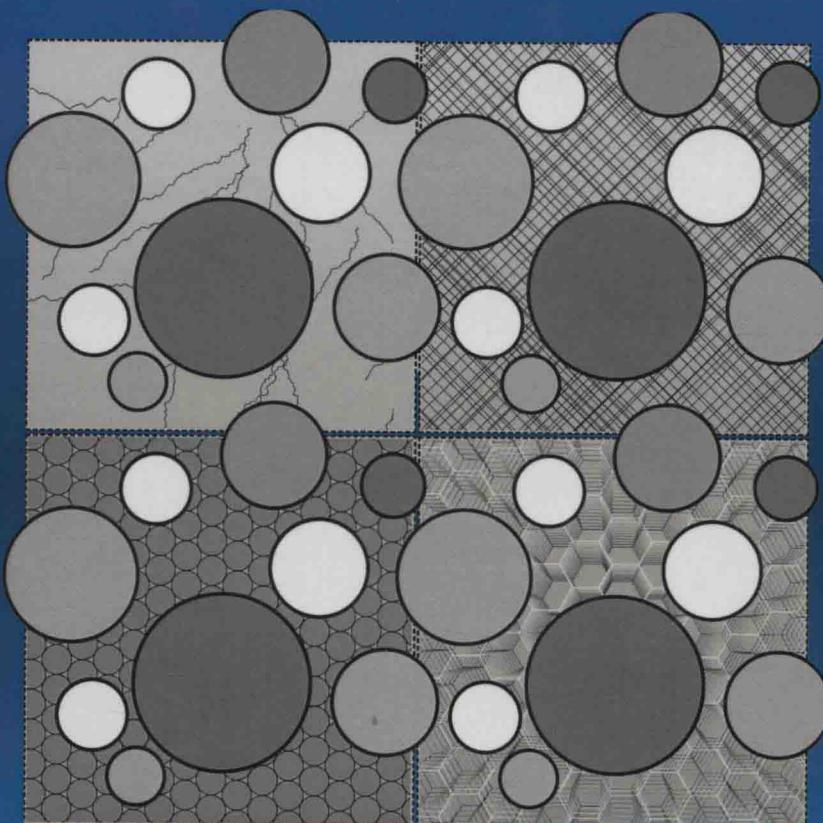


Micromechanics of Composites

Multipole Expansion Approach



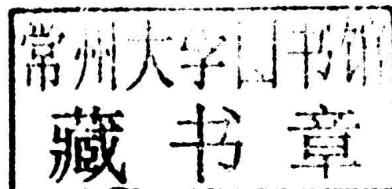
Volodymyr I. Kushch



Micromechanics of Composites

Multipole Expansion Approach

Volodymyr I. Kushch



AMSTERDAM • BOSTON • HEIDELBERG • LONDON
NEW YORK • OXFORD • PARIS • SAN DIEGO • SAN FRANCISCO
SINGAPORE • SYDNEY • TOKYO
Butterworth-Heinemann is an imprint of Elsevier



Butterworth-Heinemann is an imprint of Elsevier
The Boulevard, Langford Lane, Kidlington, Oxford, OX5 1GB, UK
225 Wyman Street, Waltham, MA 02451, USA

© 2013 Elsevier Inc. All rights reserved.

First edition 2013

No part of this publication may be reproduced, stored in a retrieval system or transmitted in any form or by any means electronic, mechanical, photocopying, recording or otherwise without the prior written permission of the publisher.

Permissions may be sought directly from Elsevier's Science & Technology Rights Department in Oxford, UK: phone (+44) (0) 1865 843830; fax (+44) (0) 1865 853333; email: permissions@elsevier.com. Alternatively you can submit your request online by visiting the Elsevier web site at <http://elsevier.com/locate/permissions>, and selecting *Obtaining permission to use Elsevier material*.

Notice

No responsibility is assumed by the publisher for any injury and/or damage to persons or property as a matter of products liability, negligence or otherwise, or from any use or operation of any methods, products, instructions or ideas contained in the material herein. Because of rapid advances in the medical sciences, in particular, independent verification of diagnoses and drug dosages should be made.

British Library Cataloguing-in-Publication Data

A catalogue record for this book is available from the British Library.

Library of Congress Cataloging-in-Publication Data

A catalog record for this book is available from the Library of Congress.

