

Index

a

- ab-initio methods
 - DFT, *see* density functional theory (DFT)
 - GW method 604
 - material properties 605
 - point defects 607
 - formation energies 613–614
 - thermodynamics 609–613
 - ZnO 614–617
 - QMC method 604
- absorptance 6, 7, 10–12, 30, 55, 56, 61, 63, 64, 66, 192–194, 196, 210
- absorption 257, 261, 262, 266, 270, 271
- absorption coefficient 11–13, 21, 22, 75, 77, 165, 192, 193
- absorptivity 277, 292
- activation energy 52–54, 96
- admittance spectroscopy (AS) 93, 96, 108–111
- AFORS-HET (program) 651–653
- AM1.5 7
- ambipolar transport 167
- AMPS-1D program 653
- angle-dispersive X-ray diffraction (ADXRD) 448–450
- annular dark-field detector 401
 - high angle (HAADF) 401
- anomalous dispersion 123–125, 136
 - correction 434
- anomalous scattering 434
- apodization 200, 204–205
- Arrhenius dependence 580
- ASA (program) 13, 653–654
- a-Si:H, *see* hydrogenated amorphous silicon (a-Si:H)
- Atlas 661
- atom probe tomography (APT) 555–562

atomic force microscopy (AFM) 344–347, 391

attempt-to-escape frequency 138

Auger electron spectroscopy (AES) 245, 373, 505, 523, 539–546

Auger recombination 17

b

- backscattered electrons 372
- band bending 14, 15, 99–101, 113
- band gap fluctuations 10
- band tail 93, 151, 191
- band tail width 137
- band–band transitions 287
- bias amplified charge extraction (BACE) 151
- bilayer process 23
- black body spectrum 7, 50, 73
- Boeing process 23
- bond order potential 626, 629
- Bragg diffraction 378, 401, 409
- Bragg's law 424
- bremssstrahlung 406, 434
- built-in field 15, 16, 21, 26, 28–30, 130–131
- built-in voltage 131, 143
- bulk heterojunction 33, 196, 654
- Burgers vector 630

c

- capacitance 93–103, 105–112, 114, 115, 128–129
- capacitance–voltage (CV) profiling 93, 648–649
 - admittance measurements 94
 - deep states 102
 - depletion approximation 98
 - instrumentation 96–98
 - sample requirements 96
- capture cross section 18, 100, 106, 107

- carrier collection
 – voltage dependent 16
 carrier lifetime 167
 cathodoluminescence 378, 386–391, 393, 396
 CdCl_2 -activation 25
 CdTe solar cells 25–27, 209, 233–241, 626–630, 645–649
 CELIV, *see* charge extraction with linearly increased voltage (CELIV)
 $\text{CH}_3\text{NH}_3\text{PbI}_3$ 4, 31, 209
 Chandeson method 261, 262
 characteristic energy 151
 charge extraction 10, 13–16, 19–21, 147–154, 156, 157, 159
 charge extraction with linearly increased voltage (CELIV) 147, 154–157
 charge-coupled device 71
 chemical bath deposition 22
 close space sublimation 389
 co-evaporation 22, 23
 coincidence-site lattice 376
 collection efficiency 86, 87
 collection function 382
 collection probability 6, 56, 196
 COMSOL Multiphysics 661
 concentric hemispherical analyzer 548
 conductive atomic force microscopy (C-AFM) 347–348
 confocal microscope 279
 contact mode atomic force microscopy 345–346
 continuity equations 662
 conventional TEM 397
 convergent-beam electron diffraction 402
 crosslight APSYS 661
 $\text{Cu}(\text{In},\text{Ga})(\text{S},\text{Se})_2$ solar cells 643
 $\text{Cu}(\text{In},\text{Ga})\text{Se}_2$ solar cells 22–25, 210, 211, 643–645
 $\text{Cu}(\text{In}_{1-x}\text{Ga}_x)\text{Se}_2$ solar cells 241–250
 current decay, 131yt de
 current/voltage curves 43
 – measurement 49
 – series resistances 50
 – shape 44–49
 – temperature dependence 52–54
 $\text{Cu}_2\text{ZnSn}(\text{S},\text{Se})_4$ solar cells 27
 cylindrical mirror analyser 541
- d**
- dangling bond 5, 28, 178
 dark conductivity 170
 dark current density 44
 Debye screening length 99
- deep level optical spectroscopy 111
 deep level transient spectroscopy (DLTS) 93, 103–107, 582
 defect 17, 29, 45, 47, 60, 125, 166, 180, 191, 192, 195, 621, 623, 625, 627, 629, 663
 – metastable 29
 demarcation energy 125, 138
 density functional theory (DFT)
 – basis sets 601
 – LDA 601
 – $+U$ method 602
 density of states 93, 100, 101, 109–111, 114, 138, 139, 141–144, 164, 184, 191
 – hydrogen 582
 depletion approximation 94, 98, 99, 108
 desorption 570, 574, 575, 579, 583, 588
 detailed balance 6, 7, 10, 99
 deuterium 574
 dielectric constant 166
 dielectric function 225, 226, 228, 229, 236, 242, 248, 251
 dielectric relaxation time 127, 135, 173
 diffraction pattern 398
 diffusion coefficient 167, 171
 – hydrogen 580
 diffusion constant 382
 diffusion length 15, 28, 75, 79–81, 163, 167–169, 172, 176, 382, 383, 395
 – hydrogen 577
 diode equation 8
 diode quality factor, *see* ideality factor
 direct semiconductor 11
 discrete Fourier transformation 199, 201
 disorder 93
 dispersion 123
 dispersion parameter 137
 dispersive transport 124
 displacability 134, 142
 displacement current 123
 donor–acceptor pair recombination 284–285
 doping density 94, 99
 drive level capacitance profiling (DLCP) 93, 110–111
 dye-sensitized solar cell 4
- e**
- EBSD, *see* electron backscatter diffraction (EBSD)
 EDMR, *see* electrically detected magnetic-resonance (EDMR)
 EELS, *see* electron energy loss spectroscopy
 effective medium theory 220
 – Bruggeman 229, 242

