

Contents

Preface	vii
1 Motivation and Overview	1
1.1 What Is a Heterogeneous Material?	1
1.2 Effective Properties and Applications	3
1.2.1 Conductivity and Analogous Properties	6
1.2.2 Elastic Moduli	7
1.2.3 Survival Time or Trapping Constant	8
1.2.4 Fluid Permeability	8
1.2.5 Diffusion and Viscous Relaxation Times	9
1.2.6 Definitions of Effective Properties	9
1.3 Importance of Microstructure	10
1.4 Development of a Systematic Theory	12
1.4.1 Microstructural Details	12
1.4.2 Multidisciplinary Research Area	14
1.5 Overview of the Book	17
1.5.1 Part I	17
1.5.2 Part II	18
1.5.3 Scope	19
I Microstructure Characterization	21
2 Microstructural Descriptors	23
2.1 Preliminaries	24

2.2	<i>n</i> -Point Probability Functions	25
2.2.1	Definitions	25
2.2.2	Symmetries and Ergodicity	28
2.2.3	Geometrical Probability Interpretation	32
2.2.4	Asymptotic Properties and Bounds	33
2.2.5	Two-Point Probability Function	34
2.3	Surface Correlation Functions	43
2.4	Lineal-Path Function	44
2.5	Chord-Length Density Function	45
2.6	Pore-Size Functions	48
2.7	Percolation and Cluster Functions	50
2.8	Nearest-Neighbor Functions	50
2.9	Point/ <i>q</i> -Particle Correlation Functions	57
2.10	Surface/Particle Correlation Function	58
3	Statistical Mechanics of Many-Particle Systems	59
3.1	Many-Particle Statistics	60
3.1.1	<i>n</i> -Particle Probability Densities	60
3.1.2	Pair Potentials	65
3.2	Ornstein–Zernike Formalism	72
3.3	Equilibrium Hard-Sphere Systems	75
3.3.1	Low-Density Expansions	79
3.3.2	Arbitrary Fluid Densities	81
3.4	Random Sequential Addition Processes	83
3.4.1	One-Dimensional Identical Hard Rods	85
3.4.2	Identical Hard Spheres in Higher Dimensions	87
3.4.3	General Hard-Particle Systems	88
3.5	Maximally Random Jammed State	88
3.5.1	Random Close Packing Is Ill-Defined	89
3.5.2	Definition of Maximally Random Jammed State	90
3.5.3	Order Metrics	92
3.5.4	Molecular Dynamics Simulations	93
3.5.5	Concluding Remarks	95
4	Unified Approach to Characterize Microstructure	96
4.1	Volume Fraction and Specific Surface	97
4.1.1	Bounding Properties	100
4.1.2	Example Calculations	102
4.2	Canonical Correlation Function H_n	104
4.2.1	Definitions	105
4.2.2	Asymptotic Properties	109
4.3	Series Representations of H_n	109
4.3.1	Mayer Representation	110

4.3.2	Kirkwood–Salsburg Representation	111
4.3.3	Bounding Properties	112
4.4	Special Cases of H_n	114
4.5	Polydispersivity	116
4.6	Other Model Microstructures	118
5	Monodisperse Spheres	119
5.1	Fully Penetrable Spheres	120
5.1.1	n -Point Probability Functions	122
5.1.2	Surface Correlation Functions	124
5.1.3	Lineal-Path Function	125
5.1.4	Chord-Length Density Function	127
5.1.5	Nearest-Neighbor Functions	128
5.1.6	Pore-Size Functions	128
5.1.7	Point/ q -Particle Correlation Functions	129
5.2	Totally Impenetrable Spheres	129
5.2.1	n -Point Probability Functions	130
5.2.2	Surface Correlation Functions	134
5.2.3	Lineal-Path Function	136
5.2.4	Chord-Length Density Function	137
5.2.5	Nearest-Neighbor Functions	139
5.2.6	Pore-Size Functions	151
5.2.7	Point/ q -Particle Correlation Functions	152
5.3	Interpenetrable Spheres	153
5.3.1	Nearest-Neighbor Functions	154
5.3.2	Volume Fraction	155
5.3.3	Specific Surface	155
5.3.4	Pore-Size Functions	157
5.3.5	Other Statistical Descriptors	157
5.4	Statistically Inhomogeneous Systems	158
6	Polydisperse Spheres	160
6.1	Fully Penetrable Spheres	161
6.1.1	n -Point Probability Functions	163
6.1.2	Surface Correlation Functions	164
6.1.3	Lineal-Path Function	165
6.1.4	Chord-Length Density Function	166
6.1.5	Nearest-Surface Functions	166
6.1.6	Pore-Size Functions	167
6.1.7	Point/ q -Particle Correlation Functions	167
6.2	Totally Impenetrable Spheres	167
6.2.1	n -Point Probability Functions	169
6.2.2	Surface Correlation Functions	170

