Index

a
Abraham’s model of surface segregation 7–8
adatoms 64, 67–70, 72, 75, 438
additive energy models, for 2D alloys 84–85
adsorbate-induced surface reconstruction 2
adsorbate-induced surface segregation 3, 38, 44–46
Al₂O₃ films, on metal alloys 614–618
alkaline halides 282–285
– and alkaline earth halides 279–281
alloys and surface properties 1–3
– applications
– – first-principle-based surface phase diagram of CoAl(100) 31–38
– – Pt₅₇Rh₄₃(100) equilibrium properties 38–52
– bulk properties
– – binary systems special properties 3–4
– – short-range order in metal alloys 4–7
– methods 7–8
– – ab initio modeling with DFT 13–15
– – alloy surfaces experimental structure determination 8–13
– – cluster expansion of surface energetics 15–31
Al-rich complex metallic alloys 371–372
Al-rich quasicrystals
– atomic structure and chemical composition 367
– electronic structure 370–371
– phonon structure 371
alumina and line defects 652–653
– alumina film on NiAl(110) 653–655
– atomic arrangement in defect networks 659–663
– atomic sites in surface unit cell 655–659
– complex domain boundary network 663–667
– spectroscopy across extended line defects 667–668
amorphous materials 383–385
– Baltic amber 412–416
– glass structures
– – continuous random network theory 385–386, 394
– – experimental 389–391
– – order ranges 388–389
– – pair-correlation function (PCF) 386–388
– – silicate glasses 392–400
– silicon–carbon alloy films 406–412
tellurium subhalides 400–405
angle-resolved photoemission spectroscopy (ARPES) spectra 204, 206, 207, 494, 498, 506–509, 511, 514, 516, 518, 523, 528
angle-resolved X-ray photoelectron spectroscopy (ARXPS) 590
antiferromagnetic coupling 422
antifreeze proteins and ice–water interface interaction
– growth inhibition by adsorption of AFGP molecules on interface 336–339
– ice–water interface MD simulation and antifreeze protein 339–343
antiphase domain boundaries (APDB) 660–664
antisites 13, 32–38
approximant 349
artificial atoms 517
asymmetric transverse wall (ATW) 577
atomic beam epitaxy (ABE). See molecular beam epitaxy (MBE)
atom chains 503
atomic diffusion 178
atomic force microscopy (AFM) 256, 284, 286, 293, 312–313, 315, 390–396, 398–411, 413–417, 641, 668, 750, 760, 773, 832, 833,
atomic force microscopy (AFM) (contd.) 840–843, 856, 914. See also noncontact atomic force microscopy (nc-AFM)
atomic layer deposition (ALD) 429–430, 589, 625
atomic scale friction 913–916
– rapid dynamics of noncontacts and dissipation new mechanisms 947
– extra friction regimes 951–953
– FFM as two-mass-two-spring system 949–951
– FFM results critical view 953
– rapid apex dynamics experimental evidence 951
– tip apex flexibility and effective mass 947–949
– stick–slip motion versus continuous sliding 922
– atomic stick–slip motion 923–927
– contact size effects 934–935
– critical dampening problem 927–928
– dimensionality 937–938
– multiple slip events and damping 936–937
– nearly vanishing friction in experiments 931–934
– from stick–slip motion to continuous sliding 929–931
– stick–slip motion universality 922–923
– stiffness 928–929
– temperature and velocity effects 938
– mechanical versus thermal excitation 946–947
– from stick–slip to thermal drift 941–944
– thermal activation effects on stick–slip motion 939–941
– thermal effects FFM observations 945–946
– thermolubricity 944–945
– tribology and nanotribology
– basic experimental approaches in nanotribology 917–920
– Da Vinci’s laws and failure at nanoscale 916–917
– frictional energy dissipation 920–921
attempt frequency 939, 947, 951, 952
Au/MgO (100) 839–843
Auger electron spectroscopy (AES) 9–10, 127, 367, 627, 696, 698, 703, 719, 818, 819, 824, 827
autocompensation. See electron counting rule
azimuthal orientation 750, 752, 755, 757, 759, 765, 768, 769, 772
b Baltic amber 412–416
band bending 154–155
Bauer’s criterion for equilibrium shape 865–869
Bergman cluster 368
Bernal–Fowler rules 307
bi-binary CE for substrate–adsorbate system 45–46
bilateral 753
bilayer islands 71, 78, 79
biphasic ordering 245, 698
Bloch function 529
Bloch wall 574–575
Bohr–Sommerfeld quantization rule. See phase accumulation model (PAM)
bottom-up approach 851–853
Brillouin light scattering (BLS) 549
broken symmetries and energy references 25–28
buffer-layer-assisted growth (BLAG) 788
Butler–Volmer equation 431
c CaF₂(111)
– atomic structure 291–299
– electron irradiation damage 299–301
CaF₂ and BaF₂ 286
canonical Monte Carlo 31
capping/decapping 122–123
carbon hydride adsorbates 165–166
carbon nanotubes (CNTs) 428, 691, 692
chemical beam epitaxy (CBE) 163–164, 168
chemical vapor deposition (CVD) 427–429, 500, 596, 695
Child’s law 739
Clausius–Clapeyron equation 748
cleavage ledges 292
cleavage plane 292
cleavage tips 292
cluster expansion (CE)
– of surface energetics 15–31
– Hamiltonian 17–25, 39
– surface applications 25–30
clusters. See metal nanoparticles
coincidence site lattice (CSL) 665–667
cold cathodes 423
collective diffusion coefficient 437
color centers 280–281, 645, 646. See also oxygen vacancies
– assignment 649–652
index

