

Contents

Preface XI

1	Spheres, Clusters and Packing of Spheres	1
1.1	Introduction	1
1.2	Geometry of Spheres	9
1.2.1	A Sphere and Its Neighbours	9
1.2.2	Neighbours by Touching	10
1.2.3	Hard and Soft Spheres	12
1.3	Geometry of Clusters	15
1.3.1	Regular Clusters	15
1.3.2	Irregular Clusters	17
1.3.3	Coordination of $(1 + k)$ Clusters	18
1.3.3.1	Blocking Model for Cluster Formation	19
1.3.3.2	Fürth Model for Cluster Formation	22
1.3.4	Configuration of $(1 + k)$ Clusters	25
1.3.4.1	Regular Clusters	25
1.3.4.2	Irregular Clusters	26
1.3.4.3	Closing Vector Based on Radial Vector Polygon	27
1.3.4.4	Physical Meaning of the Closing Vector, ζ	32
1.3.4.5	Spherical Harmonics	33
1.4	Geometry of Sphere Packings	34
1.4.1	Fixed and Loose Packings	36
1.4.2	Ordered Packing	36
1.4.3	Disordered Packing	37
1.4.4	Random Packing	38
1.4.5	Random Sequential Addition of Hard Spheres	38
1.4.6	Random Closed Packing of Spheres	40
1.4.7	Neighbours by Voronoi Tessellation	43
1.4.8	Neighbours by Coordination Shell	47
1.4.8.1	Pair Distribution Function	49
1.4.8.2	The Probability of Contacts	50
1.4.8.3	Contact Configuration Function	50

1.5	Ideal Amorphous Aolid (IAS)	51
1.6	Construction of an Ideal Amorphous Solid Class I	53
1.7	Elementary Theory of Amorphousness	59
1.7.1	Background	59
1.7.2	The Axioms	60
1.7.3	Conjecture	61
1.7.4	The Rules	62
1.7.5	Statistical Correspondence	63
1.8	Classes of Ideal Amorphous Solids	64
1.8.1	IAS Class I: Random Close Packing of Individual Atoms	64
1.8.2	IAS Class II: Random Close Packing of Linear Model Chains	64
1.8.3	IAS Class III: Random Close Packing of Three-Dimensionally cross-Linked Chains	65
1.9	Imperfections in IAS	66
1.9.1	Geometrical (local) Flaws	67
1.9.2	Statistical (global) Flaws	68
1.9.3	The Effect of Flaws on the Density of IAS	69
1.9.4	Short and Medium Range Order	72
	References	72
	Books on Crystallography	74
	Books on Glasses	74
	Books on Random Walks	74
	Books on Sphere Packings	74
	Books on Crystal Imperfections	74
2	Characteristics of Sphere Packings	75
2.1	Geometrical Properties	75
2.1.1	The Coordination Distribution Function, $\Psi(k)$	75
2.1.2	Tetrahedricity	76
2.1.3	Voronoi Polyhedra Notation	78
2.1.4	Topology of Clusters	79
2.1.4.1	Ordered Clusters	80
2.1.4.2	Irregular Clusters	81
2.1.5	The Configuration Distribution Function, $\Phi_k(\zeta)$	82
2.1.6	The Volume Fraction	83
2.1.6.1	Regular Polyhedra	84
2.1.6.2	Irregular Polyhedra	84
2.1.7	The Packing Fraction	85
2.1.7.1	The Average Packing Fraction for the Round Cell	86
2.1.7.2	The Local Packing Fraction	87
2.1.7.3	The Limits of Packing Fraction	87
2.1.8	Representative Volume Element	91
2.1.9	Density of Single Phase	92
2.1.9.1	Density of Crystalline Solid	92
2.1.9.2	Density of Amorphous Solid	92

2.1.10	Density of a Composite	93
2.1.11	Solidity of Packing	94
2.2	X-ray Scattering	96
2.2.1	Introduction	96
2.2.2	Geometry of Diffraction and Scattering	96
2.2.3	Intensity of a Scattered Wave	97
2.2.3.1	Amorphous Solid	100
2.2.3.2	Ehrenfest Formula	100
2.2.3.3	Polyatomic Solid	101
2.2.4	Factors Affecting Integrated Scattered Intensity	102
2.2.4.1	Integrated Intensity of Powder Pattern Lines from Crystalline Body	102
2.2.4.2	Integrated Scattered Intensity from Monoatomic Body	102
2.3	Glass Transition Measured by Calorimetry	103
	References	104

