



Material Substructures in Complex Bodies

From Atomic Level to Continuum



Edited by: Gianfranco Capriz and Paolo Maria Mariano

TB 383
M 425

MATERIAL SUBSTRUCTURES IN COMPLEX BODIES: FROM ATOMIC LEVEL TO CONTINUUM

Edited by

GIANFRANCO CAPRIZ

Università di Pisa

PAOLO MARIA MARIANO

D.I.C., Università di Firenze



ELSEVIER



E2009002641

Amsterdam • Boston • Heidelberg • London • New York • Oxford
Paris • San Diego • San Francisco • Singapore • Sydney • Tokyo

Elsevier

The Boulevard, Langford Lane, Kidlington, Oxford OX5 1GB, UK
84 Theobald's Road, London WC1X 8RR, UK

First edition 2007

Copyright © 2007 Elsevier BV. All rights reserved

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

Material substructures in complex bodies : from atomic level to continuum

1. Microstructure 2. Materials science 3. Atomic structure
4. Molecular structure 5. Nanostructured materials

I. Capriz, G. (Gianfranco) II. Mariano, Paolo Maria, 1966–
620.1'1299

Library of Congress Control Number: 200693845

ISBN 13: 978-0-08-044535-9

ISBN 10: 0-08-044535-7

For information on all Elsevier publications
visit our web site at books.elsevier.com

Typeset by Charon Tec Ltd (A Macmillan Company), Chennai, India.

www.charontec.com

Printed and bound in Great Britain

06 07 08 09 10 10 9 8 7 6 5 4 3 2 1

**Working together to grow
libraries in developing countries**

www.elsevier.com | www.bookaid.org | www.sabre.org

ELSEVIER

BOOK AID
International

Sabre Foundation

MATERIAL SUBSTRUCTURES IN COMPLEX BODIES

CONTRIBUTORS

Prof. Gianfranco Capriz

Dipartimento di Matematica, Università di Pisa, Largo B. Pontecorvo 5, I-56127 Pisa, Italy.
E-mail: gianfranco.capriz@mac.com

Prof. Carlo Cercignani

Dipartimento di Matematica, Politecnico di Milano, Piazza Leonardo da Vinci 32, 20133 Milano, Italy.
Phone: +39 02 2399 4557; Fax: +39 02 2399 4606; E-mail: carlo.cercignani@mate.polimi.it

Prof. Pierre Degond

Laboratoire MIP, Université Paul Sabatier, 31062 Toulouse Cedex 9, France.
Phone: +33 05 61 55 63 69; Fax: +33 05 61 55 83 85; E-mail: degond@mip.ups-tlse.fr

Prof. Antonio Fasano

Dipartimento di Matematica “U. Dini”, Università di Firenze, viale Morgani 67/A, I-50134 Firenze Italy.
Phone: +39 055 4237145; Fax: +39 055 4222695; E-mail: fasano@math.unifi.it

Dr. Harley T. Johnson

Department of Mechanical Science and Engineering, University of Illinois at Urbana-Champaign, 1206 W. Green Street, Urbana IL 61801-2906, USA.
Phone: +1 217-265-5468; Fax: +1 217-244-6534; E-mail: htj@uiuc.edu

Sukky Jun

Department of Mechanical and Materials Engineering, Florida International University, 10555 West Flagler Street, EC 3463, Miami, FL 33174, USA.
Phone: +1 305 348 1217; Fax: +1 305 348 1932; E-mail: juns@fiu.edu

K. Kannan

Department of Biomedical Engineering – Texas A&M University – 230A Engineering/Physics Building Office Wing – 3120 TAMU.

Prof. Wing Kam Liu

Northwestern University, Department of Mechanical Engineering, 2145 Sheridan, Evanston, IL 60208-3111, USA.
Phone: +1 847-491-7094; Fax: +1 847-491-3915; E-mail: w-liu@northwestern.edu

Alberto Mancini

Dipartimento di Matematica “U. Dini” – Università degli Studi di Firenze – Viale Morgagni 67/a 50134 Firenze, Italy.

Prof. Paolo Maria Mariano

D.I.C., Università di Firenze, via Santa Marta 3, I-50139 Firenze, Italy.