- in magnesia 647–649
compact adatom and vacancy islands 455–457
complementary metal oxide semiconductor (CMOS) 177, 208
complex metallic alloy 349
- Al-rich complex metallic alloys 371–372
compound semiconductors surfaces 101–102
- III–V and II–VI compound semiconductors
  - bulk properties 102
- cubic materials 103–104
- multinary and isovalent compounds 106–107
- wurzite materials 104–106
- modification, by adsorbates 162–163
- surfaces under growth conditions 163–169
- surface electronic properties 146
  - III–V(001) surfaces 148–151
  - III–V(110) surfaces 146–148
- surface steps, defects, and band bending 154–158
- wurzite III–V surfaces 152–154
- surface optical analysis 158
- optical anisotropy 159–162
- wurzite materials surfaces 141
- nonpolar surfaces 142
- polar surfaces 142–145
- zinc blende materials 103, 107–108
  - {001} surfaces 113–123, 126–141
  - {110} surfaces 108–113
  - surface structure theoretical determination 123–126
configurational entropies 15, 86
- and Monte Carlo simulations 30–31
configuration function 19–24
configuration space 19–20, 25–29
constant wavelength and energy 520
containment effects 188
continuous random network theory 385–386, 394, 670
corner-crossing 456
corundum-type surfaces 243–249
critical dampening problem 927–928
critical thickness 602
crystallization 384, 391, 398, 404, 409, 417
cubic anisotropy 566
d
2D quantum wells 500–501, 505–512
2D structures stacking 799
3D clusters 787
- metallic clusters synthesis and deposition 787–788
- small clusters magnetic properties 788–790
- surface-induced magnetic properties 790–792
3D metals 504–505
3D model and thin film magnetism 553
Da Vinci’s laws and failure at nanoscale 916–917
De Broglie relation 496
Debye–Waller effect 284, 286
dendritic ice crystal 424–425
dendritic islands. See fractals
dichromatic pattern 665
diffraction techniques 366
dimerization 114–115
Dirac points 693
disordered alloys. See solid solutions
displacements that are symmetry conserving (DSC) 1123–1124 666
divacancies (DVs) 651–652
domes 888, 895
dry friction 914–917, 923, 938, 954, 955
dynamic random access memories (DRAMs) 422
dynamic superlubricity 946
effective pair interaction (EPI) 85–86, 88, 90–93, 95
effective spin model 806
Ehrlich Schwabe barrier (ESB) 774–775
eigenstrain 881
elastic relaxation 864, 876, 879, 882–885, 897–899, 905
electrochemical deposition 430–431
electron counting rule 102, 110, 115–116, 128, 132, 139–140, 156, 157, 239
electron paramagnetic resonance (EPR) 268, 269, 646
elementary steps and ice crystals 312, 316
energy discretization spatial effects and quantum wells 497–498
energy dispersion curve (EDC) 508
energy gap 521–523
epitaxial growth 178–189, 864–865
Index

