting 718
 - extended X-ray adsorption fine structure (EXAFS) 357–358, 360, 361
 - external potential 20
 - extreme high vacuum (XHV) conditions 73
- f**
- Fabry–Perot resonator 444
 - face-centered cubic (fcc) 15
 - facilitated dewetting 467
 - Fermi’s golden rule 156, 359
 - Fermi energy 572
 - Fermi level pinning 881
 - ferromagnetic resonance (FMR) 715
 - ferromagnets 681, 684
 - Fick’s law of diffusion 748
 - field effect transistors (FETs) 893

field emission microscope (FEM) 748
 field ion microscope (FIM) 749
 first Brillouin zone 563
 first principles theory 55
 flotation 10
 flow cryostats 430
 fluorescence yield 361
 force–distance curve 446
 force theorem 729
 forward focusing 180
 Fourier filtering 375
 Fourier-transform (FT) IR spectrometers 322
 fractional coordinates 377
 fractional-order rods. *See* superstructure rods
 Franck–Condon principle 174, 175
 – envelope function and 176
 free-electron final-state approximation 192
 Frenkel–Kontorova model 759
 frequency shift 450
 Friedel oscillations 565–568, 748
 – consequences of 570–582
 Friedel's rule 378
 frozen orbital state 157
 Fuchs–Kliwer phonon 801
 full-potential linearized augmented
 plane-wave (FP-LAPW) method 26, 687,
 700

g

gas capture pumps 83
 gas exposure 76–78
 gas transfer pumps 83
 gauge 85–86
 GAUSSIAN software package 313
 generalized gradient approximation (GGA)
 23, 31, 33, 36, 52
 geometrical tensor LEED 131–133
 geometric reconstruction, of clean surfaces
 532
 – bond-breaking and bond-creating
 reconstruction
 – – compound surfaces 542–543
 – – elemental surfaces 536–542
 – elemental surface displacive reconstruction
 532–536
 Gibbs surface free energy (G^s) 49
 glide symmetry 502, 503, 504
 grazing incident X-ray scattering (GIXS)
 754
 ground-state electronic wave function 20
 group frequencies 313
 GW + T method 643
 GW method 641, 642–643

h

Hamiltonian 18, 19, 20
 Hankel function 120
 hard X-ray photoemission spectroscopy
 (HAXPES) 186
 Hartree energy 21
 Hartree–Fock approximation (HFA) 620
 Heisenberg model 681, 718
 helium atom scattering (HAS) 749, 754,
 778, 784–788
 Hellmann–Feynman theorem 580, 581
 hemispherical energy analyzer 277
 herring bone reconstruction 42
 herringbone reconstruction 438, 534
 Hertz–Knudsen formula 77
 heterogeneous catalysis 10
 hexagonal close packed (hcp) 15
 hex phases 42
 highly oriented pyrolytic graphite (HOPG)
 89
 high pressure high temperature (HPHT)
 897
 high-resolution electron energy-loss
 spectroscopy (HREELS) 175, 756, 778,
 779–784, 807
 high-resolution low-energy electron
 diffraction (HRLEED) 750
 hindered rotations 316
 hindered translations 316
 Hohenberg–Kohn theorem 20
 Hooke's law 447
 hot-cathode gauges 86
 hot electrons lifetimes 662–663
 hot filament chemical vapor deposition
 (HFCVD) 898
 hybrid functionals 23–24
 hybridization 34
 – energy 34
 hybridized orbitals 816
 hydrocarbon adsorption, at metal surfaces
 331
 hydrogen bonding 17
 H₂-dissociation 615–616

i

ideal gas 74, 75–76
 ideal surface 823
 image charge 253, 254
 image-potential states 253–256, 590–592,
 655–657, 671
 – elastic interband scattering 658–659
 – elastic intraband scattering 659–660
 – momentum dependence of lifetimes
 657–658

