Interdisciplinary Applied Mathematics

Volume 23

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Muhammad Sahimi

Heterogeneous Materials

Nonlinear and Breakdown Properties and Atomistic Modeling

With 119 Illustrations

Springer

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Cover illustration:

Mathematics Subject Classification (2000): 82-02, 65M

Library of Congress Cataloging-in-Publication Data
Sahimi, Muhammad.
Heterogeneous materials / Muhammad Sahimi.
p. cm. — (Interdisciplinary applied mathematics ; 22-23)
Includes bibliographical references and indexes.
Contents: [1] Linear transport and optical properties — [2] Nonlinear and breakdown properties and atomistic modeling.
ISBN 0-387-00167-0 (v. 1 : alk. paper) — ISBN 0-387-00166-2 (v. 2 : alk. paper)
1. Inhomogenesou materials. 2. Composite materials. I. Title. II. Interdisciplinary applied mathematiccs ; v. 22-23.
TA418.9.I53 S24 2003
620.1′1—dc21 2002042744

ISBN 0-387-95541-0 Printed on acid-free paper.

Printed in the United States of America.

9 8 7 6 5 4 3 2 1 SPIN 10885680

www.springer-ny.com

Springer-Verlag New York Berlin Heidelberg
A member of BertelsmannSpringer Science+Business Media GmbH

To children of the third world

who have the talent but not the means to succeed

and to

the memory of my father, Habibollah Sahimi,

who instilled in me, a third world child, the love of reading

Preface

Disorder plays a fundamental role in many natural and man-made systems that are of industrial and scientific importance. Of all the disordered systems, heterogeneous materials are perhaps the most heavily utilized in all aspects of our daily lives, and hence have been studied for a long time. With the advent of new experimental techniques, it is now possible to study the morphology of disordered materials and gain a much deeper understanding of their properties. Novel techniques have also allowed us to design materials of morphologies with the properties that are suitable for intended applications.

With the development of a class of powerful theoretical methods, we now have the ability for interpreting the experimental data and predicting many properties of disordered materials at many length scales. Included in this class are renormalization group theory, various versions of effective-medium approximation, percolation theory, variational principles that lead to rigorous bounds to the effective properties, and Green function formulations and perturbation expansions. The theoretical developments have been accompanied by a tremendous increase in the computational power and the emergence of massively parallel computational strategies. Hence, we are now able to model many materials at molecular scales and predict many of their properties based on first-principle computations.

In this two-volume book we describe and discuss various theoretical and computational approaches for understanding and predicting the effective macroscopic properties of heterogeneous materials. Most of the book is devoted to comparing and contrasting the two main classes of, and approaches to, disordered materials, namely, the continuum models and the discrete models. Predicting the effective properties of composite materials based on the continuum models, which are based on solving the classical continuum equations of transport, has a long history and goes back to at least the middle of the nineteenth century. Even a glance at the literature on the subject of heterogeneous materials will reveal the tremendous amount of work that has been carried out in the area of continuum modeling. Rarely, however, can such continuum models provide accurate predictions of the effective macroscopic properties of *strongly* disordered multiphase materials. In particular, if the contrast between the properties of a material's phases is large, and the phases form large clusters, most continuum models break down. At the same time, due to their very nature, the discrete models, which are based on a lattice representation of a material's morphology, have the ability for providing accurate predictions for the effective properties of heterogeneous materials, even when the heterogeneities are strong, while another class of discrete models, that represent a material as a collection of its constituent atoms and molecules, provides accurate predictions of the material's properties at mesoscopic scales, and thus, in this sense, the discrete models are complementary to the continuum models. The last three decades of the twentieth century witnessed great advances in discrete modeling of materials and predicting their macroscopic properties, and one main goal of this book is to describe these advances and compare their predictions with those of the continuum models. In Volume I we consider characterization and modeling of the morphology of disordered materials, and describe theoretical and computational approaches for predicting their *linear* transport and optical properties, while Volume II focuses on nonlinear properties, and fracture and breakdown of disordered materials, in addition to describing their atomistic modeling. Some of the theoretical and computational approaches are rather old, while others are very new, and therefore we attempt to take the reader through a journey to see the history of the development of the subjects that are discussed in this book. Most importantly, we always compare the predictions with the relevant experimental data in order to gain a better understanding of the strengths and/or shortcomings of the two classes of models.

A large number of people have helped me gain deeper understanding of the topics discussed in this book, and hence have helped me to write about them. Not being able to name them all, I limit myself to a few of them who, directly or indirectly, influenced the style and contents of this book. Dietrich Stauffer has greatly contributed to my understanding of percolation theory, disordered media, and critical phenomena, some of the main themes of this book; I am deeply grateful to him. For their tireless help in the preparation of various portions of this book, I would like to thank two of my graduate students, Sushma Dhulipala and Alberto Schroth. Although they may not be aware of it, Professors Pedro Ponte Castañeda of the University of Pennsylvania and Salvatore Torquato of Princeton University provided great help by guiding me through their excellent work, which is described in this book; I would like to thank them both. Some of my own work described in this book has been carried out in collaboration with many people; I am pleased to acknowledge their great contributions, especially those of Dr. Sepehr Arbabi, my former doctoral student. The constant encouragement and support offered by many of my colleagues, a list of whom is too long to be given here, are also gratefully acknowledged. I would like particularly to express my deep gratitude to my former doctoral student Dr. Jaleh Ghassemzadeh, who provided me with critical help at all stages of preparation of this book. Several chapters of this book have been used, in their preliminary versions, in some of the courses that I teach, and I would like to acknowledge the comments that I received from my students.

My wife, Mahnoush, and son, Ali, put up with the countless hours, days, weeks, and months that I spent in preparing this book and my almost complete absence during the time that I was writing, but never denied me their love and support without which this book would have never been completed; I love and cherish them both.

Muhammad Sahimi
Los Angeles, California, USA
May 2002

Contents

Abbreviated Contents for Volume I