

## Index

### a

*ab initio* molecular dynamics simulations 51  
 actinide carbides 155  
 actinide nitrides 160  
 adiabatic calorimetry 185, 186  
 advanced ceramics  
 – applications 27  
 alkoxide tetraethyl-ortho-silicate (TEOS) 451  
 Allen–Cahn equation 263  
 alternating network structures  
 – generation 45  
 aluminum titanate 83  
 aluminum tracer diffusion 106  
 amorphous intergranular film (IGF) 237  
 amorphous silicon oxycarbide  
 – structure 60  
 amphibole asbestos 87  
 anion volume diffusion 136  
 anisotropic crystallization 377  
 Arrhenius parameter  
 – behavior 140, 152  
 – plot 110, 119, 141, 144  
 – relations 106  
 associate model 190  
 atomic absorption spectroscopy (AAS) 22  
 atomic cluster methods 269  
 atomic emission spectroscopy (AES)  
 – techniques 21  
 atomic force microscopy (AFM) 158  
 atomistic methods 259  
 atomistic structure 41  
 Auger electron spectroscopy (AES) 22, 158

### b

barium titanate (BT) 456  
 bend stress relaxation (BSR) tests 522  
 binary oxides  
 – ceramics 4  
 – crystal chemistry 73

bioglass ceramics 378  
 – bioactivity 390, 393  
 – biocompatibility 390, 391  
 bismuth lanthanum titanate (BLT) 459  
 Boltzmann factor 268  
 Boltzmann's equation 189  
 bomb calorimetry 186  
 bond switching algorithm, *see* WWW-method  
 borates  
 – structural principles 89  
 boron-based materials 316  
 boron nitride (BN) 218  
 bottom-up approach 12  
 braiding methods  
 – circular braiding 527  
 – through-the-thickness braiding 527, 528  
 brittle fracture 2

### c

cabbage structures 389  
 Cahn–Hilliard diffusion equation 263  
 calcia-stabilized zirconia (CSZ) 110  
 calcium aluminosilicate (CAS) 31  
 calculation of phase diagrams (CALPHAD)  
 method 184, 187, 188  
 carbon fiber-reinforced composites 560  
 carbon fiber-reinforced plastics (CRFP) 522  
 carbon fibers 522  
 cart house structures 388  
 cation diffusion 112, 114, 122  
 cation-doping 252  
 cationic alkyltrimethylammonium 328  
 cation interdiffusion 118  
 cellular ceramics 409, 437  
 – properties 412  
 – structure 410  
 ceramic fiber composites 566  
 – ballistic armor applications 574  
 – energy-related applications 569