epitaxial growth, of thin films 421–422
– compact adatom and vacancy islands 455–457
– versus crystal growth 424–425
– deposition techniques 425–426
– atomic layer deposition (ALD) 429–430
– chemical vapor deposition (CVD) 427–429
– electrochemical deposition 430–431
– physical vapor deposition (PVD) 426–427
– growth manipulation 469
– periodic ion bombardment 475–477
– surfactants 470–475
– growth modes 431–435
– growth morphologies 465
– growth oscillations 465–467
– “wedding cakes” 467–468
– island shapes 449–450
– fractals 450–455
– monolayer islands coarsening 458
– Smoluchowski ripening 463–464
– nucleation 435
– atomic processes 435–438
– heterogeneous nucleation 446–449
– homogeneous nucleation 438–441
– in presence of long-range interactions 442–446
– technological applications 422–424
epitaxial organic film growth 737
erbium silicide 214
eutectics 186, 187
exchange anisotropy 937
extended X-ray absorption fine structure (EXAFS) 400

f
Fabry–Perot model 536–538
 facet plot 886
fast Fourier transformation (FFT) 678–680
Fermi surfaces 552, 553, 568
Fermi wavelength 494, 495
ferromagnetic resonance (FMR). See Brillouin light scattering (BLS)
Fibonacci sequence/chain 351
field emission resonances (FERs) 714, 715
finite element (FE) simulation 879–880, 888, 891, 892, 896–898, 900, 903
first-principles method 13
– surface phase diagram of CoAl(100) 31–38
flat-island approximation 879
fluorite silicides 191–194
Fokker–Planck equation 940
formation enthalpy. See mixing enthalpy
Fourier transform and Fourier filtering techniques 363–364
fractals 450–455
Frank’s node rule 661
Frank–van der Merve (F–vdM) growth 753, 754
free-electron model 552
Frenkel–Debye layer 299
Frenkel law 820
friction anisotropy 937
friction force microscopy (FFM) 914–919, 921–923, 925, 926, 928, 929, 933, 936, 937, 939, 947–949
– observations, of thermal effects 945–946
– results, critical view 953
– as two-mass-two-spring system 949–951
Friedel oscillations 442–444
Fuchs–Kliewer phonon 271–273
GaAs(001) (2 × 4) reconstruction 129–130
GaAs(001) (4 × 2) reconstruction 130–132
GaAs(001) (4 × 4) reconstruction 127–129
GaAs(001) surface 126–127
GaAs (111) and GaAs (T11) surfaces 139–141
Garbulsky–Ceder constraints 24
Gedanken experiment 425, 431
geometrically fully relaxed configuration 4
 giant magnetoresistance (GMR) 422, 549
Gibbs adsorption isotherm 872
Gibbs–Thomson equation 336, 458, 819
Gibbs–Thomson mechanism 336, 337, 341, 458
glass 641–642, 668–670, 675, 682
glass formers 385
glass structures
– continuous random network theory 385–386, 394
– experimental 389–391
– order ranges 388–389
– pair-correlation function (PCF) 386–388
grand-canonical Monte Carlo 31
graphene 691–692
– electronic structure and quantum properties on Ru(0001) 710–718
– epitaxial growth and structural properties on Pt(111) 702–711
– epitaxial interfacial properties, on metal substrates 718–724
– fabrication methods exploration 694–696
– millimeter scale, highly ordered, 
  single-crystalline graphene on Ru(0001)  
 696–702
– Moiré template for monodisperse Pt 
  nanoclusters formation  724–729
– unique properties and application potentials 
 692–694
grazing incidence small-angle X-ray scattering 
  (GISAXS) 836–837, 844–847
grazing incidence X-ray scattering (GIXS) 
 241, 243, 251–252. See also surface X-ray 
  diffraction (SXRD)
Green’s function 879
group III phosphide surfaces  132
growth modes  421
growth oscillations  465–467
guest atoms, floating in type1 surface alloys 
 71

\( h \)

\( H_2O \) potential model  324–326
Hall effect  215, 216
Hamiltonian equation  16–17, 21–22
Heisenberg uncertainty principle  499
helium atom scattering (HAS)  282–284, 
 286, 288, 290, 466, 473
Hertz–Knudsen equation  744
high-index surfaces  103
highly oriented pyrolytic graphite (HOPG) 
 694, 750
high-resolution electron energy loss 
  spectroscopy (HREELS)  242, 248, 252, 
 272, 273, 613, 623
high-resolution transmission electron 
  microscopy (HRTEM)  191, 622, 623, 840, 
 843, 844, 846, 847
high-temperature sputtering (HTS)  189
\( hkl \) indices 103, 105, 233
Hooke’s law  878

