Multiscale Modeling of Heterogenous Materials

From Microstructure to Macro-scale Properties

Edited by Oana Cazacu

ISTE

WILEY

Multiscale Modeling of Heterogenous Materials

From Microstructure to Macro-scale Properties

Edited by

Oana Cazacu

ISTE

E2009001051

WILEY

First published in Great Britain and the United States in 2008 by ISTE Ltd and John Wiley & Sons, Inc.

ISTE Ltd
27-37 St George's Road
London SW19 4EU
UK

www.iste.co.uk

John Wiley & Sons, Inc.
111 River Street
Hoboken, NJ 07030
USA

www.wiley.com

Library of Congress Cataloging-in-Publication Data

Multiscale modeling of heterogenous materials : from microstructure to macro-scale properties / edited by Oana Cazacu.
p. cm.
Includes bibliographical references and index.
ISBN 978-1-84821-047-9
1. Inhomogeneous materials--Mathematical models. I. Cazacu, Oana.
TA418.9.I53M85 2008
620.1'1015118--dc22

2008027555

British Library Cataloguing-in-Publication Data
A CIP record for this book is available from the British Library
ISBN: 978-1-84821-047-9

Printed and bound in Great Britain by CPI Antony Rowe, Chippenham, Wiltshire.

Multiscale Modeling of Heterogenous Materials

Foreword

For several decades, the mechanical behavior of materials has been described by phenomenological constitutive relations in the general framework of the theory of elasto-visco-plasticity. These approaches, when combined with numerical methods (e.g., finite element methods), have led to very powerful tools – tools which simulate boundary value problems in a reasonably realistic way, making them relevant for real engineering problems.

However, this methodology has reached some limits, primarily because of the great number of constitutive parameters to be determined, the recurrent difficulty in simulating cyclic loading and limitations in predicting post-failure behavior. In recognition of these basic limitations, methods based on the micromechanics of heterogenous materials have been vigorously developed through so-called homogenization techniques. Molecular dynamics also appeared as a very useful tool to simulate the mechanical behavior of materials whose internal structure is easy to identify.

This book is timely and relevant, addressing recent advances which take into account the microstructure of materials. To that end, some chapters illustrate how it is possible to improve phenomenological constitutive relations by incorporating proper micromechanical ingredients, while others propose to build macroscopic relations by using localization-homogenization methods and a local microscopic relation, describing the interaction laws between the element grains or particles. Of course these interaction laws are usually rather simple – if a proper scale has been chosen – or at least well established. For these methods the most difficult step is probably to build a localization (or projection) operator, essentially because the solutions are not unique.

Other chapters relate the application of continuum-based multi-scale methods to metallic materials or geomaterials. New powerful methodologies for describing anisotropy both at single crystal and aggregate level are presented.

Here also the mechanical parameters are very few, the local laws (grain level or single crystal level) are quite simple and the derived macroscopic properties are surprisingly realistic. Thus, the macroscopic behavior, which appears in experiments as extremely complex, can be described with few mechanical ingredients. Hence, this macro-complexity may be due to the great number of elements in interaction or texture and not to an eventual micro-complexity. As in the case of molecular dynamics, such continuum-based multi-scale methods allow the real world to be rebuilt numerically.

Some essential difficulties appearing in a continuum mechanics framework (e.g., the description of an internal length) are solved in molecular dynamics in a very natural and elegant way. On the other hand, the likely remaining difficulty is to take into account a proper geometry for the element assembly.

With respect to practical problems, we now understand that it is essential to consider materials in their own environment. From this perspective, describing environmental coupling (as induced by chemo-thermo-hydro-mechanical interactions) will be more and more important in the future. Several chapters consider these "multi-physics" couplings.

From an engineering perspective, failure is always an essential question. An efficient analysis framework is provided by the bifurcation theory. The existence of bifurcated branches and the roles of imperfections and perturbations have been investigated with success. Moreover, for non-associated materials (and all materials whose behavior depends on the mean pressure seem to behave like this), the existence of a large stress domain of bifurcations or of material/geometric instabilities has now been established on firm theoretical, experimental and numerical bases. Various failure modes are associated with these bifurcations, and diffuse and localized failures are also discussed in several chapters.