- friction-related applications 572
  - processes to fabricate 525
  - properties 550
  - space-related applications 566
  - ceramic fiber mats 436
  - ceramic injection-molding 11
  - ceramic materials
    - thermochemical properties 185
  - ceramic matrix composite (CMC) 31
  - scopes 513
  - ceramic microstructure
    - determinants 241
  - ceramic nanocomposites 351
    - properties 366
    - thermal shock resistance 370
  - ceramic powders
    - manufacture 183
    - preparation 4
    - synthesis 3
  - ceramics
    - amorphous phases in 246
    - introduction to 236
    - modeling 258
    - problems 237
    - slip casting 6
    - theory 258
  - ceramic structures
    - electrochemical approaches 308
    - from condensed phase 310
  - ceramic thermal barrier coatings
    - phase equilibria in 207
  - ceramic thin films 445
  - cerium dioxide 79
  - cerium–oxygen system
    - thermodynamic modeling 191
  - cerium sesquioxide 192, 193
  - cermets 71
  - chemical gel films 462
  - chemical sensing application 29
  - chemical solution deposition (CSD)
    - process 283, 445
    - alkoxides 448
    - carboxylates 449
    - chemical solution route 466
    - $\beta$ -diketonates 450
    - fundamentals 446
    - heteroleptic precursors 450
  - chemical vapor deposition (CVD) 11, 283, 306, 350, 435, 515
    - process 13, 534
  - chemical vapor infiltration (CVI) 530, 534
  - chemistry-based transformations 338
  - chimie douce techniques 312
  - classical powder method 20
  - Clausius–Clapeyron equation 199
  - closed cell foams 418
  - cluster variation method (CVM) 190
  - coarse-graining
    - concept 273
  - cold isostatic pressing (CIP) 6
  - colossal magnetoresistance (CMR)
    - films 454
    - oxides 475
  - complex oxide structures
    - perovskite-related structures 80
  - compound energy formalism (CEF) 190
  - computational approach 43
  - computational thermodynamics
    - methods 187
  - computer modeling studies 147
  - concurrent multiscale techniques 273
  - condensed-phase techniques 328
  - continuous random alternating networks (CRAN) 45
  - continuum modeling 260
  - continuum-phase field modeling 264
  - continuum thermodynamic model 281
  - conventional methods
    - of powder synthesis 283
  - coordination cluster model (CCM) 190
  - corundum ceramic 75
  - crack bridging mechanisms 245, 248
  - crack-free drying process 16
  - creep resistance 368
  - CSD-derived ceramic films
    - application 482
  - cubic boron nitride (CBN) 10
  - CVD coating technique 537
  - CVD-derived polycrystalline material 163
  - cyclic voltammetry (CV) 492
- d**
- deep filtration mechanism 439
  - defect-chemical model 122
  - deflection mechanisms 245
  - density functional calculations 51
  - density functional theory (DFT) 51, 268
  - DFT-optimized structures 56
  - die pressing, *see* cold isostatic pressing (CIP)
  - differential scanning calorimetry (DSC) 186
  - differential thermal analysis (DTA) 185
  - direct coagulation casting (DCC) 11
  - direct current plasma (DCP) 22
  - direct-inkjet printing (DIP) 11
  - doped corundum materials 75
  - drop solution calorimetry 186
  - dry chemical synthesis 350

**e**

- edge-defined film-fed technique 517
- electrical conductivity relaxation 141
- electrochemical approaches 299
  - porous ceramic films 328
- electrochemical impedance spectroscopy (EIS)
  - measurements 491
- electrochemical template techniques 308
- electromagnetic radiation (EMR)
  - measurements 496
- electron-beam techniques 479
- electron energy loss near edge structure (ELNES) 23
- electron energy loss spectroscopy (EELS) 22, 23
- electronic structure effects 259
- electron microscopy 24
- electron probe microanalysis (EPMA) 135
- electron spectroscopy techniques 21
- electrophoretic deposition (EPD)
  - technique 301, 537
- electrospinning 300, 309
- electrostatic spray deposition technique 330
- electrothermal vaporization 22
- embedded capacitors 483
- empirical method 62
- empirical potential approach 51
- energy band structure 269
- energy dispersive X-ray (EDX) analysis 136, 386
- energy dispersive X-ray spectroscopy 25
- environmental barrier coating (EBC) 31
- equal channel angular pressing (ECAP) 350
- evaporation-induced self assembly (EISA)
  - technique 323
- extrinsic shielding mechanisms 25

**f**

- fabrication methods 434
- face-centered cubic lattice 202
- ferroelectric random access memories (FeRAM) 482
- fiber integration
  - in the matrix 529
- fiber preforms 525
- fibers
  - basic considerations 514
  - for ceramic composites 514
  - general features 514
- Fick's equation 110
- field-assisted compaction method 9
- field-assisted sintering (FAS), *see also* spark plasma sintering (SPS) 351, 363, 364
  - field-activated sintering technique (FAST) 9
    - plasma-activated sintering (PSA) 9
    - pulse electro-discharge consolidation 9
- field emission scanning electron micrographs (FESEM) 460
- film densification 461
- finite element modeling (FEM) 261
  - atomic FEM 262
  - extended FEM (XFEM) 262
- first-principles atomic cluster method 278
- first-principles density functional method 268
- floating-zone technique 148
- fluidic templating techniques 303, 306
- fluorite oxides 109
- forced-flow thermal gradient CVI 536
- Forchheimer's equation 430
- Fourier transform infrared (FTIR) spectroscopy 456, 470
- free surface phenomena 246
- freeze-drying technique 359
- freeze granulation technique 359
- frequency agile microwave electronics (FAME) devices 488
- fresnoite glass ceramics 396
- fundamental building block (FBB) 90