\( i \)

ice
– crystalline structures  306–308
– crystals under nonequilibrium conditions 
 308–309
– ice–water interface interaction
  – equilibrium form of ice crystal in water 
    321–322
  – growth form in supercooled water 
    322–323
  – in situ observation
  – monomolecular step migrations 
    312–316
  – quasi-liquid layer dynamic behavior 
    316–321
  – molecular dynamics simulation  326–332
  – \( H_2O \) potential model  324–326
  – specific features  305–306
  – thermodynamics, near melting point 
    310–312
ice rules  307
ideal surface  108
III-(001) surfaces  135–138
image potential  528
imaging techniques  836
inclusion  881
inelastic tunneling spectroscopy  804
infinite versus finite potential wells  519–521
\( \text{InP}(001) \) (2 \( \times \) 4) reconstruction  132–135
interdiffusion  180, 182, 208, 601
interface anisotropy  556
interface barrier  521–528
interface-stabilized phases  594, 599, 606, 
 613, 627, 629, 634
interfacial chemistry  741
interfacial reactivity  181–183
interlayer diffusion  438, 468
  – barrier  468
  – intermetallic  350
ionic crystals  279–282
– \( \text{CaF}_2(111) \) and atomic structure  291–299
  – electron irradiation damage on \( \text{CaF}_2(111) \) 
    299–301
  – low-index surfaces
  – alkaline halide examples  282–285
  – \( \text{CaF}_2 \) and \( \text{BaF}_2 \)  286
  – surface phonons  288–291
ion scattering experiments  72
iron silicides  194–196, 203–206
Ising model 16–17
island shapes  449–450
  – fractals  450–455

\( k \)
Kelvin probe force microscopy (KPFM)  
 295–299, 649, 651, 652, 681, 834
kinetic Monte Carlo (KMC) simulations  825
kinetic roughening. See multilayer growth
KKY potential model 326
Knudsen cell  743, 748
Index

Knudsen method 748, 749
Kohn–Hohenberg theorem 123
Kohn–Sham equations 14
Kohn–Sham wave function 539
Kossel crystal 866, 867, 869
Kramers solutions 940

L
Langevin equation 927, 940
Langmuir–Blodgett technique 738
laser confocal microscopy – differential interference contrast microscopy (LCM-DIM) 313, 315–316
lateral atom distribution, in surface-confined alloys 79
– additive energy models, for 2D alloys 84–85
– energy parameters derived from STM data 85–86
– ordered surface alloy 88–89
– prediction and verification 90–95
– short-range order and effective pair interactions 86–88
– statistical short-range-order analysis 80–83
lattice 18
lattice matching 189
layer-by-layer growth 465
layer-by-layer self-assembly 738
layer-dependent adatom mobilities 469–470
– periodic ion bombardment 475–477
– surfactants 470–475
layer-resolved differential conductance 604
low-energy electron microscopy (LEEM) 69, 593, 601, 609, 699, 773
low-energy ion scattering (LEIS) 8, 604, 817–818
low-index surfaces 103–104, 106

