

Index

a

aggregate of spheres 8, 34, 187
 aggregate theory 198, 202
 Agricola, G. 5
 amorphous glasses 107
 amorphous solids 1, 8, 43, 75, 81, 92, 100, 123, 141, 151, 202, 215, 227, 236
 – atomic arrangements 3
 amorphous solids model
 – disordered clusters 121
 – geometrical model 121
 – irregular clusters 123
 – molecular dynamics 123
 – Monte Carlo method 124
 – packing of spheres 119
 – regular, incongruent clusters 121
 – X-ray diffraction patterns 120
 amorphous thin films 119
 amorphousness 1, 59, 63, 113, 120, 187
 Anglo-Saxon glass 107
 Angstrom, A. J. 7
 angular separation 10, 15, 19, 55
 Archimedes density 92
 argon glass
 – atomic radius 126
 – crystalline and amorphous cluster 132
 – density 126
 – physical parameters 126
 – round cell simulation
 – configuration distribution functions 129
 – coordination distribution function 129
 – vs. MD simulation 129
 – radial distribution function 129
 – Voronoi volume 129
 – volume–temperature graph 126
 – X-ray scattering 131
 argon, amorphous 15, 125, 131, 199–201
 AsGeSe glass

 – atomic arrangements
 – FSDP 186
 – IAS model 184
 – modified IAS model 186
 – coordination distribution 182
 – enthalpy of bond formation 181
 – glass transition temperature 184
 – interatomic distances 180
 – X-ray scattering pattern 183
 atomic scattering factor 99
 atomistic, simulation 3, 200, 212, 218, 239
 Avogadro, A. 7
 axiom 59, 60

b

Bernal, J.D. 3, 6, 22, 46
 Biruni, Al 5
 blocking function 20, 56
 blocking model 19, 20, 23, 86
 Born–Oppenheimer approximation 5
 Bragg's law 96
 Bravais, A. 1, 31, 37, 45, 52, 68
 Brownian motion 38
 Buckingham potential 14

c

calcite 6
 calibration 104, 149
 calorimetry, for glass transition measurement 103
 chalcogenide glass 116, 180, *see also* AsGeSe glass
 – IR optoelectronics and photonics 180
 – rewriteable (DVD+RW) optical disk 180
 chaos 38
 chord, distance 10
 circumradius 76

- close packing 4, 19, 23, 30, 35, 64, 80, 83, 87, 88, 120, 125, 215, 245
 - closed packing 40, 88, 95, 120, 132
 - closing vector 26, 30, 32
 - cluster(s)
 - configuration
 - – irregular crystals 26
 - – radial vector construction 27, *see also* random walks
 - – regular crystals 25
 - – spherical harmonics 33
 - coordination number
 - – blocking model 19
 - – definition 18
 - – Fürth model 22
 - irregular 17, 26, 40, 55, 123, 148, 236
 - – configuration 26
 - random 18, 22, 110, 124
 - regular
 - – configuration 25
 - – cubic geometry 16
 - – definition 15
 - – tetrahedral geometry 15
 - of spheres 8, 11, 15, 25, 36, 52, 75, 88, 132, 143, 236, 243
 - coercivity 33
 - combinatorics 22
 - concept, of atoms 4
 - concordant 237, 242
 - condensed matter 9, 50, 244
 - configuration 17, 25, 31, 41, 50, 75, 79, 81, 115, 129, 143, 171, 175, 193, 242
 - configuration distribution functions 82
 - argon glass 129
 - MgCuGd alloy 145
 - conical angle 10
 - contact configuration function 50
 - contact, point 10, 65, 68, 71, 85
 - convex polyhedron 78
 - convex, body 9
 - cooling, rate 4, 111, 125
 - coordination distribution function 75
 - argon glass 129
 - AsGeSe glass 182
 - MgCuGd alloy 143
 - NiNb alloy 133
 - ZrTiCuNiBe alloy 159
 - coordination, number 75, 81, 85, 114, 123, 129, 132, 181, 242
 - coordination, shell 10, 41, 44, 48, 80, 121, 181
 - correspondence, principle 63
 - crystal, lattice 2, 37
 - crystallography 66, 72, 81, 95, 111
 - geometrical 1
 - cubic, packing 5, 16, 21, 80, 126, 133, 180, 197, 219
 - cumulative distribution function 20, 22, 25
- d**
- datum 1
 - Debye equation 23, 33, 52, 98, 100, 120, 137, 138, 151, 165, 174, 177, 183, 184, 186
 - Delaunay simplexes 52
 - Delaunay tessellation 76
 - density 5, 17, 24, 35, 47, 67, 80, 103, 108, 112, 126, 132, 138, 141, 155, 167, 174, 202, 219, 233
 - MgCuGd alloy
 - – amorphous alloy 156
 - – crystalline alloy 156
 - NiNb alloy
 - – amorphous alloy 139
 - – crystalline alloy 139
 - of amorphous solid 92
 - of composite 93
 - of crystalline solid 92
 - of single phase 92
 - ZrTiCuNiBe alloy
 - – amorphous alloy 168
 - – crystalline alloy 168
 - – Vitreloy alloy 169
 - density functional theory (DFT) 15
 - differential scanning calorimeter (DSC)
 - for crystalline sapphire and diamond 104
 - for metallic glass and semi-crystalline polymers 104
 - parts of 103
 - types of 103
 - for Zr-based amorphous metallic glass 104
 - diffraction 7, 96, 102, 116, 122, 149, 159, 183
 - diffusion 67, 110, 194, 232, 234, 243
 - dislocation 194, 209, 218, 225
 - disordered crystalline solids 2
 - disordered materials 2
 - disordered sphere packing 37
 - DSC, *see* differential scanning calorimeter (DSC)
 - ductile materials 192
- e**
- Ehrenfest formula 100, 101, 131, 183
 - elasticity
 - atomistic elasticity
 - – acoustic method 201
 - – bond stiffness 200
 - – solid fcc Argon 200
 - continuum mechanics
 - – aggregate theory 198