Phone: +39.055.4796470; Fax: +39.055.4796320; E-mail: paolo.mariano@unifi.it

Prof. K. R. Rajagopal

Department of Mechanical Engineering, Texas A&M University, 230A Engineering/Physics Building Office Wing College Station, Texas 77843, USA.

Phone: +1 979-862-4552; Fax: +1 979-845-3081; E-mail: krajagopal@tamu.edu

Prof. Jan J. Sławianowski

Institute of Fundamental Technological Research, Polish Academy of Sciences, ul. Świerkowska 21, 00-049 Warsaw, Poland.

Phone: +48 (22) 8261281; Fax: +48 (22) 8269815; E-mail: jslawian@ippt.gov.pl

PREFACE

Stringent industrial requirement of sophisticated performances and of circumstantial control for micro-devices and other types of machinery at multiple scales can be satisfied often only by resort to or allowance for complex materials. The adjective “complex” beckons to the fact that the substructure influences gross mechanical behaviour in a prominent way. Interactions due to substructural changes are represented directly. Examples, just to list a few, are liquid crystals, quasi-periodic alloys, polymeric bodies, spin glasses, magnetostrictive materials and ferroelectrics, suspensions, in particular liquids with gas bubbles, polarizable fluids, etc. Hopefully, substructures can be exploited, even invented anew, to reach predetermined goals. To help in the process, theories must be developed so that severe challenging theoretical problems arise; often of fundamental nature. A precise grasp of the physical meaning of mathematical entities is critical for the correct, adequate proposal of models of behaviour and even of consequent computational analyses. A basic problem is of bridging scales even from atomic to macroscopic level, translating through continuum limit the prominent aspects of the subtle discrete substructural features. Their number and nature may be also enriched by specific circumstances. The collection of chapters composing this book aims to underline some aspects of these questions, proposing also new matter of discussion together with specific solutions.

In Chapter 1, *Pierre Degond* derives hydrodynamic models of plasmas and disparate mass binary mixtures by evaluating the continuum limit of kinetic “small-scale” events represented by means of Fokker-Planck or Boltzmann equations. Macroscopic diffusion equations for density of particles and energy follow, coupled with a Euler-type equation for ions or heavy species. Inconsistencies in existing models are evidenced.

In Chapter 2, *Carlo Cercignani* continues the discussion on how kinetic schemes based on Boltzmann equation may offer microscopic foundations of continuous dynamical models. He examines how old and new techniques in the kinetic theories of dense gases may be useful for describing the fast flow of granular materials.

Substructural kinetic effects may be not as prominent in some circumstances as quantum phenomena. In Chapter 3, *Jan Jerzy Slawianowski* develops a quantization scheme for affine bodies, a special class of complex bodies where the natural morphological descriptor is a second-order tensor: in other words, each material element is considered as a system which may (microscopically) deform independently of the neighbouring fellows.

Once reasonable models have been established, computational techniques are essential in finding explicit solutions in special cases. When phenomena at various

scales are involved, non-trivial computational problems arise and may be tackled with different methods, depending on circumstances. In their Chapter 4, *Sukky Jun* and *Wing Kam Liu* discuss computational methods appropriate to analyse the formation of electronic band structures in periodic atomic lattices. The approach makes use of periodic meshless shape functions based on the moving least-square approximation. Wave equations are analysed in the reciprocal space determined by the standard Fourier basis. The analyses of semiconductors, photonic and phononic crystals are natural applications. Complex bodies are produced in non-simple industrial processes so that the process of formation of substructures deserves to be described *per se*.

Amid possible industrial processes, in Chapter 5, *Antonio Fasano*, *Krishna Kannan*, *Alberto Mancini* and *Kumbakonam R. Rajagopal* propose a new model for the Ziegler-Natta polymerization in a high-pressure reactor by considering, after fragmentation, a single agglomerate of catalytic particles, then analyzing the mechanics of growing nano-spheres. A non-linear hyperbolic system of governing equations arises.