- effusion 569–571, 573–592
 EFTEM, *see* energy-filtered transmission electron microscopy
 Einstein relationship 546
 electrically detected magnetic-resonance (EDMR)
 – a-Si:H solar cells 334
 – history 332
 electroluminescence analysis 71–74
 – illumination 85–88
 – spatially resolved 79–81
 – spectrally resolved 74–79
 – thin-film solar cells and modules 82–85
 electron backscatter diffraction (EBSD) 358, 374, 375, 396
 electron-beam-induced current 378
 electronegativity 534
 electron energy-loss spectroscopy 403–408
 electron holography 409
 electron microscopy 371
 electron spin resonance (ESR)
 – advantage 299, 305
 – doped a-Si:H 322
 – EDMR, *see* electrically detected magnetic-resonance (EDMR)
 – g tensor 309
 – hyperfine interaction 311
 – light-induced degradation 326
 – line broadening 313
 – prerequisite 299
 – sample preparation 307
 – setup and measurement procedure 303
 – spectroscopic principle 300
 – undoped a-Si 316
 – Zeeman energy 309
 electrostatic potential 411
 ellipsometry 444
 – angles 216, 218, 219, 222–224, 252
 – real time spectroscopic 217, 226–229, 232–234, 242, 244–247, 251
 – spectroscopic 215
 energy-dispersive X-ray diffraction (EDXRD) 450–454, 530
 energy-dispersive X-ray spectroscopy (EDX) 247, 397, 408, 523, 551–555
 energy-loss near-edge structure 406
 enthalpy 580
 entropy 580
 EPR-Solar 319, 337
 equivalent-circuit modeling 95, 661, 664–665
 evanescent modes 257, 260, 261, 263, 264, 266
 exact numerical inversion 225–226
 excitons 6, 282, 386
 extended energy-loss fine-structure 406
 extinction coefficient 216–218, 252
- f**
 fast Fourier transformation 257
 Fermi level 47, 53, 125, 164, 180, 382, 588
 Fermi's golden rule 275
 field-swept pESR spectra 306
 finite-difference time-domain 263
 flatband 14–16
 fluorescence yield 505
 focused ion beam 377, 558
 four point probe technique 50
 Fourier-ratio deconvolution 407
 Fourier transform infrared (FTIR)
 spectrometer 196–204, 206, 208, 210
 Fourier-transform photocurrent spectroscopy (FTPS) 191, 195
 – data processing 198–206
 – experimental setup 196–198
 – measurement modes 208–211
 – quantum efficiency 195, 196
 – sample preparation 206–208
 free energy 579
 free-bound (FB) transitions 283–284
 Fresnel equations 218
 Fresnel fringes 411
 FTIR, *see* Fourier transform infrared (FTIR) spectrometer
 FTPS, *see* Fourier-transform photocurrent spectroscopy (FTPS)
 fullerene 4, 32, 209
- g**
 geminate recombination 150, 152, 158
 generalized gradient approximation (GGA) 601
 generalized Kirchhoff's law 277
 generalized Planck's law 277
 generation function 56
 glow discharge mass spectroscopy 523, 525, 529–532
 glow discharge optical emission spectroscopy 523, 525, 529–531
 goniometer 174
 grain boundaries 356–360, 376, 384, 624, 659, 660, 663, 665–667
 grating 165, 173
 grazing incidence X-ray diffraction (GIXRD) 424–430
 GW method 604