- impact collision ion scattering spectrometry 287
 - impact-collision ion scattering spectroscopy (ICISS) 755
 - impact scattering 783
 - importance, of surfaces and interfaces 9–12
 - incommensurate superlattice 116, 519–520
 - indirect exchange coupling 682
 - inelastic electron scattering 217, 222, 223, 224, 225, 226, 237, 243
 - inelastic electron tunneling spectroscopy (IETS) 435–436, 440, 789
 - inelastic mean free path (IMFP) 219, 221, 222, 223, 224–228
 - information depth 222, 229–233
 - infrared absorption spectroscopy (IRAS) 778, 789
 - inner potential 108
 - inner work function 572
 - instrumental transfer width 114
 - interface diffraction 386–389
 - interferometry 322–323
 - internal conversion 698
 - International Union of Crystallography (IUC) 14
 - intralayer (multiple) scattering 124, 125
 - intrinsic diffusion 746
 - inverse photoelectron spectroscopy (IPES) 753
 - ionic bonding 17
 - ionization gauges 86
 - ion pump 84
 - ion scattering spectrometry (ICISS) 282
 - ion scattering spectroscopy (ISS) 269
 - composition and structure
 - – concentration 272–275
 - – element identification 270–272
 - – structure 275–276
 - equipment 276–278
 - low-energy ion scattering
 - – compositional analysis 278–283
 - – structure analysis 283–297
 - macroscopic damage 308
 - medium-energy ion scattering (MEIS) 297–298
 - – compositional analysis 298
 - – surface crystal structure, reconstruction, and relaxation 300–304
 - – thin layer analysis 298–300
 - radiation damage and sputtering 306–308
 - secondary electron emission 304–306
 - ion-sensitive FETs (ISFETs) 893
 - Ising model 709, 723
- j**
- Jahn–Teller instability 828–831
 - jellium model 28–29, 57–61, 565
- k**
- Kelvin method 578
 - Kelvin probe force microscopy (KPFM) 451, 452, 453, 459
 - Kerr rotation 731
 - kinematic approximation, spot intensities in 106–114
 - kinetic energy 75, 76, 77, 91
 - Kirchhoff's laws 79
 - Knudsen cell 90
 - Kohn anomaly 797
 - Kohn–Sham equations 21, 25
 - Koopman's theorem 157
 - Kronig–Penney model 203
- l**
- lateral manipulation 436
 - layer doubling (LD) method 95, 127
 - linear chain 626, 790, 830
 - surface modes 774–778
 - vibrations of 773–774
 - linear magnetic dichroism in angular distribution (MLDAD) 691, 693, 702
 - linear response theory (LRT) 622
 - liquid interface composition 281–283
 - local-band theory 718
 - local density approximation 568
 - local-density approximation (LDA) 22–23, 31, 36, 52, 56, 59, 568–570, 687
 - local density of states (LDOS) 433, 434, 435, 570, 707, 708, 737
 - localized surface modes 875
 - localized surface plasmon resonance (LSPR) 346
 - low-energy electron diffraction (LEED) 40, 41, 43, 329, 375–376, 489, 526, 579, 627, 753, 782, 786, 831, 834, 836
 - basic experimental equipment 96–98
 - historical development 93–96
 - intensity measurement 98–100
 - multiple scattering and dynamical intensities 118–119
 - – dynamical diffraction and LEED pattern 129–130
 - – dynamical diffraction of atomic layer 123–125
 - – dynamical diffraction of full surface 125–129

- dynamical scattering of atom 119–123
- pattern and intensity
- coherent electron beam and periodic surface 101–106
- finite coherence and nonideal sample 114–115
- kinematic approximation and spot intensities 106–114
- superlattices and domains 115–117
- practical limitations 145–146
- direct methods 146–148
- structure determination 136
- accuracy, precision, and elemental sensitivity 141–145
- reliability factor 137–139
- structural search 139–140
- surface sensitivity 100–101
- tensor 130–131
- chemical tensor LEED 134–135
- geometrical tensor LEED 131–133
- thermal tensor LEED 135
- low-energy electron microscope (LEEM) 94
- low-energy ion scattering (LEIS) 269, 275, 306, 749
- compositional analysis 278–283
- structure analysis 283–284
- application of structure and composition techniques to $\text{Cu}_3\text{Pt}(111)$ 295–297
- Azimuthal angle scan of recoils 291–295
- Azimuthal angle scan using shadow cone 290–291
- double scattering 284–286
- polar angle scan using shadow cone 286–290
- low-temperature scanning tunneling microscopes (LT-STMs) 430, 435, 439, 440
- m**
- magnetic dichroism in angular distribution (MDAD) 691
- magnetic excitations 714
- spin waves 714–717
- thermally excited spin waves at surfaces 717–718
- thermally excited spin waves in ultrathin ferromagnetic films 721–724
- magnetic hyperfine field at surfaces, experimental methods probing 697–700
- magnetic moment 19, 679, 680, 681–685, 718
- Fe surfaces 700–704
- Fe ultrathin films 709–715
- surfaces and ultrathin films 685–688
- magnetization distribution
- imaging and magnetic domains at surfaces 734–737
- magnetic domains, and domain walls at surfaces 732–733
- magnetization-induced second-harmonic generation (MSHG) 688
- magnetocrystalline anisotropy energy (MAE) 727, 729
- magnetocrystalline volume anisotropy 728, 729
- magneto-optical Kerr effect (MOKE) method 730, 731
- MARVIN computer code 457
- mass transfer 746
- matrix notation 516
- mean escape depth (MED) 222, 229–233
- mean free path length 76
- medium-energy ion scattering (MEIS) 269, 275, 297–298, 755, 763, 764
- compositional analysis 298
- electrostatic analyzer 277
- surface crystal structure, reconstruction, and relaxation 300–304
- thin layer analysis 298–300
- meta-generalized gradient approximation 23, 31, 36
- metal cohesive properties and bonding 31–33
- metallic bonding 17, 26–27
- metallic compounds
- chemically disordered 528–530
- chemically ordered 527–528
- metallic substrates 629–632
- metal surfaces, electronic structure of 561
- band structures and Bloch functions 561–565
- density functional theory (DFT) and local density approximation (LDA) 568–570
- dimensionality reduction and electron correlation 618–619
- electron interaction and correlation 619–620
- model systems on surfaces 626–632
- screening, plasmons, and quasi-particles 620–626
- Friedel oscillations 565–568
- consequences of 570–582
- periodic potential 582–583
- image-potential surface states 590–592