Other aspects of the mechanics of polymers are further discussed by *Krishna Kannan* and *Kumbakonam R. Rajagopal* in their Chapter 7. The attention is focused on the solidification process of molten polymers where there is competition between the effects of substructural quenching and deformation of the melt: The former effect is an obstacle to the crystallization while the latter enhances it in a way in which memory effects have to be accounted for. Deformation and the corresponding macroscopic stress influence also the formation of nanostructures in semiconductors during their fabrication and the collective mechanical behaviour in applications. The modelling of these effects include atomistic, continuum and multiscale features. These topics are discussed in Chapter 8 by *Harley T. Johnson*.

Finally, our personal contributions are in Chapters 6 and 9. Basic foundations of the mechanics of bodies in which substructural phenomena have kinetic nature are discussed in Chapter 6 (by G.C.) without resorting to the use of some version of Boltzmann equation. The interaction between gross deformation and spin structures are discussed in Chapter 9 (by P.M.M.) paying attention on the evolution of disclination lines and point defects. The covariance of the relevant evolution equations is proven.

Gianfranco Capriz
Bridport (UK)

Paolo Maria Mariano
Firenze (Italy)

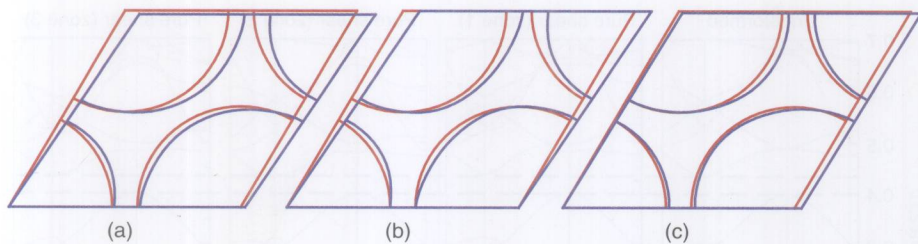


Plate 1 Undeformed (red) and deformed (blue) unit cells of 2D triangular photonic crystal with cylindrical air rods: (a) pure shear, (b) simple shear and (c) uniaxial tension. In each mode, corresponding shear or tensile strain of 3% is applied.

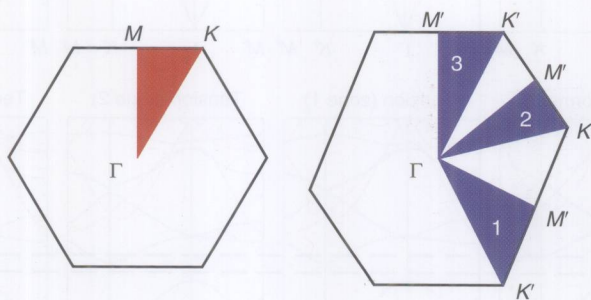


Plate 2 Schematic diagrams of symmetry points and zones in the reciprocal lattice of undeformed (left) and deformed (right) photonic crystals.

