

Qing-Hua Qin
Qing-Sheng Yang

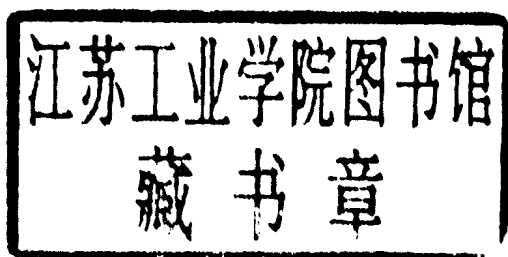
Macro-Micro Theory on Multifield Coupling Behavior of Heterogeneous Materials



高等教育出版社
HIGHER EDUCATION PRESS

Qing-Hua Qin
Qing-Sheng Yang

Macro-Micro Theory on Multifield Coupling Behavior of Heterogeneous Materials



高等教育出版社
HIGHER EDUCATION PRESS

AUTHORS:

Prof. Qing-Hua Qin
Department of Engineering
Australian National University
ACT 2601, Canberra, Australia
E-mail: qinghua.qin@anu.edu.au

Prof. Qing-Sheng Yang
Department of Engineering Mechanics
Beijing University of Technology
100022, Beijing, China
E-mail: qsyang@bjut.edu.cn

Copyright © 2008 by
Higher Education Press
4 Dewai Dajie, 100011, Beijing, P.R.China

图书在版编目 (CIP) 数据

非均匀材料多场耦合行为的宏细观理论=Macro-Micro Theory on Multifield Coupling Behavior of Heterogeneous Materials: 英文 / 秦庆华, 杨庆生著. —北京: 高等教育出版社, 2008.5

ISBN 978-7-04-022350-7

I. 非… II. ①秦… ②杨… III. 功能材料—耦合—研究—英文 IV. TB34

中国版本图书馆 CIP 数据核字 (2007) 第 162232 号

策划编辑	刘剑波	责任编辑	刘占伟	封面设计	张楠
责任绘图	宗小梅	版式设计	王莹	责任校对	姜国萍
责任印制	朱学忠				

出版发行 高等教育出版社
社 址 北京市西城区德外大街 4 号
邮政编码 100011
总 机 010-58581000

经 销 蓝色畅想图书发行有限公司
印 刷 北京佳信达艺术印刷有限公司

开 本 787×1092 1/16
印 张 21
字 数 370 000

购书热线 010-58581118
免费咨询 800-810-0598
网 址 [http:// www.hep.edu.cn](http://www.hep.edu.cn)
[http:// www.hep.com.cn](http://www.hep.com.cn)
网上订购 [http:// www.landaco.com](http://www.landaco.com)
[http:// www.landaco.com.cn](http://www.landaco.com.cn)
畅想教育 [http:// www.widedu.com](http://www.widedu.com)

版 次 2008年 5 月第 1 版
印 次 2008年 5 月第 1 次印刷
定 价 66.00 元

本书如有缺页、倒页、脱页等质量问题, 请到所购图书销售部门联系调换。

版权所有 侵权必究

物料号 22350-00

Sales only inside the mainland of China
仅限中国大陆地区销售

Qing-Hua Qin
Qing-Sheng Yang

**Macro-Micro Theory on Multifield Coupling Behavior
of Heterogeneous Materials**

Preface

Intelligent material with multifield coupling properties is an important aspect of modern science and technology with applications in many industrial fields such as biomedical, electronic and mechanical engineering.

It is well known that most engineering materials, composite materials in particular, are heterogeneous. The heterogeneity is either designed to meet engineering requirements for specific properties and functions or a natural evolution to adapt the historical architecture to changes in long term loadings and environment. Typical examples include functionally gradient materials and biomaterials. Functionally gradient materials are designed according to specific functions required by users. Biomaterials, on the other hand, remodel themselves to adapt to changes in the natural environment. Obviously, there are many heterogeneous materials in engineering including composites, defective materials and natural biomaterials. Heterogeneous materials exhibit complex properties at both microscopic and macroscopic level due to their anisotropy and interaction between components. Generally, there are two approaches used in investigating heterogeneous materials. One is the continuum mechanics approach, where the materials are assumed to be approximately homogeneous and continuous media. The other is the micromechanics approach, used for investigating the deformation and stress of heterogeneous materials by considering the interactions of the components in the microscopic scale.