- metal surfaces, electronic structure of (*contd.*)
 - nearly-free electron approximation 583–585
 - projector–operator technique 601–604
 - Shockley surface states 587–589
 - Tamm surface states 596–601
 - three-dimensional case 592–595
 - wave function matching and phase-accumulation model 585–586
- surface states
 - experimental observation of 605–609
 - influence on metal surfaces 612–618
 - modification 609–612
- metal-surface selection rule 319
- microfacet notation 509–510
- microwave chemical vapor deposition (MWCVD) 898
- Miller–Bravais indices 495
- Miller indices 495
- mirror lines 498
- mirror symmetry 499
- missing row reconstruction of fcc (110) surfaces 43
- model systems, on surfaces 626–632
- mode softening 797
- modified Pandey model 540
- molecular flow conditions 76
- molecular pumps 84
- Moliere potential 273
- Monte Carlo simulations 765
- Mott polarimeter 205
- muffin-tin constant 123
- muffin-tin potential 123
- multiple diffraction spots 129
- multiple electron capture spectroscopy (MECS) 693
- multiple scattering and dynamical intensities 118–119
 - dynamical diffraction and LEED pattern 129–130
 - dynamical diffraction of atomic layer 123–125
 - dynamical diffraction of full surface 125–129
 - dynamical scattering of atom 119–123
- multiplex (Fellgett) advantage 323
- n**
- nanobiosensors 345–346
- nanosized materials 10–11, 11
- nanotribology 449
- National Institute of Standards and Technology (NIST), US and AES and XPS 218
 - additional data and software 241, 243
 - Database, for Simulation of Electron Spectra for Surface Analysis (SESSA) (SRD 100), 237, 239, 241
 - database, relevant to AES and XPS surface sensitivity
 - depth distribution function (DDF) 218–222
 - effective attenuation length 233–238
 - inelastic mean free path 224–228
 - mean escape depth and information depth 229–233
 - parameters defining surface sensitivity 222–223
 - Electron Effective-Attenuation-Length Database 220, 235
 - Electron Elastic-Scattering Cross-Section Database (SRD 64) 220, 239
 - Electron Inelastic-Mean-Free-Path Database 227
 - selected relevant standards from ASTM International 244
 - selected standards and technical reports from International Organization for Standardization 245–246
 - standards 243–247
 - X-Ray Photoelectron Spectroscopy Database (SRD 20) 238–239
- near-edge X-ray absorption fine structures (NEXAFS) 357–358, 905, 906, 907, 908
 - examples, in surface structure determination 363–369
 - instrumentation 361–363
 - theoretical considerations 358–361
- nearly-free electron (NFE) approximation 583–585
- Néel temperature 681
- Néel-type anisotropy 728
- Néel walls 733
- negative electron affinity (NEA) 893, 918, 919, 928
- negative ion resonance, scattering via 784
- neutral projectile impact collision ion scattering spectrometry 282–283
- noncontact atomic force microscopy (NC-AFM) 449–451, 454, 456–457, 458, 459, 460, 462, 463, 464, 465, 467, 470, 472, 473
- non-empirical DFT functionals 22
- noninteracting reference system 20
- normal-incidence X-ray standing wave (NIXSW) method 187–189