ISBN: 978-0-12-407683-9

For information on all BH publications visit our website
at www.elsevierdirect.com

Printed and bound in United States of America
13 14 15 16 17 10 9 8 7 6 5 4 3 2 1



Working together
to grow libraries in
developing countries

www.elsevier.com • www.bookaid.org

Micromechanics of Composites

Preface

The subject of this book is micromechanics being the analysis of heterogeneous materials on the level of individual constituents. Number of manmade composites is permanently increasing, in parallel with the rising need to study the “structure - properties” relationships as this knowledge enables purposeful tailoring of composite materials with superior properties by rational choice of components and composition. This explains an importance of micromechanics as a science and motivates its rapid development in recent decades.

In past years, the main effort in micromechanics was focused on the macroscopic properties of heterogeneous solids and the most work in the area has been done with aid of the single inclusion (Eshelby) model being the theoretical framework of several applied theories. These theories provide useful for practice bounds and approximations for the effective constants and so they can be grouped under the title of engineering, or *applied* micromechanics. Most of the published up to now books on micromechanics fall in this category. Certainly, applied micromechanics is easy and convenient for use—but, as always, convenience comes at a price. The latter involves low or uncertain accuracy, inability to account the microstructure of composite and, as a consequence, inapplicability to study the phenomena (e.g., damage) caused by the local fields.

Now, it is well recognized that a reliable prediction of composite’s behavior must combine a realistic model of microstructure with an adequate analysis of the relevant model boundary problem. The need for an in-depth study has led to the development of *computational* micromechanics. Recent dramatic increase in computational power and available commercial FEA software made direct numerical approach accessible (not affordable for individual researcher, however) and enabled consideration of involved heterogeneous structures. The drawback of this approach is high computational effort, especially for 3D models. Another and, probably, even more substantial problem is extracting the meaningful data from a bunch of numbers generated by FEA code.

A promising alternative to computational micromechanics is the multipole expansion method also providing an efficient analysis of complex heterogeneous structures. Being mostly analytical in nature, this method constitutes a theoretical basis of high-performance computational algorithms and found numerous applications in astronomy, physics, chemistry, engineering, statistics, etc. Introduced by J.C. Maxwell in 1873 and then further developed by Lord Rayleigh in 1892, this is historically the first method of micromechanics. A substantial progress made since that time (and, especially, in recent years) in development of the multipole expansion method has been reported in numerous journal papers. However, in the author’s opinion, a true value of this method for micromechanics is still underestimated and its potential in the area is not fully discovered so far. This book is the first monograph giving systematic ac-

count of the method, with application to the actual problems of micromechanics. The multipole expansion method uses a classical approach and toolkit of mathematical physics which is a compelling reason to consider it as *theoretical* micromechanics.

The book does not pretend to cover all the aspects and methods of micromechanics. Its specific aim is to describe theory and technique of the method in detail, with application to the selected actual problems of micromechanics. This is primarily the multipole expansion approach that sets this monograph apart and is alternative one to what readers would find in the other books. In the author's opinion, the following features of this work can be of particular interest for the reader.

- The multipole expansion theory and technique have been described and further developed. In this respect, the book is of interest for a wide readership including the specialists in applied mathematics, mathematical physics, engineering, and related areas dealing with heterogeneous media.
- A detailed analysis of a variety of micromechanical multi-inclusion models has been performed. The contemporary topics include the composites with imperfect and partially debonded interface, nanostructured materials, cracked solids, statistics of the local fields, brittle strength, etc. The obtained complete analytical solutions provide a clear insight into the physical nature of the problems.
- The book contains a number of tabulated data and plots for the various problems. The results of the multipole analysis are commonly considered as the most reliable and serve as a benchmark for testing applicability of approximate models and accuracy of numerical solutions.
- The considered mechanical models are readily generalized in many ways to take the specific features of real-world heterogeneous materials into account. The Fortran source codes given in the Appendix can be used by the readers as a starting point in developing their own codes.
- An important feature of the developed approach is high numerical efficiency. In contrast to computational micromechanics, the multipole expansion does not require the powerful computers and expensive software to be used and appears probably the most efficient (especially in the fast multipole version) method of micromechanics.

The book summarizes the work done by the author with colleagues for more than 20 years in development and application of the multipole expansion method and is expected to be of particular interest to researchers and professionals in applied mathematics, physics, mechanics, materials science, engineering, and related areas dealing with the heterogeneous solids. I am very grateful to all my colleagues and friends, in Ukraine and abroad, who have contributed to this work as well as inspired and supported me in many ways in conducting the research and writing this book.