3	Glassy Materials and Ideal Amorphous Solids	107
3.1	Introduction	107
3.1.1	Solidification	108
3.1.1.1	Solidification by Means of Crystallization	110
3.1.1.2	Solidification through Vitrification	111
3.1.2	Cognate Groups of Amorphous Materials (Glasses)	114
3.1.2.1	Metallic Glasses	114
3.1.2.2	Inorganic Glasses	116
3.1.2.3	Organic Glasses	117
3.1.2.4	Amorphous Thin Films	119
3.2	Summary of Models of Amorphous Solids	119
3.2.1	Lattice with Atomic Disorder	120
3.2.2	Disordered Clusters on Lattice	121
3.2.3	Geometric Models for Amorphous Networks	121
3.2.4	Packing of Regular but Incongruent Clusters	121
3.2.5	Irregular Clusters – Random Packing	123
3.2.6	Molecular Dynamics	123
3.2.7	Monte Carlo Method	124
3.3	IAS Model of a-Argon	125
3.3.1	IAS Parameters	126
3.3.2	Round Cell Simulation and Analysis	127
3.3.2.1	Coordination Distribution Function	129
3.3.2.2	Voronoi Volume and Configuration Distribution Functions	129
3.3.2.3	Radial Distribution Function	129
3.3.2.4	X-ray Scattering from the IAS Model	131
3.3.2.5	Crystalline and Amorphous Cluster	132
3.3.3	Summary of a-Ar IAS Structure	132
3.4	IAS Model of a-NiNb Alloy	133
3.4.1	Introduction	133

3.4.2	IAS Model of a-NiNb Alloy	133
3.4.2.1	Coordination Distribution Functions	133
3.4.2.2	Voronoi Volume Distribution	135
3.4.2.3	Pair Distribution Function	135
3.4.2.4	Probability of Contacts	135
3.4.3	X-ray Scattering from a-NiNb Alloy	136
3.4.3.1	Experimental Results	136
3.4.3.2	Theoretical Results	138
3.4.4	Density of a-Ni62-Nb38 Alloy	138
3.4.4.1	Crystalline Alloy	138
3.4.4.2	Amorphous Alloy	139
3.4.5	Summary of a-NiNb IAS Structure	140
3.5	IAS Model of a-MgCuGd Alloy	140
3.5.1	Physical Properties of the Elements	140
3.5.2	IAS Simulation of a-MgCuGd Alloy	140
3.5.2.1	Coordination Distribution Functions	143
3.5.2.2	Configuration Distribution Function	143
3.5.2.3	Radial Distribution Function	143
3.5.2.4	Probability of Contacts	147
3.5.2.5	Cluster Composition According to IAS	147
3.5.2.6	Cluster Composition According to MD	148
3.5.3	X-ray Scattering from a-Mg65-Cu25-Gd10 Alloy	149
3.5.3.1	Flat Plate X-ray Scattering Pattern	149
3.5.3.2	Calibration based on Si Powder Pattern	149
3.5.3.3	Uncertainties and Corrections	153
3.5.4	Density of Mg65-Cu25-Gd10 Alloy	155
3.5.4.1	Crystalline Alloy	155
3.5.4.2	Amorphous Alloy	156
3.5.5	Summary of a-MgCuGd IAS Structure	156
3.6	IAS Model of a-ZrTiCuNiBe Alloy	157
3.6.1	Transmission Electron Microscopy	157
3.6.2	IAS Simulation of Amorphous a-ZrTiCuNiBe Alloy	159
3.6.2.1	Coordination Distribution Function	159
3.6.2.2	Voronoi Volume Distribution	161
3.6.2.3	Radial Distribution Function	161
3.6.3	Atomic Probe of the a-ZrTiCuNiBe Alloy	162
3.6.3.1	Probability of Contacts	162
3.6.4	Selected Clusters from the a-ZrTiCuNiBe Alloy	165
3.6.5	X-ray Scattering from the a-ZrTiCuNiBe Alloy	165
3.6.6	Density of ZrTiCuNiBe Alloy	167
3.6.6.1	Crystalline Alloy	167
3.6.6.2	Amorphous Alloy	168
3.6.6.3	Vitreloy Alloys	169
3.6.7	Summary of a-ZrTiCuNiBe IAS Structure	169
3.7	IAS Model of a-Polyethylene (a-PE)	169