6.2.3	Lineal-Path Function	171
6.2.4	Chord-Length Density Function	171
6.2.5	Nearest-Surface Functions	172
6.2.6	Pore-Size Functions	176
6.2.7	Point/ q -Particle Correlation Functions	176
7	Anisotropic Media	177
7.1	General Considerations	177
7.2	Fully Penetrable Oriented Inclusions	179
7.3	Impenetrable Oriented Inclusions	181
7.4	Hierarchical Laminates	183
8	Cell and Random-Field Models	188
8.1	Cell Models	188
8.1.1	Voronoi and Delaunay Tessellations	189
8.1.2	Cell Statistics	192
8.1.3	Symmetric-Cell Materials	194
8.1.4	Random Checkerboard	199
8.1.5	Ising Model	201
8.2	Random-Field Models	203
8.2.1	General Considerations	203
8.2.2	Gaussian Convolved Intensities	207
9	Percolation and Clustering	210
9.1	Lattice Percolation	211
9.1.1	Bond and Site Percolation	211
9.1.2	Percolation Properties	215
9.1.3	Scaling and Critical Exponents	217
9.1.4	Infinite Cluster and Fractality	222
9.1.5	Finite-Size Scaling	223
9.2	Continuum Percolation	224
9.2.1	Percolation Properties	227
9.2.2	Two-Point Cluster Function	230
9.2.3	Critical Exponents	231
10	Some Continuum Percolation Results	234
10.1	Exact Results for Overlapping Spheres	234
10.1.1	One Dimension	235
10.1.2	Higher Dimensions	240
10.1.3	Low-Density Expansions of Cluster Statistics	242
10.2	Ornstein–Zernike Formalism	243
10.3	Percus–Yevick Approximations	245
10.3.1	Permeable-Sphere Model	246

10.3.2	Cherry-Pit Model	248
10.3.3	Sticky Hard-Sphere Model	249
10.4	Beyond Percus–Yevick Approximations	250
10.5	Two-Point Cluster Function	250
10.6	Percolation Threshold Estimates	251
10.6.1	Overlapping Disks and Spheres	252
10.6.2	Nonspherical Overlapping Particles	254
10.6.3	Interacting Particle Systems	255
11	Local Volume Fraction Fluctuations	257
11.1	Definitions	258
11.2	Coarseness	260
11.2.1	General Formula	260
11.2.2	Asymptotic Formula	261
11.2.3	Calculations	262
11.3	Moments of Local Volume Fraction	264
11.4	Evaluations of Full Distribution	265
12	Computer Simulations, Image Analyses, and Reconstructions	269
12.1	Monte Carlo Simulations	270
12.1.1	Introduction	270
12.1.2	Importance Sampling	271
12.2	Metropolis Method for Gibbs Ensembles	273
12.2.1	Markov Chain	273
12.2.2	Algorithm	275
12.2.3	Practical Implementation	275
12.2.4	Hard Spheres	277
12.2.5	Other Particle Systems	278
12.2.6	Cell Models	279
12.3	Methods for Generating Nonequilibrium Ensembles	279
12.4	Sampling in Particle Systems	281
12.4.1	Radial Distribution Function	281
12.4.2	n -point Probability Functions	283
12.4.3	Surface Correlation Functions	285
12.4.4	Cluster-Type Functions	285
12.4.5	Other Correlation Functions	286
12.5	Sampling Images and Digitized Media	287
12.5.1	Two-Point Probability Function	289
12.5.2	Lineal-Path Function	291
12.5.3	Chord-Length Density Function	292
12.5.4	Pore-Size Functions	292
12.5.5	Two-Point Cluster Function	293