o

one-dimensional potential 255
 optical phonons 777
 optical potential 108
 optical spectroscopies 350
 optical theorem 122
 order of commensurability 516
 oscillatory relaxations 580–581

p

Patterson function 410, 411
 Pauli's principle 681, 682, 683
 Pauli correlation 22
 peculiarities, of surfaces 1–9
 Peierls instability 797
 Penn gap 893
 perfect nesting 623
 periodic crystals 14
 periodicity and simulation cells 24–25
 periodic potential 582–583
 – image-potential surface states 590–592
 – nearly-free electron approximation 583–585
 – projector–operator technique 601–604
 – Shockley surface states 587–589
 – Tamm surface states 596–601
 – three-dimensional case 592–595
 – wave function matching and phase-accumulation model 585–586
 perpendicular magnetic anisotropy (PMA) 727
 perpendicular magnetization 732
 phase boundaries 1
 phase shifts, temperature-corrected 122
 phonon–polariton coupling 798–802
 phonons at covalently bonded surfaces 802–811
 photodiodes 345
 photoelastic modulator (PEM) 350
 photoelectron microscopy (PEEM) 749
 photoelectron spectroscopy and diffraction 151
 – Auger electron spectroscopy 177–179
 – instrumentation
 – – electron energy analyzers 162–165
 – – light sources, including synchrotron radiation 161–162
 – – sample environment 165–166
 – from photoelectric effect to 151–152
 – photoemission matrix element 155–161
 – photoemission spectrum 152–155
 – photoexcitation by X-ray standing waves (XSW) 187–189
 – ultraviolet photoelectron spectroscopy (UPS)/angle-resolved photoemission spectroscopy (ARPES)
 – – ARPES for band mapping and Fermi surface mapping on surfaces 190–199
 – – extrinsic contributions to line shapes and widths 202–204
 – – spectral functions and many-body effects 199–202
 – – spin polarimetry 205–207
 – – spin-polarized photoelectron spectroscopy 204–205
 – – spin structure measurement in reciprocal space 207–210
 – – work function measurement 189–190
 – valence band XPS and resonant photoemission 186–187
 – X-ray electron spectroscopy 166
 – – core-level spectra, chemical shifts, and satellites 169–177
 – – quantifying elemental concentrations and surface cleanliness 166–169
 – X-ray photoelectron diffraction/Auger electron diffraction 179–186
 photoemission electron microscopes (PEEM) 164
 photoemission lineshape analysis 663–665
 – defects influence 665–666
 – electron–phonon coupling 666–667
 photoemission matrix element 155–161
 photoemission microspectroscopy 164
 photoemission of adsorbed xenon (PAX) method 579
 photoemission spectroscopy (PES) 690, 705, 907
 photoexcitation, by X-ray standing waves (XSW) 187–189
 photomultipliers 345
 photon-based methods
 – near-edge X-ray absorption fine structures (NEXAFS) 357–369
 – reflection–absorption infrared spectroscopy (RAIRS) 311–343
 – reflection anisotropy spectroscopy 348–357
 – ultraviolet–visible (UV–vis) absorption spectroscopy 343–348
 physisorption 613–614
 π -bonded chain model 47–48
 Pirani gauges 85
 plane groups 502–505
 point symmetry 498

positive electron affinity (PEA) 919
 projected bulk band structure (PBS) 592
 projector-augmented wave (PAW) potential 26
 projector-operator technique 601–604
 pseudopotential (PP) 26
 pumping 78–80
 – equation 80
 – speed 78
 – systems 81, 83–85
 pure dephasing 653, 654

q

quadrupol mass spectrometers 87
 quantitative surface analysis. *See* National Institute of Standards and Technology (NIST), US and AES and XPS
 quantum defect 256
 quantum well states (QWS) 729
 quartz microbalance 90
 QUASES software 243
 quasi crystals 14
 quasi-elastic approximation 650
 quasi-particle peak 201
 quasi-particles (QPs) 605, 618, 625, 628, 638, 640, 642

r

radial wave functions 158, 159
 radiation 151, 152, 155, 156, 157, 161, 178, 186, 190
 – damage and sputtering 306–308
 – synchrotron 161, 171, 187, 194, 361, 375, 421, 422
 random-phase approximation (RPA) 621
 rational directions. *See* crystallographic directions
 Rayleigh phonon 790, 791–796, 803
 Rayleigh surface mode 652
 Rayleigh wave 873
 real gas 74
 reciprocal lattice 104, 105, 106, 108, 109
 – vectors 103
 reciprocal unit-cell vectors 104
 reflection-absorption infrared spectroscopy (RAIRS) 311
 – adsorbed species on metal surfaces and 325–343
 – adsorbed species vibrations 314–316
 – current status and future 343
 – experimental considerations 320–325
 – IR spectroscopy basic principles 311–314
 – metal surfaces and 316–320