**g**

- garnets 83
- gas-phase
  - analysis 141
  - infiltration 15
- gas-phase mass spectrometry 141
- gas-phase reaction 5
- gas-phase technique 306
- generalized gradient approximation (GGA) 51
- geometrical relaxation
  - interatomic potential 46
- geometrical structure 44
- Ginzburg–Landau equation 263
- glass ceramics 377
  - for mechanical application 385
  - with high hardness 386
  - with high strength 386
  - with low thermal expansion coefficients 383
- glassy pocket
  - interfaces 247
- gradient-CVI technique 534
- grain boundary diffusion 8, 115, 116, 124, 363
- grain boundary migration 363
- grain boundary segregation 242
- grain growth anisotropy 252

- grain reinforcement 245
- grand canonical Monte Carlo (GCMC) 278
- ground state microstructures 243
- GULP modeling studies 134
- h**
- hand-crafted laminating 538
- hard thermal shock parameter R1 426
- Haven ratio 109, 111
- He–Hutchinson diagram 543
- Heuer's survey 120
- hexagonal boron nitride (h-BN) 92
- high-alumina-content ceramics 438
- high-angle annular dark-field (HAADF) detector 255
- high-melting ceramics 150
- high-pressure neutron diffraction 185
- high-pressure X-ray diffraction 185
- high-resolution electron microscopy (HREM) technique 25
- high-resolution transmission electron microscopy (HRTEM) 224
- high-silica-content ceramics 438
- high-temperature electron microscopy 185
- high-temperature oxidation
  - of BTO ceramics 131
- high-velocity oxygen fuel (HVOF) spraying 350
- high-voltage atomic resolution electron microscopy (HVAREM) 25
- honeycomb structures
  - properties 419
- honing technology
  - long-stroke 11
  - short-stroke 11
- hot isostatic pressing (HIP) 8, 364
- hot press (HP) sintering 364
- hybrid approaches 455
- hybrid multiscale modeling approach 271
- hybrid quantum-classical potential scheme 276
- hydridopolysilazane precursor (HPZ) 520
- hydrogen diffusion
  - in Si-based ceramics 163
- hydrolysis-assisted solidification (HAS) 11
- hydrothermal methods 478
- hydrothermal process conditions 315–316
- i**
- ideal substitutional solution model 189
- IGF structural model
  - electronic structure 279
- image analysis techniques 410
- indium tin oxide (ITO) 314
- inductively coupled plasma (ICP) 22
- inductively coupled plasma atomic emission spectroscopy (ICP-AES) 22
- infrequent event systems 267
- injection-molding process 6, 7, 11
- interface chemistry 355
- interface growth model 281
- intergranular films
  - chemistry 250
  - in silicon nitride 278
  - interfaces 247
- international space station (ISS) 567
- International Thermonuclear Experimental Reactor (ITER) 571
- intrinsic hydrogen diffusivity 165
- isostatic pressing 6
- j**
- Janecke prism 214
- k**
- keating-like valence-force model 46
- keating-potential approach 47
- Keramiklech flame tubes 576
- kinetic Monte Carlo (kMC) method 268
- Knoop technique 25
- l**
- La gallates values 145
- laminated object manufacturing (LOM) 11
- Landolt–Bornstein series 72
- lanthanides 118
- lanthanum chromite system 132
- lanthanum cobaltate 145
- Laplace equation 16
- laser-induced breakdown excitation sources (LIBS) 22
- lattice parameters 473
- lattice-structured foams 418
- Lazy Pulverix code 72
- light-emitted stimulation emission of radiation (LASER) 318
- liquid crystal display (LCD) 33
- liquid crystal templating approach 312
- liquid-phase sintering 7, 10, 360
- liquid polymer infiltration (LPI) 530
- liquid silicon infiltration (LSI) 531
- local density approximation (LDA) 51, 269
- localized point defects 157
- low-density models
  - of Si<sub>3</sub>N<sub>4</sub> 65
- low-density networks 50
- lower activation enthalpies 157
- low-frequency dielectric properties 485