Finally, another interesting facet of this book lies in the fact that a variety of solid materials are considered – which is quite a rare feature today. Readers will be interested in cross-linking the methods and tools developed to describe the macroscopic properties of metallic materials and geomaterials from their very different microscopic internal structures.

This book gathers together selected papers from the invited lectures presented during the 1st US-France Symposium held 28-30 March 2007 at the University of Florida in Shalimar, FL. It was locally organized by John "Row" Rogacki and Oana

Cazacu under the auspices of the International Center for Applied Computational Mechanics (ICACM) with financial support provided by the Air Force Office of Research, Program Manager Dr. Fariba Fahroo (grant # FA9550-07-1-0234). This support is gratefully acknowledged.

Félix Darve
Grenoble Institute of Technology, France

Table of Contents

Chapter 1

Accounting for Plastic Strain Heterogenities in Modeling Polycrystalline Plasticity: Microstructure-based Multi-laminate Approaches

1.1. Introduction

Models of the mechanical or physical behavior of materials are most efficient when they are microstructure-based. However, reproducing reality is not achievable and energy savings also demand models that do not become highly consumptive of computer space and time. With the goal of bridging scales in models that start from elementary atomistic models to simulate an overall response, the search for compromises between the microstructural descriptions and the resulting simulation accuracy will remain a challenging area for a long time. A smart alternative to running huge "*ab initio*" computational calculations is to anticipate which microstructural features do really matter at the macro-scale concerned according to the considered situation.

In the specific field of modeling the plastic behavior of heterogenous non-linear metallic materials, effective properties are reasonably approached when simultaneously considering i) a good enough description of the evolving morphology, ii) an appropriate homogenization scheme according to the material morphology and behavior type, iii) a relevant microstructural modeling of intra-crystalline plasticity. In all these domains the last few decades have significantly

---

Chapter written by Patrick FRANCIOSI.

enriched the available background. With regard to the third point, dislocation dynamic simulations have clarified many features that concern crystal hardening evolutions with strain [DEV 06], the anisotropy of which is one of the most complex questions not yet answered, even for the simplest cubic structures. With regard to the other two domains, enhanced morphological descriptions by integrating n-point statistics with increasing n [TAL 97], as well as improved first- and second-order developments to better describe the non-linearity of the phase plastic behavior laws [PON 98] have enabled remarkable gains in the accuracy of accessible behavior estimates or bounds. The possible further improvements in the global modeling of polycrystalline plasticity discussed here address points that concern in a combined manner the morphology description, the homogenization framework and the behavior approximation in terms of plastic flow criterion. For theoretical details and simulation examples relating to this book, see [FRA 07, FRA 08].

For such aggregates that deform by crystallographic shear mechanisms (i.e. slip, twinning or also transformation plasticity up to a volume change), we first question the granular description that is conventionally used, compared to an alternative description in terms of grain boundary and sub-boundary orientation distribution. Secondly, between the evolution of the sub-boundary spatial arrangement and the shear activity in the material, a link is made that is based on a multi-laminate approach of plastic heterogenities. Such a multi-laminate approach to describe the current morphology of the strained material in turn acts on the homogenization scheme that can be preferentially used. Comparing with the inclusion-based modeling, further advantages are pointed out, as the more natural reference to an equivalent homogenous super-crystal that justifies introducing a single plastic potential for the whole aggregate, or the possibility of accounting for a grain size effect. Section 1.2 illustrates some support to a sub-boundary based morphology description of polycrystal plasticity, section 1.3 introduces the considered multi-laminate representation and section 1.4 summarizes the proposed modeling framework that results.

1.2. Polycrystal morphology in terms of grain and sub-grain boundaries

1.2.1. *Some evidence of piece-wise regularity for grain boundaries*

When looking at micrographic or nanographic pictures of metallic aggregates, there is plenty of evidence that grains are polyhedral domains whose boundary facets result from the elaboration route. Figure 1.1 shows two examples that concern aggregates of micrometric (left) or nanometric (right) grains. On a topological ground, it is also obvious that if, ideally speaking, all the grains were convex and smooth – i.e. with rounded edges – some complementary matrix phase, of vanishing