m
Mach–Zehnder interferometry 322
Madelung energy 235, 236, 279, 598
Madelung potential 235, 256, 259, 261, 268
magnesia point defects 645–646
– color centers assignment 649–652
– color centers in magnesia 647–649
– pristine magnesia films 646–647
magnetic anisotropy 555–556
– 2D versus 1D anisotropies 562–567
– anisotropies induced by quantum well states 567–569
– exchange bias 569–571
– spin reorientation 559–562
– surface anisotropy 556–559
magnetic anisotropy energy (MAE) 802, 806, 807
magnetic clusters 785–787
– 3D clusters 787
– – metallic clusters synthesis and deposition 787–788
– – small clusters magnetic properties 788–790
– – surface-induced magnetic properties 790–792
– single atoms and few-atom clusters 801–802
– – anisotropy origins 802–803
– – dynamic properties of atoms 806–807
– – interactions between atoms 807, 808
– – quantum mechanical model 803–806
– – single-atomic magnetic bits 808
– two-dimensional magnets 792–793
– 2D structures stacking 799
– edge versus core anisotropy 793–798
– single islands experimental observation 799
magnetic domains and domain walls 571–572
– domain wall motion 577–578
– magnetic domain walls in ultrathin films 574–577
– magnetization patterns in ultrathin films 572–574
magnetic random access memories (MRAMS) 422, 423
magnetocrystalline anisotropy 787
magneto-optic Kerr effect (MOKE) 795
Markoc chain 31
McLean’s model of interfacial segregation 7
mean-field nucleation theory 439
mean separation work 866
medium-energy ion scattering (MEIS) 197, 241, 285
Mermin–Wagner theorem 560
metallic clusters synthesis and deposition 787–788
metal nanoparticles 815
– characterization techniques
– – general considerations 832
– – scanning probe techniques 832–834
– – transmission electron microscopy (TEM) 835–836
– – X-ray scattering 836–837
nanoparticles ordered growth
– general considerations 849–850
– nanoscale templates 852–855
– surfaces as templates 850–852
– template-controlled growth on oxides 855–858
– nucleation and growth kinetics
– growth kinetics 828–832
– growth mode 816–818
– nucleation kinetics 818–828
– particle shape
– Au/MgO (100) 839–843
– equilibrium shape 837–839
– kinetically controlled shape 839
– Pd/MgO 100 843–849
metal-organic vapor phase epitaxy (MOVPE) 120, 158, 163–166, 168–169
– growth 121–122
metal-to-insulator transition (MIT) 264, 265
metastable impact electron spectroscopy (MIES) 268
Metropolis algorithm 30–31
microelectromechanical system (MEMS) 918, 919, 946
microelectronics and ULSI 218–219
Miller indices. See hkl indices
miscut. See quantum dots
misfit dislocation 653
misfit plane 770
missing dimer arrangements 116–118
mixer-dimer structure 132–134
mixing enthalpy 3
molecular beam epitaxy (MBE) 119–121, 136, 165, 168–169, 178, 180, 189, 588, 694, 695, 873. See also physical vapor deposition (PVD)
– growth 121
molecular dynamics simulation 324–326, 879
– of ice crystals 326–328
– of ice–water interface 328–332
molecular organic films. See organic molecular beam deposition (OMBD)
monolayer 502–503
monolayer 753
– regions 65, 67, 69, 71–72, 77, 78, 88–91
monolayer islands coarsening 458
– Ostwald ripening 458–463
– Smoluchowski ripening 463–464
Monte Carlo (MC) simulations 15, 30–31, 62, 86, 88, 90, 93, 903
Mössbauer spectroscopy 402
mound formation. See multilayer growth
Mullins–Sekerka instability 454, 456
multichain wires 502
multiferroics 423
multilayer growth 465, 467
multisystem coupling and decreasing rank 28–30

n
nanodots 220, 504, 517–518
nanoparticles (NPs) 592, 600, 618, 632, 634
nanoparticles ordered growth
– general considerations 849–850
– nanoscale templates 852–855
– surfaces as templates 850–852
– template-controlled growth on oxides 855–858
nanoripple 893
nanosilicides 220–221
nanostripes 502, 514
nanowires 220, 513–517
near-edge X-ray absorption fine structure (NEXAFS) 709, 710, 761
nearest-neighbor correlation parameter 5
near-surface intermixing 75
Néel wall 575–576
nickel and cobalt silicides 203
normal incidence X-ray standing wave (NIXSW) 761
nucleation 435
– atomic processes 435–438
– heterogeneous nucleation 446–449
– homogeneous nucleation 438–441
– in presence of long-range interactions 442–446

o
octopolar reconstruction 241
ordered and vitreous oxide films 641–642
– experiment 642–645
– line defects in alumina 652–653
– alumina film on NiAl(110) 653–655
– atomic arrangement in defect networks 659–663
– atomic sites in surface unit cell 655–659
– complex domain boundary network 663–667
– spectroscopy across extended line defects 667–668
– magnesia point defects 645–646
– color centers assignment 649–652
– color centers in magnesia 647–649
– pristine magnesia films 646–647
ordered and vitreous oxide films (contd.)
  – thin vitreous silica film atomic structure 668–669
  – atomic positions assignment 669–681
organic field effect transistors (OFETs) 739, 741
organic light emitting devices (OLEDs) 739, 741
organic molecular beam deposition (OMBD) 737–738
  – energetic considerations
  – bonding nature at interface 761–766
  – lattice sums 769
  – layer growth and strain relief 770–772
  – molecular orientation and intermolecular interaction 766–767
  – quantitative values and remarks 767–769
  – growth morphology
  – general growth morphologies 773–775
  – methodic aspects 772–773
  – roughening and kinetic aspects 775–776
  – historical background 750–752
  – molecular materials 744–749
  – preparation chamber 742–744
  – structural relations
    – definitions 754–759
    – experimental remarks 759–761
    – general growth scenarios 753–754
    – substrate materials 749–751
organic molecular beam epitaxy (OMBE) 738, 741–742
organic photovoltaic cells (OPCs) 739, 740
Ostwald ripening 421, 458–463
overpotential deposition (OPD) 431
oxide films 832, 834, 835, 853, 856
oxide-mediated epitaxy (OME) 189
oxide surface 229
  – bulk crustal structures 230–232
  – corundum-type surfaces 243–249
  – defects 253, 265–270
  – electronic structures 257
  – core-level shifts 263–264
  – localized d–d excitations in transition metal ions 261–263
  – surface excitation 260–261
  – surface structure effect on bulk electronic properties 264–265
  – valence electronic structure 258–260
  – geometric structure 232–235
  – chemical potential, of oxygen 237–239
  – relaxation, rumpling, and reconstruction 235–236
  – stability 236–237
  – phonons 270–274
  – rock-salt-type (100) and (111) surfaces 239–242
  – wurtzite structure 249
  – oxygen chemical potential 608–614
  – oxygen vacancies 255–257. See also color centers
  – on MgO surface 267–270