In recent years, research in macro-micro mechanics of composite materials has resulted in a great many publications including journal papers and monographs. Up to the present, however, no systematic treatment of macro-micro theory of heterogeneous multifield composites has been available. The objective of this book is to fill this gap, so that the reader can obtain a sound basic knowledge of the solution methods of multifield composites. This volume details the development of linear theories of multifield materials and presents up-to-date results on magneto-electro-elastic composites. The book

consists of eight chapters. Chapters 1, 2, 5, and 7 were written by Qing-Sheng Yang, and the remaining four chapters were completed by Qing-Hua Qin. Chapter 1 describes basic concepts and solution methods of heterogeneous multifield composites. Chapter 2 introduces the essentials of homogenization approaches for heterogeneous composites. Chapter 3 deals with basic equations and solutions of linear piezoelectricity, and extensions to include magnetic effects are discussed in Chapter 4. Chapter 5 is concerned with basic equations, variational principles, and finite element solution of thermo-electro-chemo-elastic problems. Applications of multifield theories to bone remodelling process are detailed in Chapter 6. Chapter 7 examines general homogenization schemes of heterogeneous multifield composites. In Chapter 8, the final chapter, a detailed discussion of various micromechanics models of defective piezoelectricity is provided.

The main contents of this book were collected from the authors' most recent research outcomes and the research achievements of others in this field. Different parts of the research presented here were partially conducted by the authors at the Department of Engineering, Australian National University; and the Department of Mechanics of Tianjin University, the Department of Engineering Mechanics at Beijing University of Technology. Support from these universities, the National Science Foundation of China, and the Australian Research Council is gratefully acknowledged.

We are indebted to a number of individuals in academic circles and organizations who have contributed in different, but important, ways to the preparation of this book. In particular, we wish to extend our appreciation to our postgraduate students for their assistance in preparing this book. Special thanks go to Ms. Jianbo Liu of Higher Education Press for her commitment to the publication of this book. Finally, we wish to acknowledge the individuals and organizations cited in the book for permission to use their materials.

The authors would be grateful if readers would be so kind as to send us reports of any typographical and other errors, as well as their more general comments.

Qing-Hua Qin, Canberra, Australia

Qing-Sheng Yang, Beijing, China

May 2007

Contents

Chapter 1	Introduction	1
1.1	Heterogeneous materials	1
1.2	Multifield coupling properties of heterogeneous materials	3
1.3	Overview and structure of the book	5
	References	6
Chapter 2	Homogenization theory for heterogeneous materials	7
2.1	Microstructure of heterogeneous materials	7
2.2	Periodic boundary conditions	9
2.2.1	General considerations	9
2.2.2	Symmetric and periodic boundary conditions	10
2.3	Implementation of periodic boundary conditions in FE analysis	12
2.3.1	Multi-point constraints	13
2.3.2	Polynomial interpolations	14
2.3.3	Specified strain states	14
2.4	Effective fields and effective properties	15
2.4.1	Average fields	16
2.4.2	Effective properties	17
2.4.3	Homogenization methods	20
2.5	Direct homogenization	22
2.6	Indirect method	23
2.6.1	Self-consistent and generalized self-consistent scheme	24
2.6.2	Mori-Tanaka method	25
2.6.3	Self-consistent FEM and M-T FEM	27
2.6.4	Differential method	28
2.7	Variational method	30
2.8	Two-scale expansion method	31

2.8.1	Expansion of the displacement field	32
2.8.2	Establishment of basic equations of elastic microstructure	33
2.8.3	Determination of effective properties of material with microstructure	34
2.8.4	Variational forms	35
2.8.5	Finite element formulation	37
2.9	An approximate estimation of effective properties	38
2.10	Formulations and implementation for 2D problem	39
2.10.1	Formulations	39
2.10.2	FE implementation of homogenization methods	46
2.11	Numerical results	47
2.11.1	Effective stiffness of isotropic composite	49
2.11.2	Effective stiffness of anisotropic composite	52
2.11.3	Microstructural deformation	53
	References	56