Kyiv, Ukraine
October, 2012

Volodymyr I. Kushch

Contents

Preface.....	xv
--------------	----

CHAPTER 1 Introduction	1
1.1 Motivation for the Work.....	1
1.2 Geometry Models	3
1.2.1 Single Inclusion	3
1.2.2 Finite Arrays of Inclusions	4
1.2.3 Composite Band and Layer	4
1.2.4 Representative Unit Cell (RUC) Model.....	6
1.3 Method of Solution	8
1.4 Homogenization Problem: Volume vs. Surface Averaging.....	10
1.4.1 Conductivity.....	11
1.4.2 Elasticity	14
1.5 Scope and Structure of the Book	17

PART I Particulate Composites.....	19
---	-----------

CHAPTER 2 Potential Fields of Interacting Spherical Inclusions	21
2.1 Background Theory	21
2.1.1 Scalar Spherical Harmonics	21
2.1.2 Selected Properties of Solid Spherical Harmonics	24
2.1.3 Spherical Harmonics vs. Multipole Potentials.....	26
2.2 General Solution for a Single Inclusion.....	26
2.2.1 Multipole Expansion Solution	27
2.2.2 Far Field Expansion	27
2.2.3 Resolving Equations	28
2.3 Particle Coating vs. Imperfect Interface	29
2.4 Re-Expansion Formulas for the Solid Spherical Harmonics	30
2.4.1 Equally Oriented Coordinate Systems	31
2.4.2 Multipole Expansion Theorem	32
2.4.3 Arbitrarily Oriented Coordinate Systems.	33
2.5 Finite Cluster Model (FCM)	35
2.5.1 Superposition Principle.....	35
2.5.2 FCM Boundary-Value Problem	36
2.5.3 Convergence Proof.....	37

2.5.4 Modified Maxwell Method for Effective Conductivity	40
2.6 Composite Sphere.....	42
2.6.1 Outer Boundary Condition	43
2.6.2 Interface Conditions.....	43
2.6.3 RSV and Effective Conductivity of Composite	44
2.7 Half-Space FCM.....	45
2.7.1 Double Fourier Transform of Solid Spherical Harmonics.....	45
2.7.2 Homogeneous Half-Space	47
2.7.3 Superposition Sum.....	47
2.7.4 Half-Space Boundary Condition.....	48
2.7.5 Interface Conditions.....	48
CHAPTER 3 Periodic Multipoles: Application to Composites.....	51
3.1 Composite Layer.....	51
3.1.1 2P Fundamental Solution of Laplace Equation	51
3.1.2 2P Solid Harmonics	54
3.1.3 Heat Flux Through the Composite Layer	55
3.2 Periodic Composite as a Sandwich of Composite Layers	57
3.3 Representative Unit Cell Model.....	59
3.4 3P Scalar Solid Harmonics	61
3.4.1 Direct Summation	61
3.4.2 Hasimoto's Approach.....	61
3.4.3 2P Harmonics-Based Approach.....	63
3.5 Local Temperature Field.....	64
3.6 Effective Conductivity of Composite	65
CHAPTER 4 Elastic Solids with Spherical Inclusions	69
4.1 Vector Spherical Harmonics	70
4.1.1 Vector Surface Harmonics	70
4.1.2 Vector Solid Harmonics	71
4.2 Scalar and Vector Solid Spherical Biharmonics	74
4.3 Partial Solutions of Lame Equation	76
4.3.1 Definition	76
4.3.2 Properties of Spherical Lame Solutions	78
4.4 Single Inclusion in Unbounded Solid.....	81
4.4.1 Far Field Expansion	82
4.4.2 Resolving Set of Linear Equations	83
4.4.3 Single Inclusion in Viscous Fluid (Stokes's Problem).....	84
4.5 Application to Nanocomposite: Gurtin & Murdoch Theory	86
4.5.1 Imperfect Interface Conditions	86
4.5.2 Formal Solution	88