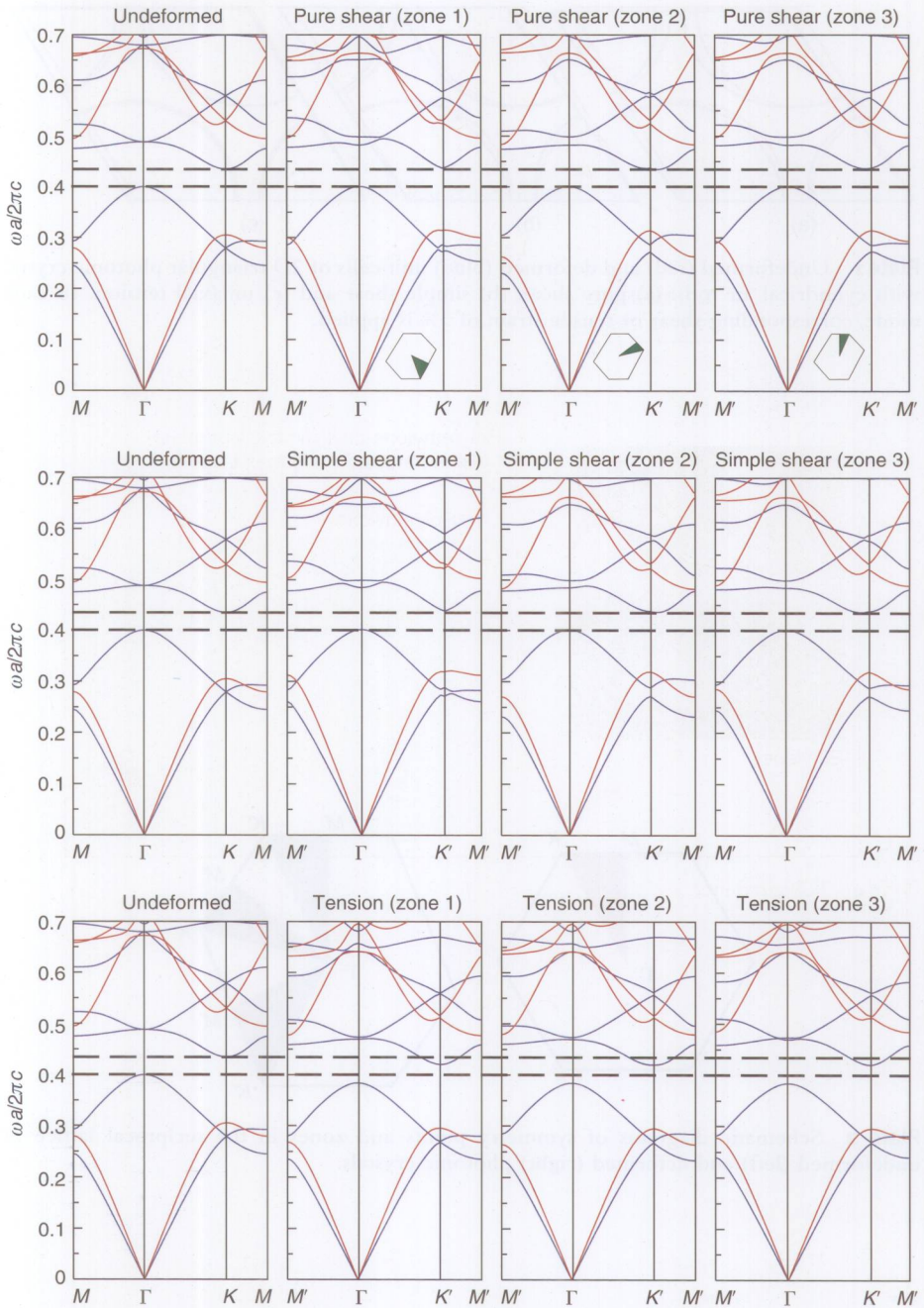


Plate 3 Photonic band structures under pure shear (top), simple shear (middle), and uniaxial tension (bottom). TM and TE modes are in blue and red, respectively. Dashed horizontal lines indicate the bandgap of undeformed original photonic crystal. Insets in top low illustrate the quasi-hexagonal symmetry zones of the deformed photonic crystal.

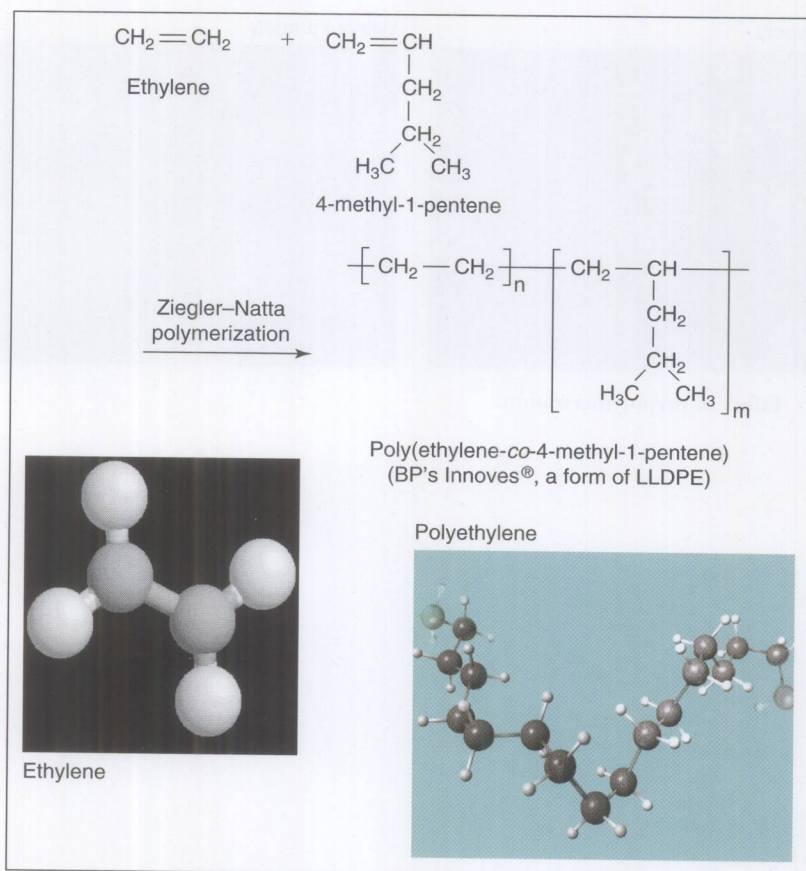
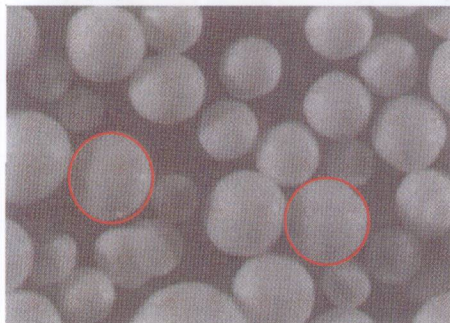