reflection anisotropy spectroscopy (RAS) 348–350
 – instrumentation 350–352
 – spectra interpretation 352–357
 reflectivity 380, 396
 – specular 396–400
 renormalized forward scattering (RFS) 95, 127
 residual gas analyzer (RGA) 87
 resonant photoemission 187
 rest atom 848, 849, 851, 861, 862
 – adatom model and 847–849
 retarding field analyzer (RFA) 97
 roasting 89
 root-mean-square (RMS) uncertainty 225
 rotary vane pumps 83
 rotational symmetry 499
 roughening pumps 83
 roughening temperature 756, 761–762, 762
 roughening transition 745, 756, 760, 761, 762, 864, 869
 rough gauge 85
 row pairing 463
 Rutherford backscattering spectrometry (RBS) 269

s

sagittal plane 873
 satellites, vibrational 174
 scanning electron microscopy (SEM) 749
 scanning electron microscopy with polarization analysis (SEMPA) 734
 scanning force microscopy (SFM) 427
 – basic principles and apparatus 444–453
 – capabilities 458–459
 – case studies 460–472
 – theory 454–458
 scanning probe microscopes (SPMs) 427
 scanning probe techniques 427. *See also* scanning force microscopy; scanning tunneling microscopy
 – outlook 472–473
 scanning tunneling microscopy (STM) 139, 427, 569, 640, 747, 749, 750, 751, 810, 822, 834, 835, 861, 862
 – basic principles and apparatus 428–431
 – capabilities 435–437
 – case studies 437–444
 – theory 431–434
 scanning tunneling spectroscopy (STS) 434, 580, 627, 640, 667, 707
 – confined electron spectroscopy 668
 – flat surface spectroscopy 667
 scattering asymmetry 205

- scattering matrix 121
- scattering vector 102
- Schrödinger equation 19, 21, 64, 118, 119, 122, 123, 255, 431–432, 565, 569, 583, 585, 597
- screening length 273
- scroll pump 83
- secondary electron coefficient 306
- secondary electron emission 304–306
- semiconducting substrates 629
- semiconductor surface states 661–662
- sensitivity factor 280
- shadow cone 275–276
 - Azimuthal angle scan using 290–291
 - polar angle scan using 286–290
- shear horizontal modes 791
- Sherman function 206, 207, 209
- Shockley-inverted gaps 588, 589
- Shockley states 64, 254, 255, 256, 587–589, 614, 655, 670–671, 705
- Si(001)-(2×1) surface electronic structure 857–859
- Si(001) surface structure 831–833
 - asymmetric (2×1) reconstruction 837–838
 - asymmetric p(2×2) reconstruction 838–839
 - asymmetric c(4×2) reconstruction 839
 - bulk terminated (1×1) 833
 - low-temperature excitation 840–841
 - order–disorder phase transition $c(4 \times 2) \leftrightarrow (2 \times 1)$ 839–840
 - surface stress anisotropy 841, 843–844
 - symmetric (2×1) reconstruction 833–837
- Si(100)-(2×1) 807–811
- Si(111)-(1×1)-H 803–807
- Si(111)-(2×1) surface electronic structure 859–860
- Si(111)-(7×7) surface electronic structure 860–863
- Si(111) and Ge(111) surface structure 844–846
 - Ge(111)-c(2×8) structure 849–850
 - Si(111)-(7×7) structure 850–855
 - (2×1) π -bonded chain structure 846–847
 - (2×2) adatom–rest atom model 847–849
- silicon nanotubes (SiNTs) 347
- Simulation of Electron Spectra for Surface Analysis (SESSA) (SRD 100) 237, 239, 241
- single crystalline surfaces 88
- single dangling bond (SDB) surface 844
- sliding 442
- Smoluchowski effect 524, 575–577
- Smoluchowski smoothing, of surface electron density 39
- snap-to-contact (jump to contact) 446–447
- sp³-hybrid functions 34
- space-charge effects 264
- Spicer's model of photoelectron emission 929
- spin polarimetry 205–207
- spin polarization in field emission spectroscopy (SP-FES) 705
- spin polarization photoemission spectroscopic analysis (SP-PES) 691, 692, 702
- spin-polarized (SP)-2PPE 706
- spin-polarized electron energy loss spectroscopy (SPEELS) 716, 717
- spin-polarized inverse photoelectron spectroscopy (SP-IPES) 691, 692, 702
- spin-polarized low energy electron diffraction (SP-LEED) 689, 690, 702
- spin-polarized photoelectron spectroscopy 204–205
- spin-polarized scanning tunneling microscopy (SP-STM) 710, 734, 735, 736
- spin-polarized STS (SP-STs) 707, 735, 736
- spin-polarized surface electronic states 704–709
- spin reorientation transition (SRT) 726, 728
- spin structure measurement in reciprocal space 207–210
- spin waves 714–717
 - thermally excited, at surfaces 717–718
 - thermally excited, in ultrathin ferromagnetic films 721–724
- split-position method 128
- spot photometer 98
- spot-profile-analysis LEED (SPA-LEED) method 94
- sputtering 89
- step modulation 595
- stepped and kinked surfaces 505–514
- sticking coefficient 77
- Stoner gap 714
- Stoner model 718
- Stoner parameter 684
- stopping power 763
- structure factor 377–378
- sudden approximation 157
- supercell approach, to model surfaces 25
- superlattices 490
 - coincidence 518–519
 - domains and 115–117
 - incommensurate 116, 519–520
 - simple 515–518