- – elastic constants 199
- – elastic strain energy 199
- – homogeneous deformation 196
- – strain ellipsoid 195
- – transverse isotropy 198
- – undeformed state 195
- – uniaxial elongation 198
- – uniaxial tension 196
- phenomenology 193
- electron, density 5, 98
- electronic, orbitals 4
- end-to-end distance 28, 31, 82
- entropy 50
- equilateral, triangle 15, 76, 80, 121
- equilibrium, separation 13, 39, 92, 109, 170, 199, 240
- Eshelby inclusion 241
- Euclidean distance, space 1, 9, 68, 77
- Euler polyhedra theorem 78
- exclusion, condition, zone 10, 19, 39

f

Fürth model 22

first sharp diffraction peak (FSDP) 183, 186

fixed sphere packing 30, 36, 40, 41, 67

flat plate camera, side-on geometry of 98

flaw, imperfection 66, 168, 215

fluctuations, density 24, 38, 88, 103, 108, 143, 158, 178, 245

Fourier transform 96, 99

fracture mechanics 204

- defects, role of 210
- elastic strain energy 207
- fracture toughness 204, 209
- Griffith's fracture stress 209
- phenomenology 203
- solid surface energy 208
- theoretical cleavage strength 212
- theoretical shear strength 213

free volume 51, 68, 86, 113, 132, 229, 234, 243

Frenkel theoretical strength 213

FSDP, *see* first sharp diffraction peak (FSDP)

Furth, R. 22, 40

g

Galileo Galilei 191

Gaussian function 42, 63, 110, 154

Gaussian random walk (GRW) 28, 29, 32, 82, 175

glass 47, 57, 68, 77

inorganic 64

metallic 64, 71, 104

transition 68, 103, 156

glassmaking 107

graphical user interface (GUI) 55, 142, 159

Green's strain energy 240

Green's theorem 242

Griffith's theory 206

h

Hamiltonian 51, 108

hard sphere(s) 12, 13

- condition 62, 70, 83, 91, 120, 140
- random sequential addition 38

Hauy, R.J. 1, 5, 6

heat flux calorimeter 103

heavy metal fluoride glass 116

hexagonal, arrangement 4, 123

hexagonal, packing 4, 35, 80, 180

high entropy alloys (HEA) 115

homogeneity of point field 35, 61

Hooke's law 193

Hooke, R. 4, 193

Huygens sum 52

i

Ideal amorphous solids (IAS) 52, 56, 60, 65, 69, 100, 143, 148, 188

- class I 64
- class II 64
- class III 66
- imperfections
- – categories 66
- – density 69
- – geometrical flaws 67
- – statistical flaws 68
- – statistical flaws
- – kappa function 68
- – zeta function 69