- low temperature co-fired ceramics (LTCC) 459  
 low-temperature techniques 351
- m**
- machinable glass ceramics 378, 388  
 magic-angle spinning nuclear magnetic resonance (MAS NMR)  
 – pulse method 400  
 magnetron-sputtered films 156, 158, 165, 166  
 Maxwell's stability criterion 414  
 McLachlan equation 428  
 melt-quench approach 41, 42, 56  
 mercury porosimetry 410  
 mesophase pitch (MPP), *see* polyacrylonitrile (PAN)  
 mesoscaled ceramic structures  
 – synthetic routes 299  
 mesoscopic thin film synthesis 459  
 metallo-organic chemical vapor deposition (MOCVD) 445, 477, 482  
 metallo-organic decomposition (MOD) 445, 451  
 metal plasma immersion methods 537  
 Metropolis algorithm 49, 64  
 micro-electromechanical system 13, 459.  
   *see also* nano-electromechanical system 13  
 microemulsion-mediated technique 459  
 micro sintering, *see* milliwave sintering  
 microstructural design  
 – factors 244  
 microwave dielectric thin films 485  
 microwave frequencies 485  
 – phase-shifter characteristics 487  
 microwave-frequency assisted CVD 535  
 microwave-induced plasma (MIP) 22  
 microwave sintering 8  
 milliwave sintering 364  
 minimum solid area (MSA) model 413  
 mixed spinel phase 207  
 modified-vacuum-infusion (MVI) 531  
 molecular beam epitaxy (MBE) 482  
 molecular dynamics (MD) 41, 236  
 – accelerated MD methods 267–268  
 – advantages 265  
 – classical 265  
 – interatomic interactions 265  
 molecular precursor technique 318  
 monolithic functional ceramics 125  
 monolithic polycrystalline alumina 357  
 Monte Carlo (MC) methodology 49, 268  
 morphotropic phase boundary (MPB) 499  
 multiferroic thin films 495  
 multi-layer ceramic capacitor (MLCC) 33, 459  
 multiscale methodologies 271  
 multi-wall carbon nanotubes (MWCNT) 371
- n**
- nanocrystalline coatings 350  
 nano-electromechanical systems 13  
 nano-inclusions  
 – formation 354  
 nano glass ceramics 402  
 nano infiltration and transient eutectics (NITE) process 539  
 nano test tubes 312  
 near-net-shape technologies 11  
 near-net-shape weaving 527  
 network algorithm 46  
 network-forming systems 42  
 Neumann–Kopp rule 199  
 neutron diffraction (ND) 24  
 nitridosilicates  
 – structural principles 95  
 nitrogen self-diffusion 160  
 non-brittle composites 540  
 non-centrosymmetric space group 93  
 non-fluorite-structured oxide 109  
 non-gelling films 462  
 non-ionic poly-ethyleneoxide 328  
 nonlinear optical (NLO) materials 90  
 non-Newtonian flow 398  
 non-oxide ceramics  
 – diffusion 149  
 non-oxide fibers  
 – Si-based 518  
 non-stationary nucleation rate 381  
 non-tetrahedral connectivity 46  
 nuclear magnetic resonance (NMR) 253, 456  
 nuclear reaction analysis (NRA) 149  
 nuclear resonance reflectivity 159  
 nucleation rate 379
- o**
- Oak Ridge National Laboratory (ORNL) 534  
 one-dimensional (1-D) ceramic structures 308, 318  
 optimum foam density 424  
 oriented glass ceramics  
 – kinetic control 395  
 – routes to 394  
 – thermodynamic control 395  
 oxidation protection systems (OPS) 567  
 oxide fibers 516  
 oxygen diffusion 109, 120, 124