- superparamagnetic limit 710
- superstructure 490, 516
 - rods 384
- surface alloys 542
- Surface Analysis Society of Japan 243
- Surface Chemical Analysis Technical Working Area (SCATWA) 246–247
- surface composition 6
- surface conductivity (SC) 890, 893, 908, 926, 935
- surface core level shifts (SCLS) 62–63, 170–173
- surface coverage 77
- surface crystal field effect 197
- surface crystallography 489–493
 - adsorbate-induced relaxation and reconstruction 550
 - – surface relaxation change 550–551
 - – surface restructuring 551–555
 - clean compound surfaces, chemical reconstruction of 543
 - – compound semiconductors 545–550
 - – ordered alloys 544–545
 - – random alloys 543–544
 - clean surfaces, geometric reconstruction of 532
 - – bond-breaking and bond-creating reconstruction of compound surfaces 542–543
 - – bond-breaking and bond-creating reconstruction of elemental surfaces 536–542
 - – elemental surface displacive reconstruction 532–536
 - layer relaxation in clean and unreconstructed surfaces
 - – compound semiconductors 530–532
 - – elemental semiconductors 525–527
 - – metallic compounds 527–530
 - – multilayer relaxation 520–524
 - – registry shifts 524–525
 - two-dimensional lattices and structures
 - – Bravais lattices 497, 498, 499–500
 - – crystallographic 2D point groups 500–502
 - – plane groups 502–505
 - – rotational and mirror symmetry 499
 - – stepped and kinked surfaces 505–514
 - – superlattices 514–520
 - – surface orientation 494–496
 - – from 2D to 3D crystallography 496–497
- surface density of states (SDOS) 433, 434
- surface diffraction 382–385
- surface diffusion 746–750
- surface dipole 59, 570–571
- surface electronic structure 57, 67
 - Jellium surfaces 57–61
 - surface states 63–65
 - transition metal surfaces 61–63
- surface energies 66
 - anisotropy 55–57
 - cohesive energies and 53–55
 - experimental considerations 49–52
 - theoretical considerations 52–53
- surface-enhanced Raman spectroscopy (SERS) 789
- surface free energy 4, 9
- surface layer atomic density changes 41–43
- surface magnetism 679–681
 - experimental methods probing magnetic hyperfine field at surfaces 697–700
 - experimental methods probing magnetization at surfaces 688–693
 - experimental methods probing X-ray magnetic circular dichroism (XMCD) in absorption 693–697
 - low dimensions 681–685
 - – magnetic moment at surfaces and in ultrathin films 685–688
 - magnetic anisotropy and magnetization distribution 724–726
 - – dipolar/shape anisotropy and magnetocrystalline anisotropy 726–729
 - – magnetization distribution imaging and magnetic domains at surfaces 734–737
 - – magnetization distribution, magnetic domains, and domain walls at surfaces 732–733
 - – thin films and surface magnetic determination and experimental determination 730–732
 - magnetic excitations 714
 - – spin waves 714–717
 - – thermally excited spin waves at surfaces 717–718
 - – thermally excited spin waves in ultrathin ferromagnetic films 721–724
 - magnetic moments at Fe surfaces 700–704
 - magnetic moments in Fe ultrathin films 709–715
 - spin-polarized surface electronic states 704–709
- surface melting 762–767
- surface morphologies 345, 346, 352–353, 355