Chapter 3 Thermo-electro-elastic problems59

3.1	Introduction	59
3.2	Linear theory of piezoelectricity	61
3.2.1	Basic equations of linear piezoelectricity	61
3.2.2	Two-dimensional simplification	66
3.3	Two classical solution approaches for piezoelectricity	67
3.3.1	Solution with Stroh formalism	68
3.3.2	Solution with Lekhnitskii formalism	69
3.3.3	Some identities	73
3.4	Logarithmic singularity of crack-tip fields in homogeneous piezoelectricity	75
3.4.1	General solution for crack-tip fields	75
3.4.2	Modified solution for p being a multiple root	77
3.4.3	Modified solution for η being a multiple root	77
3.5	Trefftz finite element method for piezoelectricity	78
3.5.1	Basic field equations and boundary conditions	79
3.5.2	Assumed displacement and electric potential fields	80
3.5.3	Variational principles	83

3.5.4	Elemental stiffness matrix	86
3.5.5	Application to anti-plane problem	87
3.5.6	Numerical examples	94
3.6	Theory of coupled thermo-piezoelectricity	95
3.6.1	Basic equations	95
3.6.2	Uniqueness of the solution	97
3.7	Solutions by Fourier transform method	99
3.7.1	Fourier transform method and induced general solution ...	100
3.7.2	Crack-tip singularity	103
3.7.3	Griffith crack in homogeneous piezoelectricity	106
3.8	Penny-shaped cracks	111
3.8.1	Problem statement and basic equation	112
3.8.2	Reduction of crack problem to the solution of a Fredholm integral equation	115
3.8.3	Numerical assessment	126
3.9	Piezoelectric fibre composites	128
3.9.1	Theoretical model for piezoelectric fibre push-out	128
3.9.2	Stress transfer in the bonded interface	131
3.9.3	Frictional sliding	133
3.9.4	Partially debonding model	135
3.9.5	Interfacial debonding criterion	139
3.9.6	Numerical examples	141
	References	144

Chapter 4 Thermo-magneto-electro-elastic problems149

4.1	Introduction	149
4.2	Basic field equations for magneto-electro-elastic solids	150
4.2.1	Basic equations of general anisotropy	150
4.2.2	Eight forms of constitutive equations	152
4.2.3	Transversely isotropic simplification	153
4.2.4	Extension to include thermal effect	154
4.3	Variational formulation	155
4.4	General solution for 3D transversely isotropic magneto-electro-elastic solids	157

4.5	Green's function for half-plane and bimaterial problems	160
4.5.1	Preliminary formulations	161
4.5.2	New coordinate variables	162
4.5.3	Green's function for full space	162
4.5.4	Green's function for half-space	164
4.5.5	Green's function for a bimaterial problem	165
4.5.6	Green's function for an inclined interface or half-plane boundary	166
4.6	Green's function for wedge problems	168
4.6.1	Basic formulations	168
4.6.2	Green's function for a wedge or a semi-infinite crack	169
4.7	Antiplane shear crack in a magneto-electro-elastic layer	172
4.7.1	Statement of the problem	172
4.7.2	Solution procedure	175
	References	178

Chapter 5 Thermo-electro-chemo-mechanical coupling183

5.1	Introduction	183
5.2	Governing equations of fields	185
5.3	Free energy and constitutive laws	188
5.4	Variational principle	190
5.5	Finite element formulation	193
5.6	Chemo-mechanical coupling	195
5.7	FE procedure and numerical examples	199
	References	203

Chapter 6 Thermo-electro-elastic bone remodelling207

6.1	Introduction	207
6.2	Thermo-electro-elastic internal bone remodelling	208
6.2.1	Linear theory of thermo-electro-elastic bone	208
6.2.2	Adaptive elastic theory	209
6.2.3	Analytical solution of a homogeneous hollow circular cylindrical bone	211