Ideal amorphous solids (IAS) model

- argon
- – atomic radius 126
- – crystalline and amorphous cluster 132
- – density 126
- – physical parameters 126
- – round cell simulation 127
- – volume–temperature graph 126
- – X-ray scattering 131
- AsGeSe glass 184
- construction
- – IAS parameters 58
- – IAS software 53
- – outer spheres 58
- – primary cluster creation 54
- – Round Cell 59
- – coordination numbers 52
- – geometrical construction 52
- MgCuGd alloy

Ideal amorphous solids (IAS) model (*contd.*)

- physical properties 140
- round cell simulation 141
- X-ray scattering 149
- NiNb alloy
 - physical properties 133
 - primary uses 133
 - round cell simulation 133
 - X-ray scattering 136
- packed spheres 187
- polyethylene
 - crystal structure 170
 - radial distribution function 171
 - specific volume 171
 - uses 170
 - X-ray scattering 173
- random atomic arrangement 51
- silica
 - formation 176
 - modified glasses 176
 - molecular parameters 176
 - round cell simulation 177
 - short range order 179
 - united atom model 177
 - X-ray scattering 177
- statistical functions 52
- X-ray scattering 52
- ZrTiCuNiBe alloy
 - mechanical properties 157
 - physical properties 157
 - round cell simulation 159
 - transmission electron microscopy 157
 - X-ray scattering 165
- ideal crystal 72, 83, 111
- ideal Greek solids 1, 53
- imperfection, defect 66, 102, 192, 210, 229
- incongruent 121
- indivisible, object 4
- inherently non-crystallizable (equable) glasses 114
- inhomogeneity 51
- inner sphere 10, 21, 36, 45, 55, 75, 83, 134, 159, 236
- inorganic glasses 116
- inorganic silica-based glasses 107
- intermolecular, forces 14, 112, 215
- irregular clusters 17, 40, 45, 54, 79, 236
 - blocking function 21
 - configuration 26
- irregular, triangle 56
- isosceles triangle 40, 56, 80, 121
- isotropy, point field 42, 61, 198, 202

j

- jammed, configuration 68, 77

k

- Kepler, J. 4

l

- lattice 7, 31, 45, 68, 69, 95, 112, 120, 200, 221
- Lennard–Jones potential 12, 14, 15, 200
- local relaxation event (LRE) 248
- London dispersion forces 14
- loose sphere packing 19, 36, 51, 67, 83
- Lorentz function 153
- Lucretius 4

m

- Markov chains 43
- mechanical behavior
 - elastic modulus of amorphous solids 202
 - elasticity 193
 - fracture 203
 - viscoelasticity 243
- metallic glass 49, 64, 71, 104, 114, 157, 166, 192, 239
- metastable 114, 238
- metastable (crystallizable) glasses 114
- Mg65–Cu25–Gd10 alloy 149, 155
- MgCuGd alloy
 - density
 - amorphous alloy 156
 - crystalline alloy 156
 - round cell simulation
 - atomic parameters 141
 - cluster composition 148
 - configuration distribution functions 145
 - coordination distribution functions 143
 - interatomic distances 146
 - vs. MD simulation 143
 - probability of contacts 147
 - radial distribution functions 143
 - X-ray scattering 149
- Miller indices 2, 6
- Miller, W.H. 6
- mineralogy 5
- Minkowski distance 78
- molecular dynamics 3, 13, 34, 46, 120, 123, 163
- Monte Carlo method 124
- motion invariance 42