Plate 4 Polyethylene.

With prepoly



Without prepoly

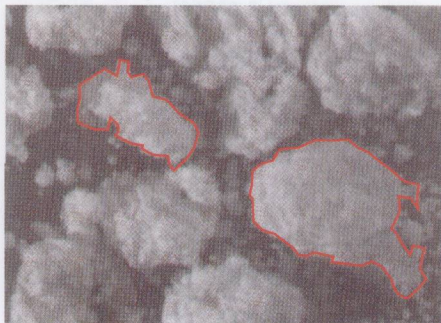
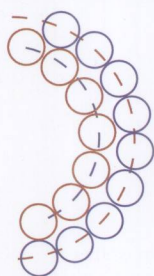


Plate 5 Effect of prepolymerization.



Ideal packing of the growing microspheres



Neighbouring spheres
have similar histories
and approximately the
same radius

Plate 6 Porosity ϵ constant.



Plate 7 Schematic of three thin film growth modes. Left: Frank–van der Merwe or planar layer-by-layer growth. Center: Stransk–Krastanow or island growth on a wetting layer. Right: Volmer–Weber or island growth with no wetting of the substrate.

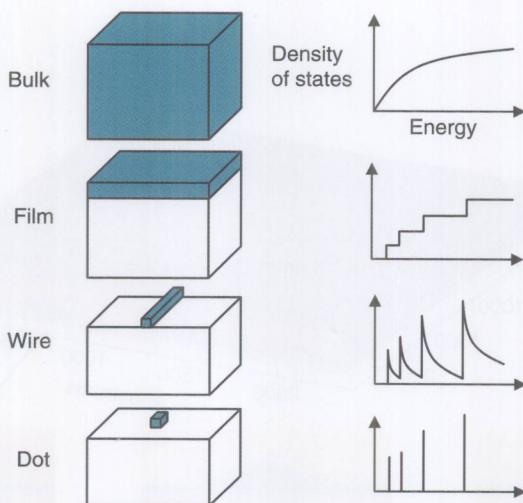


Plate 8 Schematic of the electron density of states in bulk and quantum confined material systems. The delta-function-like densities of states in quantum wire and quantum dot configurations are desirable for many nanoelectronic and optoelectronic devices.

