

# Contents

<b>Preface</b>	<b>vii</b>
<b>1 Motivation and Overview</b>	<b>1</b>
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
<b>I Microstructure Characterization</b>	<b>21</b>
<b>2 Microstructural Descriptors</b>	<b>23</b>
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
<b>3</b>	<b>Statistical Mechanics of Many-Particle Systems</b>	<b>59</b>
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
<b>4</b>	<b>Unified Approach to Characterize Microstructure</b>	<b>96</b>
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
<b>5</b>	<b>Monodisperse Spheres</b> . . . . .	<b>119</b>
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
<b>6</b>	<b>Polydisperse Spheres</b> . . . . .	<b>160</b>
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
<b>7</b>	<b>Anisotropic Media</b>	<b>177</b>
7.1	General Considerations . . . . .	177
7.2	Fully Penetrable Oriented Inclusions . . . . .	179
7.3	Impenetrable Oriented Inclusions . . . . .	181
7.4	Hierarchical Laminates . . . . .	183
<b>8</b>	<b>Cell and Random-Field Models</b>	<b>188</b>
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
<b>9</b>	<b>Percolation and Clustering</b>	<b>210</b>
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
<b>10</b>	<b>Some Continuum Percolation Results</b>	<b>234</b>
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
<b>11</b>	<b>Local Volume Fraction Fluctuations</b>	<b>257</b>
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
<b>12</b>	<b>Computer Simulations, Image Analyses, and Reconstructions</b>	<b>269</b>
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 $\mathbb{R}^d$ . . . . .	315
13.2.5	Homogenization of Random Problem in $\mathbb{R}^d$ . . . . .	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 $\mathbb{R}^d$ . . . . .	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 $\mathbb{R}^d$ . . . . .	341
13.5	Steady-State Fluid Permeability Problem . . . . .	344
13.5.1	Local Relations . . . . .	345
13.5.2	Homogenization of Random Problem in $\mathbb{R}^d$ . . . . .	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
<b>15</b>	<b>Phase-Interchange Relations</b>	<b>390</b>
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
<b>16</b>	<b>Exact Results</b>	<b>403</b>
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
<b>17 Single-Inclusion Solutions</b>	<b>437</b>
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
<b>18 Effective-Medium Approximations</b>	<b>459</b>
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
<b>19 Cluster Expansions</b>	<b>485</b>
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
<b>20</b>	<b>Exact Contrast Expansions</b>	<b>509</b>
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
<b>21</b>	<b>Rigorous Bounds</b>	<b>552</b>
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
<b>22</b>	<b>Evaluation of Bounds</b>	<b>593</b>
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
<b>23</b>	<b>Cross-Property Relations</b>	<b>632</b>
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
<b>A</b>	<b>Equilibrium Hard-Disk Program</b>	<b>656</b>
<b>B</b>	<b>Interrelations Among Two- and Three-Dimensional Moduli</b>	<b>661</b>

CONTENTS	xxi
<b>References</b>	<b>663</b>
<b>Index</b>	<b>693</b>



Random Heterogeneous Materials  
Microstructure and Macroscopic Properties  
Torquato, S.  
2002, XXI, 703 p. 111 illus., Hardcover  
ISBN: 978-0-387-95167-6