n

- neighbour, touching 8, 15, 29, 36, 64, 69, 75, 143, 160, 187, 200, 236

- neighbouring, sphere 2, 9, 19, 43, 53, 79, 124, 220
- network 64, 76, 114, 120, 177
- Ni62-Nb38 alloy 138
- NiNb alloy
 - density
 - – amorphous alloy 139
 - – crystalline alloy 139
 - round cell simulation
 - – atomic parameters 133
 - – coordination distribution functions 133
 - – pair distribution function 135
 - – probability of contacts 135
 - – Voronoi volume 135
 - X-ray scattering 136
- 2-norm distance 77
- o**
- ordered cluster 17, 45, 70, 80, 121
- ordered packing 6, 36, 45, 76, 87
- ordered sphere packing 36
- organic glasses 117
- outer sphere 10, 18, 27, 36, 55, 75, 81, 134, 236
- p**
- packing, dense 49, 91, 119, 239
- packing, disordered 37
- packing, fraction 8, 35, 54, 68, 80, 85, 86, 129, 139, 157, 169
- packing, geometric 13
- packing, of spheres 3, 18, 34, 40, 41, 61, 69, 71, 82, 95, 119, 143, 171, 185
- packing, random 18, 34, 44, 60, 76, 84, 95, 113, 124, 164, 175
- pair distribution function (PDF) 49
 - NiNb alloy 135
- pattern, repeating 1
- Peierls–Nabarro stress 218
- percolation 47
- plasticity 215, 227
 - amorphous solids 227
 - continuum mechanics 217
 - crystalline solids, atomistic mechanics
 - – atoms displacement 224
 - – critical shear stress 226
 - – grain boundary strengthening 220
 - – plastic flow mechanism 224
 - – precipitation hardening 223
 - – solid solution hardening 221
 - – strain hardening 218
 - phenomenology 215
 - superplasticity
 - – bulk metallic glasses 234
- – concordant deformation mechanism 236
- – continuum mechanics 195
- – phenomenology 193
- Platonic solids 53
- Pliny the Elder 5
- polarity, cluster 33
- polyethylene
 - crystal structure 170
 - radial distribution function 171
 - specific volume 171
 - uses 170
 - X-ray scattering 173
- polygon 15, 43, 53, 76
- polyhedron 44, 53, 78
 - convex 78
 - topology of 79
- polytope 76
- potential 12, 95, 113, 129, 146, 161, 173, 199, 237
- power compensation calorimeter 103
- primary cluster 9, 18, 41, 54, 129, 148
- principle 2, 15, 53, 115, 120, 199, 225, 233
- probability 17, 22, 31, 43, 72, 81, 98, 124, 135, 146, 160, 204, 239
 - density 17, 38
- probability of contacts 50
 - MgCuGd alloy 147
 - NiNb alloy 135
 - ZrTiCuNiBe alloy 162
- properties, of matter 4
- pseudo-random 38
 - packing 41
- pseudo-randomness 38
- pulse echo technique 201
- Pythagoras 2
- r**
- radial distribution function
 - argon glass 129
 - MgCuGd alloy 143
 - polyethylene 171
 - silica glass 116
 - ZrTiCuNiBe alloy 161
- radial pair distribution function 50
- random closed packing 8, 24, 34, 38, 40, 46, 64, 76, 85
- random sequential addition (RSA) 38
- random sequential packing 39
- random sphere packing 38
- random walk, Gaussian (GRW) 28
- random walk, self avoiding, space limited (SASLRW) 28
- random walk, self-avoiding (SARW) 28

- random walks 28, 43, 83
 - Markov chains 43
- random, addition 16
- random, atomic arrangement 3, 21, 58, 69, 92, 103
- random, configuration 17, 61
- random, patterns 2, 66, 82
- randomness 21, 38
- rational ratios 2
- regular clusters 15, 21, 25, 32, 56, 122, 133
 - blocking function 21
 - configuration 25
 - cubic geometry 16
 - definition 15
 - polygon 15
 - shape 15
 - tetrahedral geometry 15
- representative volume element (RVE) 53, 71, 91
- rigidity 12, 52, 94
- rotational symmetry 16, 25, 71, 122, 132
- round cell 8, 54, 126, 134, 161, 176, 184
- round cell simulation
 - argon glass
 - – configuration distribution functions 129
 - – coordination distribution function 129
 - – vs. MD simulation 129
 - – radial distribution function 129
 - – Voronoi volume 129
 - MgCuGd alloy
 - – atomic parameters 141
 - – cluster composition 148
 - – configuration distribution functions 145
 - – coordination distribution functions 143
 - – interatomic distances 146
 - – vs. MD simulation 143
 - – probability of contacts 147
 - – radial distribution functions 143
 - NiNb alloy
 - – atomic parameters 133
 - – coordination distribution functions 133
 - – pair distribution function 135
 - – probability of contacts 135
 - – Voronoi volume 135
 - silica glass 177
 - ZrTiCuNiBe alloy
 - – atomic parameters 159
 - – coordination distribution function 159
 - – graphical user interface 159
 - – radial distribution functions 161
 - – Voronoi volume distribution 161
- 5
 - saturation density 39
 - scale invariance 35, 61
 - self-avoiding random walks (SARWs) 29, 31, 64
 - self avoiding space limited random walk (SASLRW) 29
 - silica glass
 - formation 176
 - modified glasses 176
 - molecular parameters 176
 - radial distribution function 116
 - round cell simulation 177
 - short range order 179
 - united atom model 177
 - X-ray scattering 177
 - simplex, simplicial 52, 76
 - soft spheres 12
 - solid, angle 19, 198
 - solidification 108, 111
 - solidity 36, 51, 62, 94, 193
 - solidity of packing 94
 - space-filling model 7
 - sphere packing characteristics 75
 - geometrical properties 75
 - – configuration distribution function 82
 - – coordination distribution function 75
 - – density 92
 - – packing fraction 85
 - – representative volume element 91
 - – solidity of packing 94
 - – tetrahedrality 76
 - – topology of clusters 79
 - – volume fraction 83
 - – Voronoi polyhedra notation 78
 - glass transition 103
 - X-ray scattering 96
 - sphere packings 35, 48, 53, 69, 87, 156
 - disordered packing 37
 - fixed 31, 36, 40, 67
 - loose 11, 19, 36, 39, 51, 67
 - ordered packing 36
 - random closed packing 40
 - random packing 38
 - spheres
 - definition 9
 - force
 - – electrical and magnetic forces 14
 - – gravitational forces 14
 - – interatomic forces 14
 - – work function 13
 - hard 4, 12, 13, 35
 - neighbours
 - – categories 9