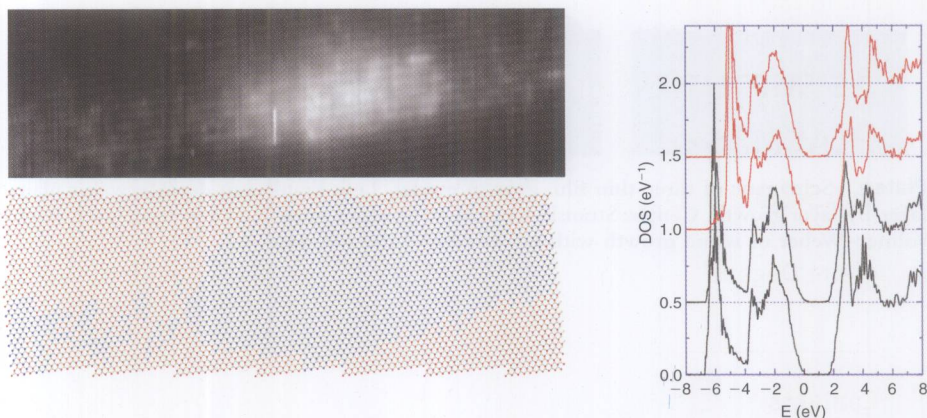


Plate 9 Combined experimental and computational study of electronic structure of individual embedded quantum dot at the atomistic scale. Atom positions are determined using high resolution cross-sectional scanning tunneling microscopy (upper left) and then converted to an atomistic computational input file (lower left). Using a novel tight-binding method, the local density of states is determined at various positions (right) and compared to experimental data [56].

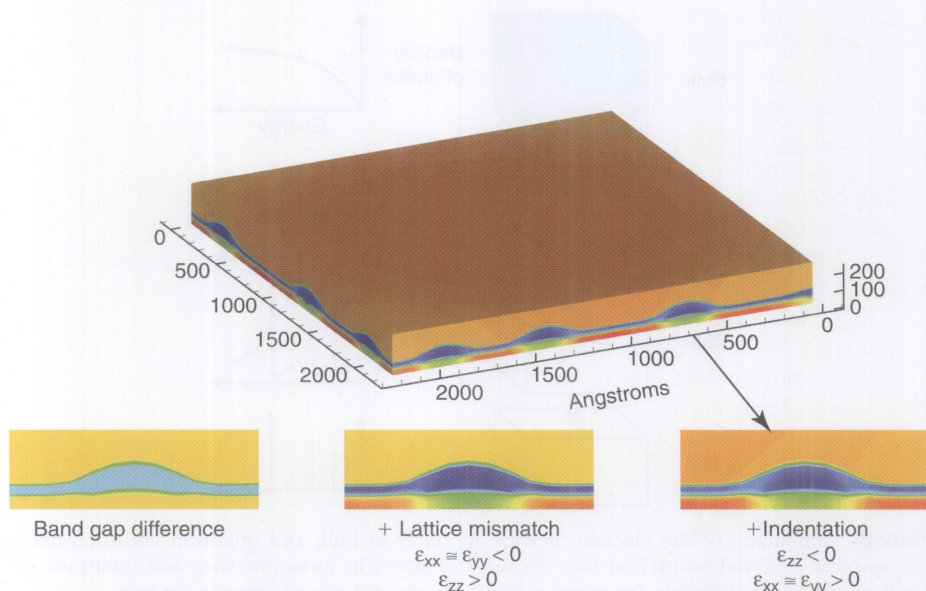


Plate 10 Embedded quantum dot array finite element mesh. The color contour shows the electrostatic potential for a single electron in the system when the surface is nanoindented to a small depth. The three inset images show how bandgap difference, lattice mismatch strain, and nanoindentation strain contribute to the total potential field [64].

CONTENTS

Contributors

xi

Preface

xiii

1. Asymptotic Continuum Models for Plasmas and Disparate Mass Gaseous Binary Mixtures

1

Pierre Degond

1.1	Introduction	2
1.2	The Kinetic Model	6
1.3	Moment Method and Conservation Laws for Gas Mixtures: Why it Cannot Apply to Plasmas	11
1.3.1	Properties of the collision operators	11
1.3.2	Moments and conservation laws	13
1.3.3	Closure of the moment system: LTE	14
1.3.4	Why the standard mixture model does not apply to plasmas	17
1.4	The Plasma Fluid Model	18
1.4.1	Energy-transport form of the system	18
1.4.2	Hydrodynamic form of the system	21
1.4.3	Discussion of the plasma fluid model and applications	22
1.4.4	Approximate expression of the diffusion matrices	24
1.5	Scaling Hypotheses	29
1.6	Expansion of the Interspecies Collision Operators	34
1.7	Moment Method and Conservation Laws for Plasmas	40
1.7.1	Properties of the expanded collision operators	40
1.7.2	Moments and conservation laws for the scaled kinetic model	42
1.7.3	Closure of the plasma moment system	44
1.8	Computation of the Fluxes and of the Collision Terms	49
1.8.1	Preliminaries	49
1.8.2	Properties of \mathcal{L}_B	50
1.8.3	Resolution of the perturbation equation (1.242)	51
1.8.4	Computation of the fluxes	52
1.8.5	Expression of the fluxes in terms of n_e and T_e	54
1.8.6	Expression of the collision terms	56
1.8.7	Back to physical variables	57
1.9	Conclusion	57