\( P \)

pair-distance histograms (PDHs) 675–676
parent lattice 18
Pd/MgO 100 843–849
periodic ion bombardment 475–477
periodic potential 529–532
phase accumulation model (PAM) 532–536
phase diagram 7, 31–38, 124–126, 433, 434, 607, 930
phase formation 178, 185–187
phase separation 17
phonons
  – at ionic crystals 288–291
  – at oxide surfaces 270–274
photoelectron spectroscopy (PES) 709
physical vapor deposition (PVD) 426–427, 624. See also molecular beam epitaxy (MBE)
polarization catastrophe 619
postoxidation (PO) 596
Prandtl–Tomlinson model 914, 915, 924–930, 933–935, 937, 938, 943, 944, 947, 950, 953
prepyramids 885, 886
properties, of surface alloys
  – annealing effect
  – guest atoms floating in type I surface alloys 71
  – surface and subsurface alloying 75–77
    – type I 63–71
    – type II 71–75
    – type III 78–79
    – classification 62–63
  – lateral atom distribution in surface-confined alloys 79
  – additive energy models, for 2D alloys 84–85
  – energy parameters derived from STM data 85–86
  – ordered surface alloy 88–89
  – prediction and verification 90–95
  – short-range order and effective pair interactions 86–88
Index

- statistical short-range-order analysis 80–83
- role in surface science 61–62
pseudogap 370, 372
pseudo-MacKay cluster 368
Pt$_{35}$Rh$_{65}$(100) equilibrium properties 38
- adsorbate-induced segregation 44–46
- results and discussion 46–52
- surface structure and stability 38–43
pulsed laser deposition (PLD) 596

q
quadrupole mass spectrometer (QMS) 743–744
quantum dots 863–864
- elastic interaction between Ge islands on vicinal Si substrates 903–909
- growth mode thermodynamic criterion
  - Bauer’s criterion for equilibrium shape 865–869
  - epitaxial growth 864–865
  - generalized criterion for growth mechanism 871–873
  - thickness variation of chemical potential 869–871
- intermixing effect on nucleation 897–903
- morphology stability 873–888
- vicinality effect on shape 888–897
quantum Hall effect 693
quantum mechanical model 803–806
quantum well resonance (QWR) 714, 715
quantum well states, in metallic films, wires, and dots 493–494
- critical dimensions 494–495
- discretization and temperature 496
- energy discretization spatial effects 497–498
- discrete states momentum 498–499
- electronic properties
  - 0D quantum wells 517–518
  - 1D quantum wells 513–517
  - 2D quantum wells 505–512
  - 3D metals 504–505
- modeling
  - density functional theory 538–541
  - Fabry–Perot model 536–538
  - phase accumulation model (PAM) 532–536
- potentials 518
- infinite versus finite potential wells 519–521
- interface barrier 521–528
- periodic potential 529–532
- vacuum barrier 528
- types 499–500
- 0D quantum wells 504
- 1D quantum nanowires 501–504
- 2D quantum wells 500–501
quartz crystal balance (QCB) 919, 921
quartz microbalance (QMB) 743–744
quartz-tuning-fork-based sensor device 644–645
quasicrystals 349
- alloy and intermetallic 350
- Al-rich CMAs 371–372
- Al-rich quasicrystals
  - atomic structure and chemical composition 367
  - electronic structure 370–371
  - phonon structure 371
  - approximant 349
  - background 350
  - complex metallic alloy 349
  - compositions 350
  - history 353
  - non-Al-based QCs 372–373
  - phases 350
  - sample preparation and surface evolution 353–356
  - spacings between similar features 350
  - special considerations 356
  - diffraction techniques 366
  - scanning tunneling microscopy 356–365
  - XPS and AES 367
quasiepitaxy 752
quasi-liquid layer (QLL) 308–313, 316–321, 326–328, 338