4.5.3 Single Cavity Under Hydrostatic Far Field Load	89
4.5.4 Single Cavity Under Uniaxial Far Field Load	90
4.6 Re-Expansion Formulas for the Vector Harmonics and Biharmonics	91
4.6.1 Translation of Scalar Biharmonics.....	91
4.6.2 Translation of Vector Harmonics	94
4.6.3 Translation of Vector Biharmonics	96
4.6.4 Translation of Lame Solutions.....	97
4.6.5 Re-Expansion Due to Rotation	99
4.7 Finite Array of Inclusions (FCM)	99
4.7.1 Direct (Superposition) Sum	100
4.7.2 Local Expansion Sum.....	101
4.7.3 Infinite System of Linear Equations	101
4.7.4 Two Cavities Under Uniaxial Far Tension.....	102
4.7.5 Interface-Induced Stress Concentration in Nanostructured Solid	103
4.7.6 Stress Concentration Factors of Interacting Inclusions	104
4.8 Isotropic Solid with Anisotropic Inclusion	105
4.8.1 Formal Solution	106
4.8.2 Resolving Set of Equations.....	107
4.9 Effective Stiffness of Composite: Modified Maxwell Approach.....	109
4.9.1 Cubic Symmetry	110
4.9.2 Bulk Modulus k^*	111
4.9.3 Shear Modulus μ_1^*	112
4.9.4 Shear Modulus μ_2^*	112
4.10 Elastic Composite Sphere	113
4.11 RSV and Effective Elastic Moduli.....	114
4.11.1 Macroscopic Strain and Stress Tensors	114
4.11.2 Effective Bulk Modulus.....	115
4.11.3 Effective Shear Modulus.....	116
CHAPTER 5 Elasticity of Composite Half-Space, Layer, and Bulk	119
5.1 Vector Harmonics and Biharmonics for Half-Space	119
5.1.1 Definition	119
5.1.2 Integral Transforms.....	121
5.1.3 Series Expansions	123
5.2 Vector Lame Solutions for Half-Space	124
5.2.1 Definition	124
5.2.2 Properties of Lame Solutions $h_{\alpha\beta}^{(i)\pm}$	125

5.2.3 Integral Transforms and Series Expansions	127
5.3 FCM for Elastic Half-Space	127
5.3.1 Problem Statement.....	127
5.3.2 Solution for Homogeneous Half-Space	128
5.3.3 Heterogeneous Half-Space	129
5.4 Doubly Periodic Models	131
5.4.1 2P Lame Solutions	132
5.4.2 Composite Layer.....	134
5.4.3 Periodic Composite as a Sandwich of Composite Layers	137
5.5 Triply Periodic Vector Multipoles.....	137
5.5.1 Scalar Biharmonics.....	137
5.5.2 Periodic Solutions of Lame Equation	139
5.6 RUC Model of Elastic Spherical Particle Composite	140
5.6.1 Formal Solution	140
5.6.2 Effective Stiffness Tensor	142
5.7 Numerical Study	145
5.7.1 Local Stress Fields.....	145
5.7.2 Effective Stiffness Tensor	148
CHAPTER 6 Conductivity of a Solid with Spheroidal Inclusions	155
6.1 Scalar Spheroidal Solid Harmonics	155
6.1.1 Laplace Equation in Spheroidal Coordinates	155
6.1.2 Spheroidal Solid Harmonics: Definition and Properties....	157
6.1.3 Relationships Between the Spherical and Spheroidal Harmonics.....	159
6.1.4 Alternate Set of Spheroidal Harmonics	161
6.2 Single Inclusion: Conductivity Problem.....	162
6.2.1 Series Solution	163
6.2.2 Resolving Equations	163
6.2.3 Limiting Cases: Spherical, Penny-Shaped, and Needle-Like Inclusions	164
6.3 Re-Expansion Formulas for Spheroidal Solid Harmonics.....	168
6.3.1 Formal Series Expansion	169
6.3.2 Translation: Integral Form of Expansion Coefficients.....	170
6.3.3 Translation: Rational Form of Expansion Coefficients.....	172
6.3.4 Translation: General Formula	174
6.3.5 Rotation.....	177
6.4 Finite Cluster Model of Spheroidal Particle Composite.....	179
6.4.1 Formal Solution	179