2. Microscopic Foundations of the Mechanics of Gases and Granular Materials	63
Carlo Cercignani	
2.1 Introduction	63
2.2 Kinetic Theory of Smooth Spheres	65
2.3 Collision Dynamics of Rough Spheres	69
2.4 The Boltzmann–Enskog Equation	72
2.5 The Macroscopic Balance Equations	74
2.6 Concluding Remarks	76
3. Quantization of Affine Bodies: Theory and Applications in Mechanics of Structured Media	80
Jan J. Sławianowski	
3.1 Introduction	80
3.2 Classical Preliminaries	82
3.3 General Ideas of Quantization	125
4. Moving Least-Square Basis for Band-Structure Calculations of Natural and Artificial Crystals	163
Sukky Jun and Wing Kam Liu	
4.1 Introduction	164
4.1.1 Electronic band structures	164
4.1.2 Photonic and acoustic band structures	165
4.1.3 Meshless methods and moving least-square basis	166
4.1.4 Periodicity	166
4.2 MLS Basis and Periodicity	167
4.2.1 MLS approximation	168
4.2.2 Implementation of periodicity condition	169
4.3 Atomic Crystals and Semiconductors	174
4.3.1 Galerkin formulation of Schrödinger equation	175
4.3.2 The Kronig–Penney model potential	177
4.3.3 Empirical pseudopotentials of Si and GaAs	178
4.3.4 Strain effect in compound semiconductors	180
4.4 PhoXonic Crystals	183
4.4.1 Maxwell equations for 2D photonic crystals	183
4.4.2 Band structures of various 2D photonic crystals	185
4.4.3 Acoustic bandgap materials	194
4.5 Strain-Tunable Photonic Bandgap Materials	195
4.5.1 Deformations of 2D triangular photonic crystals	196
4.5.2 Band structures of deformed photonic crystals	198
4.6 Concluding Remarks	201

5. Modelling Ziegler–Natta Polymerization in High Pressure Reactors	206
Antonio Fasano, K. Kannan, Alberto Mancini and K. R. Rajagopal	
5.1 Introduction	208
Modelling the Growth of the Agglomerate (Macroscale)	212
5.2 Governing Equations	212
5.2.1 Constancy of porosity	212
5.2.2 Density of microspheres	213
5.2.3 Liquid monomer balance	213
5.2.4 Solid mass balance	214
5.2.5 Relating the agglomerate expansion to microspheres growth	214
5.2.6 Liquid flow	215
5.2.7 Energy balance	215
5.3 Initial and Boundary Conditions	216
Modelling the Growth of Microspheres	217
5.4 Kinematics	217
5.5 The Governing Equations	218
5.5.1 Mass balance	219
5.5.2 Momentum balance	219
5.5.3 Constitutive equations	220
5.6 Initial and Boundary Conditions	222
5.7 Analysis of the Equations in the Microscale with Spherical Symmetry	224
5.8 Consistency of the Boundary Conditions	228
Bridging the Two Scales. The Complete Model	232
5.9 Determining the Free Terms in the Macroscopic Transport Equations	232
5.10 The Complete Model	232
5.10.1 Macroscale	232
5.10.2 Microscale	233
5.11 Not Evolving Natural Configuration	234
5.12 Conclusions	235
 6. Pseudofluids	 238
Gianfranco Capriz	
6.1 Preamble	238
6.2 Material Element	239
6.3 Basic Fields	242
6.4 Measures of Deformation and Distorsion	245
6.5 Strain Rates and Distorsion Rates	248
6.6 Inertia Measures	250
6.7 Relations with Thermal Concepts	252