h

- Hall measurement 121
Hahn-echo function 306
 Hamaker constant 345
 Hecht plot 130
 high injection condition 276
 hopping 123
 Hough space 376
 hydrogen effusion 569–570, 573–592
 – data analysis 573–592
 – experimental setups 570
 – passivation 5
 – surface desorption 579
 hydrogenated amorphous silicon (a-Si:H) 27–29, 178–182, 209, 210, 228–231, 587–588, 635–638
 hydrogenated microcrystalline silicon (μ c-Si:H) 29–30, 182–183, 209, 211, 590–591, 638–639

i

- ideality factor 46, 47, 52, 661
 in-line electron holography 409–412
 instrumental line shape 204–205
 interface recombination 52
 interface states 113
 interfacial barrier 54
 interference 12, 56, 57, 62, 63, 165, 422, 423, 431
 inverse photoemission spectroscopy (IPES) 504, 505
 ion bombardment 545, 548
 ion-beam sputtering 539

k

- Kelvin probe force microscopy (KPFM) 350–352
 kesterite 21, 27
 Kikuchi pattern 375
 Kirchhoff's law 7
 – Würfel's generalization 7
 Kramers–Kronig transformation 108, 225, 226, 436

l

- Lambert–Beer law 426
 Lambertian distribution 11
 Langevin recombination 156
 Laplace transform 143
 Large-scale atomic/molecular massively parallel simulator (LAMMPS) 622
 laser 80, 127, 194, 197, 201–204, 211
 – dye 127
 laser light scattering (LLS) 454–459

- LDA, *see* local density approximation (LDA)
 least squares regression 226
 lifetime 15, 18, 28, 45, 49, 65, 171, 172, 276, 660, 663, 665, 666
 light scattering 257, 258, 263, 267, 272
 light trapping 5, 10–13, 19–21, 257, 260, 263, 266, 272
 light-induced degradation 180
 light-induced ESR (LESR) 305
 light-soaking 180
 light-trapping 257, 266
 liquid-phase crystallized Si 30–31
 local density approximation (LDA) 601
 local magnification effect (LME) 558
 lock-in amplifier 195, 208
 long-range order 125

m

- Malus's Law 221
 Maxwell–Boltzmann approximation 634
 mean-inner potential 409
 metal-halide perovskite solar cells 31–32
 metastability 115
 Meyer–Neldel rule 110, 112–113
 microcrystalline germanium 183
 micromorph tandem solar cells 30
 micro-PL 293
 microRaman configuration 475
 Miller indices 423
 misfit dislocations 624, 626
 mobility 10, 15, 16, 18, 21, 28, 29, 44, 93, 108, 114, 123, 130, 166, 170, 172
 – edge 136
 – gap 28
 – lifetime product 164
 molecular dynamics 621–623
 monochromator 194, 195, 209
 Monte Carlo simulation 382
 Mueller matrices 224
 multijunction solar cell 59, 78
 multiple-trapping model 133, 136–140
 multithrough-interface model 650–651

n

- nanoparticles 4, 32, 33
 near-field scanning optical microscopy 391
 neutron scattering 421–423, 431–434
 non-contact mode atomic force microscopy 346
 nongeminate recombination 158, 159
 nonradiative recombination 17–19, 665
 Nose–Hoover dragging forces 622

o

off-axis electron holography 409–412
 Ohm’s law 166
 open-circuit voltage 8, 9, 16–18, 21, 54
 optical emission spectroscopy
 (OES) 445
 optical transitions 275, 282
 organic 4, 6, 11, 21, 31–33, 147–149, 152,
 154, 157, 158, 195
 OTRACE 157