- oxygen self-diffusion 141
- oxygen tracer diffusion 106, 139, 145
  - coefficient 140
- oxygen vacancy
  - diffusion coefficients 141
- p**
- PARATEC code 56
- partial Schottky equilibrium 126
- perovskite group
  - complex perovskites 125
- perovskite structure 82
- phase diagrams
  - determination 184
  - dynamic methods 184
  - static methods 184
- phase field method (PFM) 244, 262, 263
- phosphor-converted light-emitting diode (pc-LED) 96
- photonic technologies 378
- physical gel films 462
- physical vapor deposition (PVD) 283, 350
- piezoceramics 28
- piezoelectric films
  - for MEMS 498
- plasma spraying 350
- polyacrylonitrile (PAN) 524
- polycarbosilanes (PCS) 20, 518
- polycrystalline diamond (PCD) 10
- polycrystalline lead zirconium titanate (PLZT) ceramics 81
- polycrystalline samples 156
- polycrystalline silicon-based materials 163
- polycrystalline silicon nitride 157
- polycrystalline zirconia ceramics 241
- polymer-derived ceramic (PDC) 18, 166
- polymer-derived material 67
- polymer-derived SiC fibers 519
- polymer infiltration and pyrolysis (PIP)
  - process, *see* liquid polymer infiltration (LPI)
- poly(organo)silazanes 20
- poly(organo)siloxanes 19
- polysilanes 20
- polysilylcarbodiimides 20
- poly(titano) carbosilane (PTC) 518
- porous cellular structure model 333
- positive electrode materials 490
- potential intermittent titration technique (PITT) 491
- potential step chronoamperometry (PSCA) 491
- potentiostatic step measurements 146
- pre-ceramic polymers 160
- pressure-assisted consolidation
  - methods 8
- pressure pulsed CVI 535
- printed wiring boards (PWB) 484
- probabilistic design codes 237
- pulsed-laser deposition (PLD) 28
- pulse electric current sintering 364
- q**
- quantum chemical methods 270
- quantum interactions 236
- quantum molecular dynamics (QMD) 265
- quasi-continuum method 261, 273
- quenching method 184
  - advantage 185
- r**
- radioactive tracers 155
- radiotracer methods 112, 149
- rapid-CVI 536
- rapid densification process 9
- rapid prototyping 333
- rapid thermal annealing (RTA) 447
- rare earth additions
  - adsorption behavior 254
- rare-earth metal oxides (REO) 30
- reactive force field (RFF) methodologies 271, 276
- reactive melt infiltration (RMI),
  - see* liquid silicon infiltration (LSI)
- relic process 515
- resin transfer molding (RTM) process 530
- reticulated ceramics 435
- reverse microemulsion technique 312
- reversible polyamorphic transitions 267
- rolling assisted biaxially textured substrates (RABiTs) 485
- Rutherford backscattering spectrometry (RBS) 149
- s**
- scanning transmission electron microscopy (STEM) 255
- Schottky defect formation 129, 156
- Schrödinger equation 268
- Scientific Group Thermodata Europe (SGTE) 189
- SciFinder system 72
- secondary ion mass spectrometry (SIMS) 106, 149
- selective laser sintering (SLS) 11
- self-assembly approach 477
- self-consistent field (SCF) method 269
- self-organization technique 316