6.4.2 Modified Maxwell Method for Effective Conductivity.....	180
6.5 Double Fourier Integral Transform of Spheroidal Harmonics.....	183
6.6 Doubly Periodic Harmonics	185
6.7 Triply Periodic Harmonics.....	187
6.8 Heat Conduction in Periodic Composite	188
6.8.1 Problem Statement.....	188
6.8.2 Temperature Field in Periodic Composite: 3P Approach.....	188
6.8.3 Temperature Field in Periodic Composite: 2P Approach.....	191
6.8.4 Multiple Inclusion RUC Model	192
6.8.5 Effective Conductivity	193
6.9 Numerical Examples.....	195
6.9.1 Spheroidal Cavities and Inclusions.....	195
6.9.2 Penny-Shaped Cracks	196
6.9.3 Superconducting Flakes	200
CHAPTER 7 Elastic Solid with Spheroidal Inclusions	203
7.1 Background Theory	203
7.1.1 Vector Solid Harmonics in Spheroidal Coordinates	203
7.1.2 Scalar and Vector Biharmonics. Spheroidal Lame Solutions	206
7.1.3 Selected Properties of Spheroidal Lame Solutions.....	209
7.2 Single-Inclusion Problem	215
7.2.1 Single Particle in Unbounded Solid.....	215
7.2.2 Single Particle in an Unbounded Fluid.....	218
7.2.3 Stress Intensity Factors for the Penny-Shaped Crack	219
7.3 Re-Expansion Formulas for the Spheroidal Lame Solutions.....	222
7.3.1 Translation	224
7.3.2 Rotation.....	227
7.4 Finite Cluster Model of Composite with Spheroidal Inclusions	228
7.4.1 Problem Statement.....	228
7.4.2 Formal Solution	229
7.4.3 Local Expansion	230
7.4.4 Numerical Example: Penny-Shaped Crack Interacting with Another Crack or Inclusion.....	231
7.5 Half-Space Problem.....	236
7.5.1 Integral Transforms of the Spheroidal Lame Solutions	236

7.5.2 Elastic Half-Space Containing a Finite Array of Spheroidal Inclusions.....	238
7.6 RUC Model of Elastic Spheroidal Particle Composite.....	239
7.6.1 Periodic Solutions of the Lame Equation	239
7.6.2 Formal Solution	240
7.6.3 Effective Stiffness Tensor of the Spheroidal Particle Composite	242
7.6.4 Numerical Study	242
CHAPTER 8 Composites with Transversely Isotropic Constituents	251
8.1 Transversely Isotropic Conductivity.....	251
8.1.1 Partial Solutions.....	252
8.1.2 Problem Statement.....	253
8.1.3 Series Solution	253
8.1.4 Effective Conductivity Tensor	256
8.2 Transversely Isotropic Elastic Solid with Spherical Inclusions	258
8.2.1 Partial Vector Solutions.....	258
8.2.2 Single Inclusion Problem.....	263
8.2.3 Finite Array of Inclusions	266
8.3 RUC Model.....	269
8.3.1 Formal Solution	269
8.3.2 Effective Stiffness Tensor	270
8.4 Numerical Examples.....	271
8.4.1 Stress Concentration	271
8.4.2 Effective Stiffness	275
PART II Fibrous Composites: Two-Dimensional Models	281
CHAPTER 9 Circular Fiber Composite with Perfect Interfaces	283
9.1 In-Plane Conductivity and Out-of-Plane Shear: The Governing Equations	284
9.1.1 Conductivity.....	284
9.1.2 Out-of-Plane Shear	284
9.2 Finite Array of Circular Inclusions	285
9.2.1 General Solution for a Single Inclusion.....	285
9.2.2 Finite Array of Inclusions in Unbounded Plane	286
9.2.3 Convergence Proof.....	290

9.3	Half Plane with Circular Inclusions.....	291
9.4	Infinite Arrays of Circular Inclusions	295
9.4.1	Periodic Complex Potentials.....	295
9.4.2	Composite Band.....	296
9.4.3	Composite Layer.....	298
9.5	Representative Unit Cell Model.....	301
9.5.1	Problem Statement.....	301
9.5.2	Local Thermal Fields: 1P Approach	302
9.5.3	Local Thermal Fields: 2P Approach	304
9.5.4	Averaged Fields and Effective Conductivity.....	306
9.6	Finite Array of Circular Inclusions: In-Plane Elasticity Problem.....	307
9.6.1	Basic Equations in Terms of Complex Potentials.....	307
9.6.2	Solution for an Unbounded Plane.....	309
9.7	Circular Inclusions in Half-Plane	312
9.7.1	Problem Statement.....	312
9.7.2	Determination of the Integral Densities $p(\beta)$ and $q(\beta)$	314
9.7.3	Resolving Linear System: Integrals vs. Rational Expressions	315
9.8	RUC Model of Fibrous Composite: Elasticity.....	318
9.8.1	The Problem Statement.....	318
9.8.2	Displacement Solution.....	319
9.8.3	Transverse Effective Stiffness of Fibrous Composite	321
9.9	Statistics of MicroStructure, Peak Stress and Interface Damage in Fibrous Composite	323
9.9.1	MicroStructure Statistics: Nearest Neighbor Distance	324
9.9.2	Peak Interface Stress and Statistics of Extremes	325
9.9.3	Stress Concentration vs. Nearest Neighbor Distance	326
9.9.4	Micro Damage Model of FRC.....	329
CHAPTER 10	Fibrous Composite with Interface Cracks	331
10.1	General Solution for a Single, Partially Debonded Inclusion	331
10.1.1	The Problem Statement.....	331
10.1.2	The $R(\zeta)$ Function	332
10.1.3	Formal Solution	334
10.1.4	Heat Flux Intensity Factor	337
10.2	Finite Array of Partially Debonded Inclusions	337
10.3	Conductivity of Fibrous Composite with Interface Damage	340
10.3.1	Formal Solution	340
10.3.2	Evaluation of the Lattice Sums	342