p

parasitic absorption 55, 56, 65
 Parrinello–Rahman algorithm 622
 partial electron yield 505
 passage effect 304
 PC1D program 654
 perovskite 4, 21, 31, 32, 209
 phase correction 206
 photocapacitance 93, 111–112
 photoconductivity 164
 photocurrent 8, 13, 44, 48, 49, 60,
 63, 64, 66
 – decay 123
 photoelectron spectroscopy 502
 photoluminescence 386
 – calibration 280
 – setup 278
 photomultiplier tube 528
 photon flux 277
 photon recycling 78
 photothermal deflection spectroscopy (PDS)
 63, 193–195
 plasmon 540
 point defects 607
 – formation energies 613–614
 – thermodynamics 609–613
 – ZnO 614–617
 Poisson equation 163, 409, 662
 polarization 166, 173, 215–218, 220, 221,
 223, 224, 252
 polarized light 217–218, 223
 polymer 4, 32, 209
 post-transit 124, 139
 potential fluctuations 285
 pre-transit 124
 profilometer 538
 pulse (p) ESR 306

q

QMC, *see* quantum Monte Carlo (QMC)
 method
 quadrupole 533, 570

quantum efficiency 55, 56, 58, 60–64, 66,
 195, 196, 201, 209, 227, 237, 248, 251, 263,
 268
 – of a light emitting diode 76, 77
 – of a solar cell 73–76
 quantum Monte Carlo (QMC) method 604
 quasi-Fermi level 46
 – splitting 276, 277

r

radiative lifetime 276
 Raman microscopy 477–479
 Raman spectroscopy 444, 470–472, 481
 rate-limiting effusion processes 575–578
 Rayleigh scattering 471
 real-time *in situ* characterization 442
 reciprocity 72, 75, 76, 88
 recombination 44–47, 52–56, 60, 63, 65,
 71–77, 79, 82, 180, 181, 387, 662, 663,
 665–669
 recombination current density 44
 reflection 11, 13, 19, 20, 55, 56, 62
 reflection coefficients 216, 218, 252
 reflection of high energy electrons 445
 refractive index 11, 164, 216, 218, 221, 252,
 260–262, 266, 426
 relative sensitivity factor 530
 remote electron beam induced current 395
 resonant inelastic (soft) X-ray scattering 505
resonant Raman effects 477
 Rietveld analysis 431–433
 Ritter–Zeldov–Weiser analysis 167–170
 rotating-analyzer SE 221–222
 rotating-compensator SE 222–224
 Rutherford scattering 401

s

SAED, *see* selected-area electron diffraction
 saturation current density 44, 47, 53
 – Shockley–Queisser theory 9
 Savitzky–Golay filter 543
 SC-Simul program 654–655
 scanning capacitance microscopy (SCM)
 348–350
 scanning electron microscopy (SEM) 371,
 412–413
 scanning near-field optical microscopy
 (SNOM) 257–272
 scanning TEM 397
 scanning tunneling microscopy 352–353,
 391
 SCAPS 102, 654
 scattering cross section 423
 Schottky contact 663