- self-propagating high-temperature synthesis (SHS) 364
- self-reinforced microstructures 249
- self-reinforced silicon nitride (SRSN) 238
- serpentine asbestos 87
- shallow-bed filtration mechanism 439
- shear stress 398
- short-lived radioactive isotopes 162
- SiCN network model 62
- silicon-based polymers 19
- silicon carbides 150
- silicon carbonitrides 160
- silicon nitride-based material 43
- silicon nitride ceramics 250
- silicon oxycarbide glasses 19
- silicon tracer diffusion 106
- simple conceptual model 278
- simulated annealing process 49, 265
- simulation method 261
- single crystal fiber concept 517
- single-edge notch beam tests (SENB) 550
- single-line-injection (SLI) 531
- single-wall carbon nanotubes (SWCNT) 371
- sinoite  
– structure 97
- sintered glass ceramics 377
- sintering process 7  
– reactive process 8
- slow crack growth 246
- small-angle scattering (SAS) 24
- small angle X-ray spectroscopy (SAXS) 326
- smear-out thermal vacancies 162
- sol-gel process 15, 17, 18, 451
- sol-gel synthetic approach 301
- sol-gel techniques 302
- solid electrolyte interface (SEI) films 492
- solid freeform fabrication (SFF) 11
- solid oxide fuel cells (SOFC) 29, 197, 440
- solid-state NMR spectroscopy 22
- solid-state sintering 359
- spark plasma sintering (SPS) 9, 351, 363, 364
- spectroscopic techniques 456
- spinel phases  
– modeling 202
- spinel structure 82
- spray pyrolysis 307
- stereolithography process 333
- stress-strain curve 416
- strontium bismuth niobate (SBN) 459
- strontium bismuth tantalate (SBT) 459
- strontium titanate (ST) 456
- strontium-doped lanthanum manganite 330
- structure-directing templates 323
- structure-insensitive properties 261
- structure-property relationships 469
- surfactant-mediated template methods 316
- suspension processes 458
- Sylramic fibers 519
- synthetic techniques 323
- t**
- tailor ceramic microstructure  
– approaches to 243
- tape casting technique 7, 459
- temperature coefficient of capacitance (TCC) 488
- temperature tunneling  
magneto-resistance 475
- template-assisted fabrication 316
- template-assisted methods 312
- template-steered approach 318
- template-steered sol-gel templating 333
- templating technique  
– for non-siliceous ceramics 323  
– using monodisperse spheres 328
- tetraethyl orthosilicate 309
- thermal barrier coating (TBC) 30, 207
- thermal expansion coefficient 26
- thermal processing parameters 471
- thermal shock phenomenon 425
- thermal shock resistance 425
- thermal spraying 350
- thermodynamic modeling 201, 244  
– parameters 188
- thermodynamic properties  
– of liquid 193
- thermogravimetry (TG) 185
- thick film synthesis 451
- thin film electrodes  
– for Li ion rechargeable batteries 490
- thin-film multilayer capacitor (TMC) 483
- thin film synthesis, *see* thick film synthesis
- three-dimensional (3-D) ceramic structures 332, 349  
– condensed-phase routes 333  
– electrochemical routes 333
- three-dimensional nanostructures 475
- three-dimensional periodic structures 436
- three-dimensional piezoresponse force microscopy (PFM) 477
- titanate perovskites 126  
– cation diffusion 126  
– in oxygen diffusion 137
- titaniozirconate (PZT) ceramic 333
- topological relaxations  
– simulated annealing 49
- topological structure 44

- tracer  
 – diffusion 118  
 – interdiffusion 118  
 – self-diffusion studies 157  
 tractable theory 238  
 transient-enhanced diffusion process (TED) 153  
 transition metal carbides 154  
 transition metal diffusion 166  
 transition metal nitrides 157  
 translationengleiche subgroup 93  
 transmission electron microscopy (TEM) 19, 24, 326, 386, 463  
 – image 356  
 transparent conducting oxide (TCO) material 325  
 trap-limited diffusion mechanism 163, 165  
 trifluoroacetic acid (TFA)-based process 485  
 two-dimensional ceramic structures 323  
 two-step sintering 351, 363
- u**  
 universal property-porosity curve 419  
 UV-emitting medical lamps 90
- v**  
 vacancy diffusion coefficient 141, 145  
 vapor–liquid solid (VLS) process 307  
 vapor–solid (VS) process 307  
 Vegard's law 66  
 Vickers technique 25  
 Vienna Ab-Initio Simulation Package (VASP) 51  
 viscoelastic models 262  
 VLS growth type mechanism 312  
 volatile organic compound (VOC) 439
- w**  
 weak interface composites (WIC) 514, 541  
 weak matrix composites (WMC) 514, 541, 547  
 weaving technique 527  
 Weibull modulus 417  
 wet chemical synthesis, *see* dry chemical synthesis  
 wet-shaping techniques 359  
 Whipple model 158  
 wurtzite-type modification 93  
 wurtzite-type structure 73, 74  
 WWW-method 42, 43
- x**  
 X-ray absorption fine structure (XAFS) 22  
 – extended (EXAFS) 22, 155, 325, 456  
 X-ray absorption near edge structures (XANES) 22, 325  
 X-ray absorption spectra (XAS) 22  
 X-ray diffraction (XRD) 24, 386, 477  
 X-ray microtomography (XMT), *see* electron microscopy  
 X-ray photoelectron spectroscopy (XPS) 22, 253, 496  
 X-ray tomography 410
- y**  
 Yajima process 18, 20  
 Young's modulus 262, 412, 553  
 yttria-stabilized zirconia (YSZ) 29, 110, 207, 314, 330  
 yttrium dislocations diffusivities 117
- z**  
 Zachariasen's model 41  
 zeolites 89  
 zircon dioxide 79