r
radial distribution function (RDF) 364. See also pair correlation function (PCF)
rare earth/silicon interfaces electronic structure 209–211
- chemical bond formation 211
- electronic band structure and surface states 211–214
- Schottky barrier heights 214–215
rare-earth silicides 196–198
reactive deposition epitaxy (RDE) 178
reactive evaporation (RE) 596
rebonded-step structure 886
reflectance anisotropy spectroscopy (RAS) 120, 158–159, 162, 165, 168
reflection domain boundaries (RDBs) 659–660, 664–666
reflection high-energy electron diffraction (RHEED) 119, 120, 136, 137, 142, 565, 627–629, 631, 752, 761, 773, 791
reflectivity 537, 538
rehybridization and charge transfer 109–113
rock-salt-like oxides
– cube-on-cube epitaxy 621–623
– on different metals 602–608
rock-salt-type (100) and (111) surfaces 239–242
Ronay’s rule 187
Ruderman–Kittel–Kasuya–Yosida (RKKY) interaction 552, 792, 808
rumpling 236, 283, 934
Ru-terminated surface 239
Rutherford backscattering spectroscopy (RBS) 191
scanning electron microscopy (SEM) 312, 433
scanning probe microscopies (SPMs) 401, 853
scanning probe techniques 832–834
scanning transmission electron microscopy (STEM) 668
Schottky barrier
– electrical properties 206–209
– heights 214–215
Schrödinger equation 538, 714, 715
selectron energy loss spectroscopy (EELS) 262, 263, 269, 272
self-aligned silicide (SALICIDE) 218
self-trapped excitons (STEs) 299
selvedge definition and different depth regimes 586–587
short-range order (SRO) 2–5, 86
– in metal alloys 4–7
– statistical analysis 80–83
silicate glasses 392–400
silicon–carbon alloy films 406–412
simulated annealing procedure 88–89
six-site model 324–327, 329, 331, 340
Smoluchowski ripening 422, 463–464
soft X-ray photoemission spectroscopy (SXPS) 134
solidification 383–385
solid phase epitaxy (SPE) 178, 180, 186, 189, 196
solid solutions 3
space charge layer 598
spatial distribution of the nearest-neighbor distances (SDNN) 907
spectroscopic effects 530–532
spincasting and doctor blade technique 738
spin reorientation 559–562
spins 17
spin valve 569
sputter annealing 367, 372
stability line 42
statistical multilayer growth 467
stick–slip motion versus continuous sliding 922
– atomic stick–slip motion 923–927
– contact size effects 934–935
– critical dampening problem 927–928
– dimensionality 937–938
– multiple slip events and damping 936–937
– nearly vanishing friction in experiments 931–934
– from stick–slip motion to continuous sliding 929–931
– stick–slip motion universality 922–923
– stiffness 928–929
Stranski–Krastanov (S–K) growth 753, 754, 760, 771, 863, 873, 874
superlattice 18
superlubricity 932–934
superparamagnetic instability 786
supersaturation 425
surface’s Gibb’s function 34
surface anisotropy 556–559
surface core-level shifts (SCLS) 112
surface forces apparatus (SFA) 919
surface segregation 1–2, 7
surface silicides physical properties 177
– and thin-film silicides applications 177–178
– applications
– – coatings 219
– – microelectronics and ULSI 218–219
– – nanosilicides 220–221
– – conductivity and transport properties 215
– – electrical transport in semiconducting silicides 216, 217
– – metallic silicides electrical transport 215–216
Index

magnetic properties 217
optical properties 217, 218
rare earth/silicon interfaces electronic structure 209–211
– chemical bond formation 211
– electronic band structure and surface states 211–214
– Schottky barrier heights 214–215
structural properties
– thin epitaxial silicide films structure and interfaces 189–198
surface silicide formation and epitaxial growth
– containment effects 188
– fabrication technologies 189
– growth methods 178–180
– interface growth kinetics 180–183
– therodynamical aspects 184–188
transition metal silicides electronic structure
– chemical bond formation 198–201
– electronic band structure and surface states 203–206
– interface electronic structure formation 201–202
– Schottky barrier electrical properties 206–209
– silicide/silicon heterojunctions 208, 209
surface slab 26
surface stabilization, by hydrogen 166–169
surface X-ray diffraction (SXRD) 191, 590, 622, 645, 659. See also grazing incidence X-ray scattering (GIXS)
(III) surfaces 138–139
surfactants 470–475
symmetric and asymmetric dimer structures 118–119
symmetry gap 523–526
– hybridization effects 526–528