6.2.4	Semi-analytical solution for inhomogeneous cylindrical bone layers	215
6.2.5	Internal surface pressure induced by a medullar pin	218
6.2.6	Numerical examples	221
6.3	Thermo-electro-elastic surface bone remodelling	227
6.3.1	Equation for surface bone remodelling	227
6.3.2	Differential field equation for surface remodelling rate	228
6.3.3	Approximation for small changes in radii	230
6.3.4	Analytical solution of surface remodelling	232
6.3.5	Application of semi-analytical solution to surface remodelling of inhomogeneous bone	235
6.3.6	Surface remodelling equation modified by an inserting medullar pin	236
6.3.7	Numerical examples	238
6.4	Extension to thermo-magneto-electro-elastic problem	241
6.4.1	Linear theory of thermo-magneto-electro-elastic solid	241
6.4.2	Solution for internal bone remodelling	242
6.4.3	Solution for surface bone remodelling	246
	References	251

Chapter 7 Effective coupling properties of heterogeneous materials.....255

7.1	Basic equations for multifield coupling	256
7.2	Direct method	259
7.3	Indirect method	260
7.4	Two-scale expansion method	264
7.4.1	Asymptotic expansion of fields	264
7.4.2	Effective coupling properties	267
7.5	FE computation of effective coupling properties	269
7.6	Numerical examples	271
7.6.1	Piezoelectric solid with voids	272
7.6.2	Rigid inclusions	273
7.6.3	Piezoelectric composite	275
	References	277

Chapter 8 Effective properties of thermo-piezoelectricity279

8.1 Introduction 279

8.2 Micromechanics model of thermo-piezoelectricity with microcracks 281

8.2.1 Basic formulation of two-phase thermo-piezoelectricity 281

8.2.2 Effective conductivity 285

8.2.3 Effective electroelastic constants 292

8.2.4 Effective thermal expansion and pyroelectric constants 297

8.3 Micromechanics model of thermo-piezoelectricity with microvoids 298

8.3.1 Effective conductivity 299

8.3.2 Effective electroelastic constants 299

8.3.3 Effective concentration factors based on various micromechanics models 301

8.4 Micromechanics model of piezoelectricity with inclusions 302

8.4.1 Eshelby’s tensors for a composite with an ellipsoidal inclusion 302

8.4.2 Effective elastoelectric moduli 305

8.4.3 Effective thermal expansion and pyroelectric coefficients 306

8.5 Micromechanics-boundary element mixed approach 310

8.5.1 Two-phase BE formulation 310

8.5.2 Algorithms for self-consistent and Mori-Tanaka approaches 312

References 313

Index317

Chapter 1 Introduction

1.1 Heterogeneous materials

In classical continuum mechanics, materials are viewed as ideal, continuous, homogeneous media. The aim of continuum mechanics is to describe the response of homogeneous materials to external forces using approximate constitutive relations without microstructural considerations. In fact, all materials are inhomogeneous in the microscopic scale. Manufactured composites, natural soils and rocks as well as biological tissues are typical examples. The continuum is a model of materials in the macroscopic scale. Therefore, the homogeneity of materials depends on the scale of measurement. The magnitude of the micro-scale used differs for specific materials. In general, the approximate range of the micro-scale is 10^{-7} m to 10^{-4} m.

Heterogeneous materials exist in both synthetic products and nature. Synthetic examples include aligned and chopped fiber composites, particulate composites, interpenetrating multiphase composites, cellular solids, colloids, gels, foams, microemulsions, block copolymers, fluidized beds, and concrete. Some examples of natural heterogeneous materials are polycrystals, soils, sandstone, granular media, earth's crust, sea ice, wood, bone, lungs, blood, animal and plant tissue, cell aggregates, and tumors [1]. These heterogeneous materials have a legible microstructure. Figs.1.1 to 1.3 show microscopic pictures of some inhomogeneous materials.