12.6	Reconstructing Heterogeneous Materials	294
12.6.1	Reconstruction Procedure	295
12.6.2	Illustrative Examples	297
II	Microstructure/Property Connection	303
13	Local and Homogenized Equations	305
13.1	Preliminaries	306
13.2	Conduction Problem	308
13.2.1	Local Relations	308
13.2.2	Conduction Symmetry	311
13.2.3	Model One-Dimensional Problem	313
13.2.4	Homogenization of Periodic Problem in \mathfrak{R}^d	315
13.2.5	Homogenization of Random Problem in \mathfrak{R}^d	318
13.2.6	Frequency-Dependent Conductivity	321
13.3	Elastic Problem	321
13.3.1	Local Relations	321
13.3.2	Elastic Symmetry	324
13.3.3	Homogenization of Random Problem in \mathfrak{R}^d	332
13.3.4	Heterogeneous Materials	334
13.3.5	Relationship Between Elasticity and Viscous Fluid Theory	337
13.3.6	Viscosity of a Suspension	338
13.3.7	Viscoelasticity	339
13.4	Steady-State Trapping Problem	339
13.4.1	Local Relations	341
13.4.2	Homogenization of Random Problem in \mathfrak{R}^d	341
13.5	Steady-State Fluid Permeability Problem	344
13.5.1	Local Relations	345
13.5.2	Homogenization of Random Problem in \mathfrak{R}^d	346
13.5.3	Relationship to Sedimentation Rate	348
13.6	Classification of Steady-State Problems	349
13.7	Time-Dependent Trapping Problem	350
13.7.1	Basic Equations	350
13.7.2	Relationship Between Survival and Relaxation Times	353
13.8	Time-Dependent Flow Problem	354
13.8.1	Basic Equations	354
13.8.2	Relationship Between Permeability and Relaxation Times	356
14	Variational Principles	357
14.1	Conductivity	359
14.1.1	Field Fluctuations	359
14.1.2	Energy Representation	361

14.1.3	Minimum Energy Principles	363
14.1.4	Hashin–Shtrikman Principle	367
14.2	Elastic Moduli	368
14.2.1	Field Fluctuations	369
14.2.2	Energy Representation	370
14.2.3	Minimum Energy Principles	373
14.2.4	Hashin–Shtrikman Principle	377
14.3	Trapping Constant	379
14.3.1	Energy Representation	379
14.3.2	Minimum Energy Principles	380
14.4	Fluid Permeability	383
14.4.1	Energy Representation	383
14.4.2	Minimum Energy Principles	385
15	Phase-Interchange Relations	390
15.1	Conductivity	390
15.1.1	Duality for Two-Dimensional Media	390
15.1.2	Three-Dimensional Media	397
15.2	Elastic Moduli	398
15.2.1	Two-Dimensional Media	398
15.2.2	Three-Dimensional Media	401
15.3	Trapping Constant and Fluid Permeability	402
16	Exact Results	403
16.1	Conductivity	404
16.1.1	Coated-Spheres Model	404
16.1.2	Simple Laminates	407
16.1.3	Higher-Order Laminates and Attainability	410
16.1.4	Fiber-Reinforced Materials	413
16.1.5	Periodic Arrays of Inclusions	413
16.1.6	Low-Density Cellular Solids	415
16.1.7	Field Fluctuations	416
16.2	Elastic Moduli	417
16.2.1	Coated-Spheres Model	417
16.2.2	Simple Laminates	419
16.2.3	Higher-Order Laminates and Attainability	424
16.2.4	Periodic Arrays of Inclusions	426
16.2.5	Low-Density Cellular Solids	428
16.2.6	Equal Phase Shear Moduli	429
16.2.7	Sheets with Holes	429
16.2.8	Dispersions of Particles in a Liquid	429
16.2.9	Cavities (Bubbles) in an Incompressible Matrix (Liquid)	429
16.2.10	Field Fluctuations	430

16.2.11	Link to Two-Dimensional Conductivity	430
16.2.12	Link to Thermoelastic Constants	431
16.3	Trapping Constant	432
16.3.1	Diffusion Inside Hyperspheres	432
16.3.2	Periodic Arrays of Traps	433
16.4	Fluid Permeability	434
16.4.1	Flow Between Plates and Inside Tubes	434
16.4.2	Periodic Arrays of Obstacles	436
17	Single-Inclusion Solutions	437
17.1	Conduction Problem	437
17.1.1	Spherical Inclusion	437
17.1.2	Polarization Within an Ellipsoid	441
17.2	Elasticity Problem	442
17.2.1	Spherical Inclusion	442
17.2.2	Polarization Within an Ellipsoid	448
17.3	Trapping Problem	451
17.3.1	Spherical Trap	451
17.3.2	Spheroidal Trap	453
17.4	Flow Problem	455
17.4.1	Spherical Obstacle	455
17.4.2	Spheroidal Obstacle	457
18	Effective-Medium Approximations	459
18.1	Conductivity	459
18.1.1	Maxwell Approximations	460
18.1.2	Self-Consistent Approximations	462
18.1.3	Differential Effective-Medium Approximations	467
18.2	Elastic Moduli	470
18.2.1	Maxwell Approximations	470
18.2.2	Self-Consistent Approximations	474
18.2.3	Differential Effective-Medium Approximations	477
18.3	Trapping Constant	479
18.4	Fluid Permeability	481
19	Cluster Expansions	485
19.1	Conductivity	486
19.1.1	Dilute Dispersions of Spheres	488
19.1.2	Dilute Dispersions of Ellipsoids	490
19.1.3	Nondilute Concentrations	491
19.2	Elastic Moduli	496
19.2.1	Dilute Dispersions of Spheres	497
19.2.2	Dilute Dispersions of Ellipsoids	500