- surface phonon 873–877
 - anharmonicity and 754–757
 - dispersion 789
 - – Rayleigh phonon 791–796
 - from single 2D layers to finite slabs 789–791
 - – surface Brillouin zones 791
 - studies
 - phonon–polariton coupling 798–802
 - phonons at covalently bonded surfaces 802–811
 - – reconstruction and relaxation 796–798
- surface phonon–polariton. *See* Fuchs–Kliwer phonon
- surface photovoltage 883–884
- surface plasmon resonance (SPR) absorption 347
- surface reconstruction 7, 39, 40, 490, 532
 - elemental metals 41–43
 - elemental semiconductors 43–49
- surface relaxation 6, 7, 39–40
- surface resonance 875
- surface rippling 491
- surface roughening 760–762
- surface roughness 385–386
- surface science approach 73–74
 - sample preparation
 - – clean surface preparation 87–89
 - – controlled adsorption and deposition 89–90
 - surface analytical methods 90–92
 - vacuum physical background 74
 - – gas exposure 76–78
 - – ideal gas 75–76
 - – pumping 78–80
 - vacuum technology technical background
 - – pressure measurements 85–87
 - – pumping systems 81, 83–85
 - – ultrahigh vacuum materials 80–81
- surface segregation 492
- surface-state mediated interactions 616–618
- surface states 258, 259, 261, 349, 350, 565, 637–640, 647–648, 655, 661–662, 670–671, 704–705, 707, 748, 833, 837, 856, 857, 904–907, 911, 913, 917–918, 927
 - band bending and 879–883
 - experimental observation of 605–609
 - influence on metal surfaces 612–618
 - modification 609–612
- surface stress 581–582
- surface structure
 - basic considerations 823, 825–828
 - Jahn–Teller instability 828–831
 - Si(001) surface structure 831–844
 - Si(001)-(2×1) surface electronic structure 857–859
 - Si(111) and Ge(111) surface structure 844–855
 - Si(111)-(2×1) surface electronic structure 859–860
 - Si(111)-(7×7) surface electronic structure 860–863
- surface topography 427
- surface vibrations 773, 788–789
 - experimental techniques 778–779
 - – helium atom scattering (HAS) 784–788
 - – high-resolution electron energy loss spectroscopy (HREELS) 779–784
- phonons, in one dimension
 - – surface modes of linear chain 774–778
 - – vibrations of linear chain 773–774
- surface phonon dispersion 789
- – Rayleigh phonon 791–796
- from single 2D layers to finite slabs 789–791
 - – surface Brillouin zones 791
- surface phonon studies
 - – phonon–polariton coupling 798–802
 - – phonons at covalently bonded surfaces 802–811
 - – reconstruction and relaxation 796–798
- surface X-ray diffraction (SXRD) 375–376
 - bulk X-ray crystallography 376–378
 - crystal shape function and diffraction rods 389–392
 - crystal truncation rods 379–382
 - data analysis
 - – averaging 404–406
 - – Fourier methods 409–411
 - – model calculations 408–409
 - – obtaining of accurate data 407
 - interface diffraction 386–389
 - line shapes
 - – antiphase domains 417–419
 - – correlation function 411–413
 - – multidomain system integrated intensity 419–421
 - – two-level roughness model 413–417
 - reflection and refraction
 - – specular reflectivity 396–400
 - – structure factor effects 401–404
 - – transmitted beam 400–401
 - single layer 378–379
 - structure factor measurement

surface X-ray diffraction (SXRD) (*contd.*)
 – – correction factors 393–395
 – – experimental geometries 392–393
 – – stationary geometry 396
 – surface diffraction 382–385
 – surface roughness 385–386
 – trends 421–423
 symmetric dimer model (SDM) 45
 synchrotron radiation 161, 171, 187, 194,
 361, 375, 421, 422
 systematic extinctions 129

t

Tamm states 64, 596–601
 tensor LEED 130–131
 – chemical tensor 134–135
 – geometrical tensor 131–133
 – thermal tensor 135
 terrace modulation 595
 Tersoff–Hamann model 434
 thermal conductivity 892
 thermal desorption spectroscopy (TDS)
 751
 thermal dynamics, at surfaces 743–745
 – surface diffusion 746–750
 – surface melting 762–767
 – surface phonons and anharmonicity
 754–757
 – surface roughening 760–762
 – thermal surface reconstructions
 757–760
 – two-dimensional adatom and vacancy gas
 750–754
 thermal surface reconstructions 757–760
 thermal tensor LEED 135
 thermocouple 90
 thin films and surface magnetic
 determination and experimental
 determination 730–732
 throughput (Jacquinot) advantage 322–323
 titanium sublimation pumps 85
 topography mode 450
 total symmetry 502
 transfer doping mechanism 893
 transition metals
 – surfaces 61–63
 – tight binding and 29–31
 transition state theory (TST) 746
 transmission electron microscopy (TEM)
 541, 758
 transmitted beam 400–401
 transport approximation (TA) 219
 transport cross section (TCS) 220
 transport mean free path (TMFP) 220