t
tellurium subhalides 400–405
temperature desorption spectroscopy (TDS) 743–744, 762
TensErLEED code 12
thermal desorption spectroscopy 768
thermal drift 943–944
thermal excitation 67, 86, 89
thermal expansion 284
thermal hysteresis region 334
thermal roughening transition 322
thermolubricity 915, 934, 944–947, 952
thin film
– characterization 589–590
– preparation 587–589
– science, historical overview 585–586
thin film magnetism 545–547
– magnetic anisotropy 555–556
– 2D versus 1D anisotropies 562–567
– anisotropies induced by quantum well states 567–569
– exchange bias 569–571
– spin reorientation 559–562
– surface anisotropy 556–559
– magnetic domains and domain walls 571–572
– domain wall motion 577–578
– magnetic domain walls in ultrathin films 574–577
– magnetization patterns in ultrathin films 572–574
– oscillatory interlayer exchange
– coupling history 547–548
– experimental approaches 548–550
– quantum-well states 552–555
– spacer materials, periods, and coupling strengths 550–551
Ti-interlayer-mediated epitaxy (TIME) 189
TIP4P model 324–326, 328–329
top-down approach 852
tracer diffusion coefficient 437
transition metal silicides electronic structure
– chemical bond formation 198–201
– electronic band structure and surface states 203–206
– interface electronic structure formation 201–202
– Schottky barrier electrical properties 206–209
– silicide/silicon heterojunctions 208
transition metals 695, 696, 703, 709, 724, 728
transition-state theory (TST) 436
translation domain boundaries (TDBs) 660, 663–665, 667
transmission electron microscopy (TEM) 312, 390, 622, 835–836
tribology and nanotribology
– basic experimental approaches in nanotribology 917–920
– Da Vinci’s laws and failure at nanoscale 916–917
– frictional energy dissipation 920–921
tunnel magnetoresistances (TMRs) 422–423
two-dimensional silicides 212–213

u
ultra-large-scale integration (ULSI) 218
ultrathin films 500, 505–512, 556
- magnetic domain walls 574–577
- magnetization patterns 572–574
- multilayer 500–501
- single-layer 501
ultrathin oxide films 592
- case studies 602–618
- on metal substrates
  - specific aspects 599–602
- on oxide substrates 618
- case studies 621–635
- specific aspects of oxide and oxide interface 618–621
- physicochemical aspects of interfaces with oxides
  - generic interface equilibrium structure and chemistry 597–598
  - interface peculiarities involving oxides 598–599
- preparative aspects 593–594
  - film deposition and postdeposition treatments 596–597
  - surface oxidation (SO) of substrate 594–595
- reasons to use 592–593
ultraviolet photoelectron spectroscopic (UPS) 250, 259, 264, 265, 268, 627, 629, 632, 634
UNCLE code 33, 45
underpotential deposition (UPD) 431
van der Waals epitaxy 752
Van Hove singularity 516
variable valence oxides 623
- on different metals 608–614
- oxides with different lattices 631–635
- quasi-isostuctural oxides 623–631
Vegard’s law 40, 898
Vienna ab initio simulation package (VASP) 90, 647
viscous friction 927
Vollmer–Weber (V-M) growth 753

W
Walker field 577
Walser–Bené rule 187
Warren–Couley SRO parameter 5, 80, 83
wave vector 553
“wedding cakes” 467–468
wetting layer 771, 863, 873, 876, 882
Wulff–Kaischew theorem 817, 837, 847
Wulff theorem 816, 837
wurtzite materials surfaces 141
- nonpolar surfaces 142
- polar surfaces 142–145
wurtzite structure 249

X
X-ray absorption spectroscopy (XAS) 604, 623, 802
X-ray diffraction (XRD) 590, 629, 641–642, 671, 673, 674, 676, 749, 752, 759, 760, 773
X-ray magnetic circular dichroism (XMCD) 791, 802, 803, 807
X-ray photoelectron diffraction (XPD) 604, 606, 610, 612, 624–627, 629
X-ray photoelectron spectroscopy (XPS) 245, 264, 367, 623
X-ray scattering 836–837

Y
Young–Dupré equation 817
Young equation 816

Z
Zeeman energy 549, 564
zinc blende materials 103, 107–108
- {001} surfaces 113–123, 126–141
- {110} surfaces 108–113
- surface structure theoretical determination 123–126
Zinsmeister equations 820–821
(0001)-Zn surface stabilization 252–253
Zn(00–1)–O surface stabilization 253
ZnO polar surfaces 251–252