19.2.3 Nondilute Concentrations	501
19.3 Trapping Constant	502
19.3.1 Dilute Dispersions of Spherical Traps	502
19.3.2 Dilute Dispersions of Spheroidal Traps	503
19.3.3 Nondilute Concentrations	504
19.4 Fluid Permeability	505
19.4.1 Dilute Beds of Spheres	505
19.4.2 Dilute Beds of Spheroids	506
19.4.3 Nondilute Concentrations	507
20 Exact Contrast Expansions	509
20.1 Conductivity Tensor	510
20.1.1 Integral Equation for Cavity Electric Field	511
20.1.2 Strong-Contrast Expansions	514
20.1.3 Some Tensor Properties	519
20.1.4 Weak-Contrast Expansions	520
20.1.5 Expansion of Local Electric Field	521
20.1.6 Isotropic Media	521
20.2 Stiffness Tensor	530
20.2.1 Integral Equation for the Cavity Strain Field	530
20.2.2 Strong-Contrast Expansions	534
20.2.3 Weak-Contrast Expansions	539
20.2.4 Expansion of Local Strain Field	540
20.2.5 Isotropic Media	541
21 Rigorous Bounds	552
21.1 Conductivity	554
21.1.1 General Considerations	554
21.1.2 Contrast Bounds	555
21.1.3 Cluster Bounds	563
21.1.4 Security-Spheres Bounds	564
21.2 Elastic Moduli	566
21.2.1 General Considerations	566
21.2.2 Contrast Bounds	568
21.2.3 Cluster Bounds	576
21.2.4 Security-Spheres Bounds	577
21.3 Trapping Constant	578
21.3.1 Interfacial-Surface Lower Bound	579
21.3.2 Void Lower Bound	580
21.3.3 Cluster Lower Bounds	581
21.3.4 Security-Spheres Upper Bound	582
21.3.5 Pore-Size Upper Bound	584

21.4	Fluid Permeability	585
21.4.1	Interfacial-Surface Upper Bound	585
21.4.2	Void Upper Bound	586
21.4.3	Cluster Upper Bounds	587
21.4.4	Security-Spheres Lower Bound	589
21.5	Structural Optimization	590
21.6	Utility of Bounds	592
22	Evaluation of Bounds	593
22.1	Conductivity	594
22.1.1	Contrast Bounds	594
22.1.2	Cluster Bounds	609
22.1.3	Security-Spheres Bounds	610
22.2	Elastic Moduli	611
22.2.1	Contrast Bounds	611
22.2.2	Cluster Bounds	620
22.2.3	Security-Spheres Bounds	620
22.3	Trapping Constant	621
22.3.1	Interfacial-Surface Lower Bound	621
22.3.2	Void Lower Bound	623
22.3.3	Cluster Lower Bounds	624
22.3.4	Security-Spheres Upper Bound	625
22.3.5	Pore-Size Upper Bound	625
22.4	Fluid Permeability	627
22.4.1	Interfacial-Surface Upper Bound	627
22.4.2	Void Upper Bound	629
22.4.3	Cluster Upper Bounds	630
22.4.4	Security-Spheres Lower Bound	631
23	Cross-Property Relations	632
23.1	Conductivity and Elastic Moduli	633
23.1.1	Elementary Bounds	633
23.1.2	Translation Bounds for $d = 2$	636
23.1.3	Translation Bounds for $d = 3$	642
23.2	Flow and Diffusion Parameters	647
23.2.1	Permeability and Survival Time	647
23.2.2	Permeability, Formation Factor, and Viscous Relaxation Times	650
23.2.3	Viscous and Diffusion Relaxation Times	654
A	Equilibrium Hard-Disk Program	656
B	Interrelations Among Two- and Three-Dimensional Moduli	661

CONTENTS	xxi
References	663
Index	693

— This is page xxii
Printer: Opaque this