It is noted that an important class of heterogeneous media is composites which are manufactured mixtures of two or more constituents, firmly (as a rule, but not always) bonded together [2]. The composites have inhomogeneous properties for different domains or different directions due to the inhomogeneity of their microstructures. This is an important feature and merit of heteroge-

neous materials. The microstructures of the composite materials can be designed to meet various desired properties and functions. The materials may possess very high properties in one or two directions and very weak properties in other directions, depending on the design for structural performance. Because of their excellent designable characteristics, composite materials are increasingly applied to industrial fields, for example, aeronautics and astronautics, electronics, chemical engineering, biomedical fields and so on.

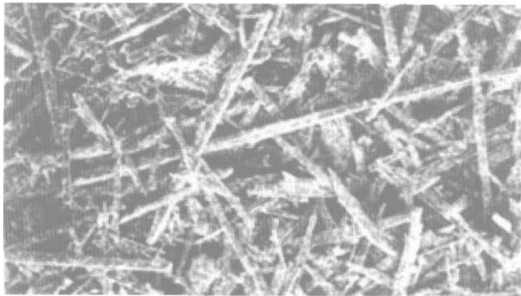


Fig. 1.1 Fiber reinforced composite

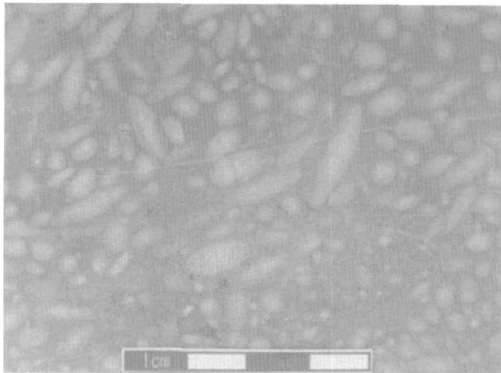


Fig. 1.2 Microstructure of concrete

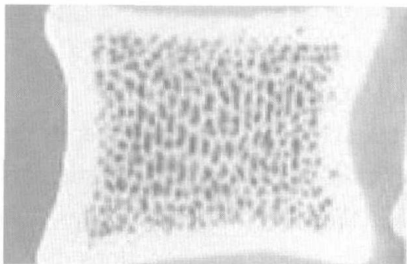


Fig. 1.3 Microstructure of a bone

Heterogeneous materials often exhibit very complex properties, presenting new challenges and opportunities to scientists and engineers. In recent years several new composite materials have been developed which display not only good mechanical properties but also some new functions such as thermal, electric, magnetic, photic, and chemical effects. At the same time, composite materials can create new functions and performance which are absent in their constituents. Such multiple physical properties are usually coupled with each other. Consequently, the coupling properties and deformation behavior of heterogeneous materials are topics of great interest for qualitative and quantitative investigation.

1.2 Multifield coupling properties of heterogeneous materials

A number of heterogeneous materials can fulfill the transfer between mechanical and non-mechanical energy (thermal, electrical, chemical energy, etc). Such materials are usually called *intelligent materials*. These materials can be used in adaptive structures, sensors, and actuators. Intelligent materials are sensitive to variables of the external environment, adjusting their shape or size to adapt to changes in that environment. This multifield coupling behavior is a unique characteristic of intelligent materials. For instance, piezoelectric ceramics, piezoelectric polymers, and some biological tissues (e.g. bone, skin, etc) exhibit thermo-electro-elastic coupling properties [3]. Electric current and heat flow will be excited when the material is subject to a mechanical loading, and vice versa.

As an example, a composite material consisting of a piezoelectric phase and a piezomagnetic phase exhibits considerable multifield coupling properties, i.e. both electro-mechanical and magneto-mechanical coupling. In addition, it displays a remarkably large coupling coefficient between static electric and magnetic fields, which is absent in either constituent. The magnetoelectric coupling in the composite is created through the interaction between the piezoelectric phase and the piezomagnetic phase, which is called a *product property*. The product property of composites offers great engineering opportunities to develop new materials.

In a different example, biological tissues, a form of natural material, can

perform energy transfer between chemical and mechanical energy. In this process electric and thermal effects are coupled. This phenomenon can also be found in clay, gel, and so on, and can be described by thermo-electro-chemo-mechanical coupling theory.