- – coordination shell 47
- – touching neighbours 10
- – Voronoi tessellation 43
- random assemblage 18
- random closed packing 40
- soft 12
- unequal sizes 11
- spherical cap 10, 19
- spherical harmonics 27, 33
- statistical mechanics 47, 158
- statistics, mathematical 3, 71, 82
- Steno, N. 6
- strain ellipsoid 195
- superplasticity 231
 - bulk metallic glasses 234
 - concordant deformation mechanism
 - – density variation, amorphous solids 238
 - – transformation 241
 - continuum mechanics 195
 - phenomenology 193
- superplasticity: concordant deformation mechanism: 5-atom subcluster 236
- symmetry
 - rotational 1, 16, 25, 71, 122
 - translational 1, 52, 71

t

- tessellation 10, 43, 52, 76, 133
- tetrahedral 15, 44
- tetrahedrality 76
- tetrahedron 53
- tetrahedron, irregularity of
 - Gamma parameter 77
 - Minkowski measure 76
- theory of amorphousness 1
 - axioms 60
 - conjecture 61
 - rules 62
 - statistical correspondence 63
- topology 78
- topology of clusters
 - classification of 80
 - crystalline clusters 81
 - irregular clusters 81
 - ordered clusters 80
- touching spheres 10
- translational symmetry 1, 52, 71
- triangulation 44

u

- united atom model 177
- unpredictable 3

v

- van der Waals force 14
- vector, polygon 10, 26, 54, 59, 72
- viscoelasticity
 - phenomenology 243
 - temperature effect, viscoelastic behaviour 247
 - time and temperature dependent behaviour 245
- viscosity 15, 111, 176, 233, 244
- Vitreloy 157
- volume fraction 35, 83, 111, 139, 155, 167, 223
 - irregular polyhedra 84
 - regular polyhedra 84
 - Voronoi polyhedron 84
- volume, occupied 35, 92
- volume, unoccupied 35
- Voronoi polyhedra notation 78
- Voronoi tessellation 35, 43
- Voronoi volume distribution
 - argon glass 129
 - NiNb alloy 135
 - ZrTiCuNiBe alloy 161
- Voronoi, H. 46

w

- Warren method 179
- Weibull probability 204
- Wigner-Seitz cells 45

x

- X-ray diffractometer
 - for amorphous samples 96
- X-ray scattering 7, 52, 70, 96, 113, 131, 137, 150, 165, 175, 183
 - argon glass 131
 - diffraction and scattering, geometry of 96
 - factors affecting integrated scattered intensity 102
 - MgCuGd alloy 149
 - NiNb alloy 136
 - polyethylene 173
 - scattered wave, intensity of 97
 - silica glass 177
 - ZrTiCuNiBe alloy 165

y

- Young's modulus 201

z

- Zarzycki, J. 188
- ZrTiCuNiBe alloy
 - atomic probe 162

ZrTiCuNiBe alloy (*contd.*)

- clusters 165
- density
 - - amorphous alloy 168
 - - crystalline alloy 168
 - - Vitreloy alloy 169
- mechanical properties 157
- physical properties 157
- probability of contacts 162
 - round cell simulation
 - - atomic parameters 159
 - - coordination distribution function 159
 - - graphical user interface 159
 - - radial distribution functions 161
 - - Voronoi volume distribution 161
- transmission electron microscopy 157
- X-ray scattering 165