triple dangling bond (TDB) 844
 tunable lasers 257
 turbomolecular pump 84
 two-dimensional adatom and vacancy gas
 750–754
 two-dimensional lattices and structures
 – Bravais lattices 497, 498, 499–500
 – crystallographic 2D point groups
 500–502
 – plane groups 502–505
 – rotational and mirror symmetry 499
 – stepped and kinked surfaces 505–514
 – superlattices 514–520
 – surface orientation 494–496
 – from 2D to 3D crystallography 496–497
 two-level roughness model 413–417
 two-photon photoelectron spectroscopy
 253
 – energy-resolved spectroscopy 256–258
 – experimental setup 262–264
 – image-potential states 253–256
 – theoretical aspects 264–267
 – time-resolved measurements 258–262
 two-photon photoemission (2PPE)
 580, 706

u

UK Surface Analysis Forum 243
 ultrahigh vacuum (UHV) 3, 76, 83, 84, 85,
 88–90, 96, 98, 165, 324, 348, 350, 357,
 361–362, 429, 451, 458, 459, 464–465, 538,
 579, 760, 901–902, 916, 922
 – conditions 73
 – materials 80–81
 ultraviolet photoelectron spectroscopy
 (UPS)/angle-resolved photoemission
 spectroscopy (ARPES)
 – ARPES for band mapping and Fermi
 surface mapping on surfaces 190–199
 – extrinsic contributions to line shapes and
 widths 202–204
 – spectral functions and many-body effects
 199–202
 – spin polarimetry 205–207
 – spin-polarized photoelectron spectroscopy
 204–205
 – spin structure measurement in reciprocal
 space 207–210
 – work function measurement 189–190
 ultraviolet–visible (UV–vis) absorption
 spectroscopy 343–344, 347, 348
 – applications 345–348
 – instrumentation 344–345
 uniaxial anisotropy 710, 724

universal potential. *See*
 Ziegler–Biersack–Littmark (ZBL)
 up atom 837

v

vacuum gauges 85
 vacuum level 575
 valence band maximum (VBM) 905, 920
 van der Waals bonding 16–17
 Versailles Project on Advanced Materials and
 Standards (VAMAS) 246
 vertical manipulation 436
 vibrational coupling, in organic molecules
 369
 vibrational properties, surface-specific 8
 vibrational spectroscopy 311–314, 316, 331,
 334, 341

w

wave function matching, and
 phase-accumulation model 585–586
 wave vector 563
 wet pumps 83
 Wigner–Seitz cell 498
 Wood notation 515–516
 work function 59–60, 878, 918
 – basic considerations 571–575
 – experimental determination 577–580
 – measurement 189–190
 Wulff construction 50–51, 56

x

X-ray absorption cross section 359
 X-ray absorption near-edge structure
 (XANES) 360

X-ray absorption spectroscopy 62
 X-ray absorption spectrum (XAS) 358, 360
 X-ray diffraction (XRD) 93, 107, 145, 389,
 421, 489
 X-ray fluorescence process 177
 X-ray fluorescence yield 178
 X-ray magnetic circular dichroism (XMCD)
 727
 – absorption 693–697
 X-ray photoelectron diffraction (XPD) 152,
 179–186
 – Auger electron diffraction and 179–186
 X-ray photoelectron spectroscopy (XPS)
 152, 154, 168–169, 178, 215–217, 349.
See also National Institute of Standards and
 Technology (NIST), US and AES and XPS
 – core-level spectra, chemical shifts, and
 satellites 169–177
 – quantifying elemental concentrations and
 surface cleanliness 166–169
 – valence band, and resonant photoemission
 186–187
 X-Ray Photoelectron Spectroscopy Database
 (SRD 20) 238–239
 X-ray resonant magnetic reflectivity (XRMR)
 method 697
 X-rays 86
 – scattering 91
 X-ray standing waves (XSW), photoexcitation
 by 187–189

z

Zeeman splitting 686
 Ziegler–Biersack–Littmark (ZBL) 274
 Z+1 approximation 174