3.7.1	Radial Distribution Function	171
3.7.2	X-ray Scattering	173
3.7.2.1	Short-Range Order	174
3.7.3	Summary of a-PE IAS Structure	174
3.8	IAS Model of a-Silica (a-SiO ₂)	176
3.8.1	Molecular Parameters for SiO ₂	176
3.8.2	IAS and United Atom Models for SiO ₂	176
3.8.3	Summary of a-SiO ₂ IAS Structure	179
3.9	Chalcogenide Glasses	179
3.9.1	As12–Ge33–Se55 Chalcogenide Glass	180
3.9.2	Measured Coordination Distribution	181
3.9.3	Measured X-ray Scattering	182
3.9.4	Glass-Transition Temperature of AsGeSe Glasses	184
3.9.5	Models of Atomic Arrangements in AsGeSe Glass	184
3.9.5.1	IAS Model of AsGeSe Glass	184
3.9.5.2	Other Models of AsGeSe Glass	185
3.9.6	Summary of a-AsGeSe IAS Structure	186
3.10	Concluding Remarks	186
3.10.1	Chapter 3	186
3.10.2	Chapter 2	187
	References	187

4 Mechanical Behaviour 191

4.1	Introduction	191
4.2	Elasticity	193
4.2.1	Phenomenology	193
4.2.2	Continuum Mechanics	195
4.2.2.1	Calculation of Average Elastic Constants – Aggregate Theory	198
4.2.2.2	Green's Elastic Strain Energy	199
4.2.3	Atomistic Elasticity	200
4.2.3.1	Calculation of an Elastic Constant for Single Crystal of Argon	200
4.3	Elastic Properties of Amorphous Solids	202
4.3.1	Elastic Modulus of Amorphous Argon	202
4.4	Fracture	203
4.4.1	Phenomenology	203
4.4.2	Continuum Mechanics	204
4.4.2.1	Definition of Fracture Mechanics: Fracture Toughness	204
4.4.2.2	Elastic Strain Energy Release	207
4.4.2.3	Solid Surface Energy	208
4.4.2.4	Griffith's Fracture Stress	209
4.4.2.5	The Role of Defects	210
4.4.3	Atomistic Fracture Mechanics of Solids	212
4.4.3.1	Theoretical Cleavage Strength	212
4.4.3.2	Theoretical Shear Strength	213
4.5	Plasticity	215

4.5.1	Phenomenology	215
4.5.2	Continuum Mechanics	217
4.5.2.1	Tresca Yield Criterion	217
4.5.2.2	Huber–von Mises Criterion	217
4.5.3	Atomistic Mechanics of Crystalline Solids	218
4.5.3.1	Strain Hardening	218
4.5.3.2	Grain Boundary Strengthening	220
4.5.3.3	Solid Solution Hardening	221
4.5.3.4	Precipitation Hardening	223
4.5.3.5	Mechanisms of Plastic Flow in Crystalline Materials	224
4.5.3.6	Displacement of Atoms Around Dislocations	224
4.5.3.7	Critical Shear Stress to Move Dislocation	226
4.6	Plasticity in Plasticity: Amorphous Solids	227
4.6.1	Plastic Deformation by Shear Band Propagation	228
4.7	Superplasticity	231
4.7.1	Phenomenology	231
4.7.2	Continuum Mechanics	233
4.7.3	Superplasticity in Bulk Metallic Glasses	234
4.7.3.1	Calculation of Strain Rate for Superplasticity	234
4.7.4	Concordant Deformation Mechanism	236
4.7.4.1	Density Variation in Amorphous Solids	238
4.7.4.2	The ‘Inclusion’ Problem	240
4.7.4.3	The System without Transformation	240
4.7.4.4	The System with Transformation	241
4.7.4.5	Conclusions	242
4.8	Viscoelasticity	243
4.8.1	Phenomenology	244
4.8.2	Time- and Temperature-Dependent Behaviour	245
4.8.2.1	Definitions of Viscosity	245
4.8.2.2	Order of Magnitude Calculations	246
4.8.3	Temperature Effect on Viscoelastic Behaviour	247
4.8.3.1	Arrhenius Behaviour	247
4.8.3.2	Vogel–Fulcher – Tammann Behaviour	247
	References	248