- secondary electrons 372, 373
 secondary ion mass spectroscopy (SIMS) 248, 523, 532–539, 574
 secondary neutral mass spectrometry 535
 selected-area electron diffraction 401
 selenisation 23
 Sentaurus Device 661
 series resistance 47, 48, 50–52, 81, 82, 85, 95, 96, 106
 sheet resistance 72, 84, 85, 87
 Shockley–Queisser theory 6–9, 44, 55
 Shockley–Read–Hall (SRH) recombination 15, 45, 60, 639–641
 short-circuit current density 7, 8, 12, 13, 15, 16, 18, 44, 49–53, 55
 shunt 47, 48, 52, 82–84, 661, 668
 site-specific sample preparation 558
 small signal response 95
 Snell's law 164, 218
 space charge region 13, 45–47, 53, 96, 100, 101, 104–106
 spatial inhomogeneities 113–115, 293
 spectral absorptivity 277
 spectral response 55, 60
 spectroscopic ellipsometry (SE) 56, 251, *see also* ellipsometry
 spectrum imaging 387
 SPICE program 48, 661, 662
 spontaneous emission rate 275
 sputter deposition 22
 sputtered neutral mass spectroscopy 523
 S-shape 16
 stacking fault 625–627
 Staebler–Wronski effect 29
 steady-state photocarrier grating (SSPG)
 method 163
 – dark conductivity 170
 – data analysis 175–177
 – diffusion length 167–170
 – DOS determination 184
 – experimental setups 173–175
 – mobility-lifetime products 172
 – optical model 164–166
 – semiconductor equations 166–167
 – trapped charge 170
 Stillinger–Weber potential 623, 629
 Stokes vectors 224
 substrate 20, 22, 23, 28
 superposition principle 8, 60, 88
 superstrate 4, 19, 20, 28
 surface recombination 15–19, 170, 179
 surface recombination velocity 75, 79, 80, 382
 surface-enhanced Raman scattering (SERS) 480
 synchrotron-assisted growth analysis 441
t
 tail 10, 17, 82, 170, 181
 – states 151, 156
 tandem solar cell 59, 265
 Tauc–Lorentz (TL) oscillator 236
 TDCF, *see* time-delayed collection field method (TDCF)
 temperature-programmed desorption 570
 thermal desorption spectroscopy 570
 thermal velocity 18
 thermalization 6, 30
 thermometry 443
 thin-film solar cell simulation
 – basic equations 633
 – CdTe solar cells 645
 – Cu(In,Ga)(S,Se)₂ solar cells 643
 – density of states 635
 – flat interfaces 649
 – recombination statistics 643
 – rough interfaces 649–651
 – tools
 – AFORS-HET 651–653
 – AMPS-1D 653
 – ASA 653–654
 – PC1D 654
 – SCAPS 654
 – SC-Simul program 654–655
 three-stage deposition process for CIGS 241, 242, 245, 246, 248
 three-stage process 23
 time-delayed collection field method (TDCF) 147, 154, 157–159
 time-of-flight mass spectrometer 528
 time-of-flight (TOF) analysis 121, 147, 155, 159
 – anomalous dispersion 123–125
 – basic procedure 122
 – caveats 135
 – density of states 141–142
 – multiple-trapping model 136–140
 – spatial charge distribution 140
 – vertical time-of-flight experiments 126–128
 tip-enhanced Raman spectroscopy (TERS) 480
 topography 384
 total electron yield 505
 total internal reflection 11
 TPV, *see* transient photovoltage (TPV)
 transient photocapacitance spectroscopy 111

transient photovoltaic (TPV) 147–149, 152
 transit time 123, 131, 134
 transmission electron microscopy (TEM)

- 371, 396, 413–415, 625, 626
- bright-field 398
- conventional (CTEM) 398
- cross sectional 238
- dark-field 398
- energ-filtered (EFTEM) 403
- high resolution (HR-TEM) 400
- scanning (STEM) 398
- transparent-conductive oxide (TCO) 25, 665
- trap 46, 94, 100–114, 123, 136, 137, 139, 387
- trapped charge 166, 170
- tripod polishing 414–415
- tritium 574
- tunneling luminescence microscopy 392
- tunnelling enhanced recombination 46
- two-diode model 47
- type inversion 26

u

ultraviolet-excited photoelectron spectroscopy 502
 undersampling 202
 Urbach tail 191, 236, 247

v

vapor deposition simulations 623–625
 vibrational modes 472
 virtual interface analysis 225, 226, 232, 244
 voids 235, 242, 246, 582, 586, 589–591

w

waveguide mode 258, 266–268
 wavelength-dispersive X-ray spectrometry 433
 white light reflectometry (WLR) 459–462
 Wong/Green theorem 86
 workfunction 547

x

X-ray absorption spectroscopy 504
 X-ray diffraction 376, 424, 431
 X-ray emission spectroscopy 503
 X-ray-excited Auger electron spectroscopy 503
 X-ray-excited photoelectron spectroscopy 502
 X-ray fluorescence 408, 547, 552
 X-ray photoelectron spectroscopy (XPS) 523, 539, 546–551
 X-rays 421–427, 431, 432
 X-ray scattering 421, 422
 X-ray spectrometry
 – energy-dispersive 378
 – wavelength-dispersive 378

z

Z contrast imaging 374, 401
 zero filling 200–202
 ZnO/CdS/Cu(In,Ga)Se₂ heterojunction 23
 ZnO films
 – hydrogen effusion measurements 591
 – point defects 614–617