10.3.3 Effective Conductivity Tensor	343
10.3.4 Numerical Examples.....	344
10.4 In-Plane Elasticity: General Form of the Displacement Solution.....	346
10.5 Displacement Solution for the Partially Debonded Inclusion	348
10.5.1 Problem Statement.....	348
10.5.2 General Form of Potentials	349
10.5.3 The $R_\lambda(\zeta)$ and $X_\lambda(\zeta)$ Functions.....	350
10.5.4 Analytical Solution	352
10.5.5 Stress Intensity Factor.....	354
10.6 A Finite Number of Interacting Inclusions with Interface Cracks	355
10.6.1 Problem Statement and Iterative Solution Procedure	355
10.6.2 Evaluation of Integrals in Eq. (10.87).....	357
10.7 RUC Model of Fibrous Composite with Interface Cracks.....	359
10.7.1 Formal Solution	359
10.7.2 Effective Stiffness Tensor	360
10.7.3 Numerical Study: Stiffness Reduction vs. Interface Crack Density	362
CHAPTER 11 Solids with Elliptic Inclusions	367
11.1 Single Elliptic Inclusion in an Inhomogeneous Far Field	367
11.1.1 Problem Statement and Form of Solution.....	367
11.1.2 Displacement and Traction at the Elliptic Interface.....	369
11.1.3 Formal Solution	371
11.1.4 Stress Intensity Factor.....	374
11.2 Re-Expansion Formulas for the Elliptic Solid Harmonics	374
11.3 Finite Array of Inclusions	378
11.4 Half-Space Containing a Finite Array of Elliptic Fibers	382
11.4.1 Integral Transforms for Elliptic Harmonics.....	382
11.4.2 Half-Plane with Elliptic Hole: Out-of-Plane Elasticity/Conductivity Problem	383
11.4.3 Half-Plane with Elliptic Inclusion: Plane Elasticity Problem.....	386
11.4.4 FCM in Half-Plane	389
11.5 Periodic Complex Potentials.....	390
11.6 Micromechanical Model of Cracked Solid.....	391
11.6.1 Geometry	392
11.6.2 Boundary-Value Problem.....	393
11.6.3 Out-of-Plane Shear	394
11.6.4 Plane Strain.....	395

11.6.5 Effective Stiffness Tensor	399
11.6.6 Stress Intensity Factors	400
11.7 Numerical Examples	401
11.7.1 Geometry with Pre-Defined Crack Orientation Statistics	401
11.7.2 Effective Stiffness vs. Crack Density and Orientation	402
11.7.3 SIF Statistics	406
CHAPTER 12 Fibrous Composite with Anisotropic Constituents	411
12.1 Out-of-Plane Shear	411
12.1.1 Outline of the Approach and Basic Formulas.....	411
12.1.2 Single Inclusion Problem.....	414
12.1.3 Finite Array of Inclusions	416
12.2 Periodic Complex Potentials.....	418
12.2.1 RUC Model.....	419
12.3 Plane Strain	420
12.3.1 General Solution	421
12.3.2 Single Inclusion Problem.....	421
12.3.3 Array of Inclusions	423
12.4 Effective Stiffness Tensor	424
APPENDIX A Sample Fortran Codes.....	427
A.1 FCM Conductivity Problem (Chapter 2)	428
A.2 RUC Conductivity Problem for Spherical Particle Composite (Chapter 3).....	436
A.3 FCM Elasticity Problem (Chapter 4).....	440
A.4 RUC Elasticity Problem for Spherical Particle Composite (Chapter 5)	453
A.5 RUC Conductivity and Elasticity Problems for Fibrous Composite (Chapter 9).....	459
A.6 Standard Lattice Sums	465
A.6.1 Triple Harmonic and Biharmonic Sums for Simple Cubic Lattice	465
A.6.2 Double Harmonic and Biharmonic Sums for Square Lattice	469
Bibliography	471
Index.....	485