Research into heterogeneous media has a long history. Two approaches have been adopted: macro-mechanical and micro-mechanical approaches. Macromechanics deals with material as a homogeneous continuum based on the approximate constitutive model, ignoring heterogeneity of the microstructure. The macroscopic or averaged properties of heterogeneous materials are studied. However, the macroscopic properties of materials depend on micro-structural information, such as the geometric and physical properties of the constituents and the behavior of their interface. Micromechanics has been developed to investigate the relations between the effective properties and microstructures of heterogeneous materials and the interactions among the constituents[4,5]. As the characteristic length of microstructure is far less than the characteristic length of the whole body, a homogenization is carried out to capture the macroscopic behavior of the materials, as shown in Fig.1.4. Denoting y as the microscopic scale and x as the structural scale, since $y \ll x$, the composite is replaced by the homogenized continuum.

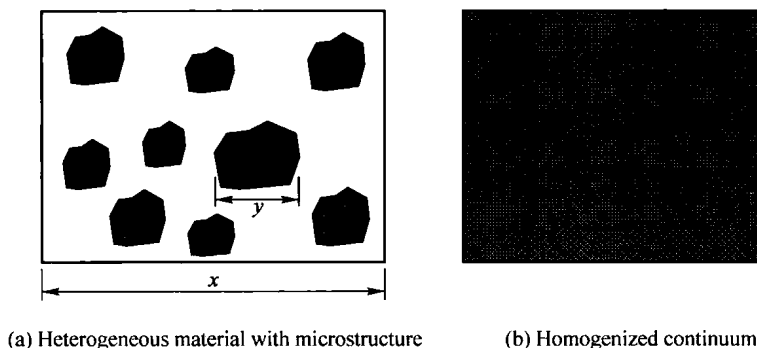


Fig.1.4 Homogenization of heterogeneous materials

In the frame of micromechanics, the emphasis is placed on the bridging of effective properties and micro-structure parameters of materials. Effective properties that can be measured experimentally include effective elastic stiffness, conductivity of electricity and heat, permeability coefficient of fluid and coupling coefficients among physical fields. An understanding of the relations

of effective properties and microstructure of materials is very vital in the design of new composite materials.

1.3 Overview and structure of the book

The multifield coupling behavior of the heterogeneous material is a multi-disciplinary subject. This book focuses on the multifield coupling properties of several intelligent materials, investigating them by means of macro- and micro-mechanics. The first group of materials involved is artificially intelligent materials, such as piezoelectric solids, piezomagnetic materials, and electric activity polymers which are sensitive to stimuli from the external environment. The second group of materials includes natural materials, such as biological materials (bone, soft tissue, articular cartilage). These materials exhibit thermo-electro-chemo-mechanical coupling effects. Investigation of the behavior of such materials can contribute to understanding of the interaction of the fields and mechanism of deformation, growth, aging and rebuilding of the biological system.

This book is divided into two parts: macromechanics and micromechanics. Macromechanical analysis is covered in Chapters 3 to 6. The phenomenological theory of continuous media is applied in the investigation of multifield coupling behavior of heterogeneous materials. In Chapter 3 the linear theory and general solutions of piezoelectric materials are described. In Chapter 4 electro-elastic coupling theory is extended to magneto-electro-elastic coupling problems. In Chapter 5 we discuss fundamental equations and analytical methods of thermo-electro-chemo-mechanical coupling problem. Chapter 6 involves applications of thermo-electro-elastic coupling in bone remodeling.

Micro-mechanical analysis focuses on the connection between macro-properties and micro-structure parameters, devoting attention to establishing analytical methods for the effective coupling properties of materials. Micro-mechanical analysis is dealt with in Chapters 2, 7, and 8. Chapter 2 discusses the homogenization theory of microstructure and the method of calculation of the effective properties of heterogeneous elastic materials. In Chapter 7, we introduce the homogenization methods in the general sense, including the direct average method, the indirect average method, and the mathematical homogenization method. In Chapter 8, a micro-mechanical model of thermo-piezoelectric solid is described, and the effective properties of