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Edited by

Erik van der Giessen
Theodore Y. Wu

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Erik van der Giessen

DELFT UNIVERSITY
OF TECHNOLOGY
DELFT, THE NETHERLANDS

Theodore Y. Wu

DIVISION OF ENGINEERING AND APPLIED SCIENCE
CALIFORNIA INSTITUTE OF TECHNOLOGY
PASADENA, CALIFORNIA

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Editorial Board

Contributors to Volume 36

Alan C. F. Cocks

W. A. Curtin

Simon P. A. Gill

Michael Ortiz

Jingzhe Pan

Rob Phillips

List of Contributors

Numbers in parentheses indicate the pages on which the authors' contributions begin.

ALAN C. F. COCKS (81) Department of Engineering, Leicester University, Leicester LE1 7RH

W. A. CURTIN (163), Division of Engineering, Brown University, Providence, Rhode Island, 02912

SIMON P. A. GILL (81), Department of Engineering, Leicester University, Leicester LE1 7RH

MICHAEL ORTIZ (1), Graduate Aeronautical Laboratories, California Institute of Technology, Pasadena, California 91125

JINGZHE PAN (81), School of Mechanical and Material Engineering, University of Surrey, Guildford, Surrey GU2 5XH

ROB PHILLIPS (1), Division of Engineering, Brown University, Providence, Rhode Island 02912

Preface

Since the first issue of Advances in Applied Mechanics in 1948, the field of applied mechanics has witnessed numerous changes in focal points. One of the most noticeable areas of intense activity today is the application of mechanics in materials science. One of the central issues is to explain the relationship between a material's microstructure and its mechanical properties. The work in the past on the deformation of purely elasticmicrostructured systems is classical by now. In recent years, attention is focussing on more complicated phenomena, which have posed challenging issues on the interface between mechanics and other disciplines. Three articles in the present volume highlight some of the recent advances in these areas.

Microstructures exist at various length scales. In metals, atomic defects such as dislocations can control the mechanical behaviour at length scales several orders of magnitude larger than the atomic scale. Structure-property relationships require the bridging of many length scales. One of the most difficult, and least understood scale transitions is that from the atomic scale to the continuum level. The article by Michael Ortiz and Rob Phillips addresses this subject from a novel point of view by which the standard continuum description of the material is imbued with atomistic content. Numerous examples show that this approach promises to be an effective method to link the behavior of individual atomic defects to macroscopic inelastic behavior.

A different class of microstructural changes are considered in the article by Alan C. F. Cocks, Simon P. A. Gill and Jingzhe Pan. The kinetic processes addressed here include grain-boundary and surface diffusion, interface reactions and grain-boundary migration, which can be modeled by continuum theory. The authors present a comprehensive variational framework for the description of all these processes in competition with each other and in dependence of their respective thermodynamic forces. The emphasis in this article is on numerical techniques, and in this sense supplements the article by Z. Suo in Advances in Applied Mechanics, Vol. 33, 1997, pp. 193–294.

The last article, by W. A. Curtin, addresses failure in fiber-reinforced composite materials. Rather than concentrating on the details of elementary fracture events locally in the microstructure, the main emphasis is on the role of stochastic variations in fiber strengths on macroscopic failure. Starting from the consideration of a single-fiber composite, the author addresses the modeling of damage evolution in multifiber composites, emphasizing the role of accompanying internal stress redistributions. Results of detailed simulations of damage development are used to guide a number of relatively simple analytical models, both are confronted against a wealth of experimental observations.

Theodore Y. Wu and E. van der Giessen

Contents

Nanomechanics of Defects in Solids

MICHAEL ORTIZ

Graduate Aeronautical Laboratories
California Institute of Technology
Pasadena, California

and

ROB PHILLIPS

Division of Engineering
Brown University
Providence, Rhode Island

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I. Introduction

The mechanics of materials is played out against a background of structural imperfection in which defects mediate the inelastic deformation of materials. The recent development of microscopies that allow for the examination of defects at the atomic scale now permit a more direct connection between the defects and the response they engender. Techniques ranging from high-resolution electron microscopy, which makes possible the determination of the atomic-level structure of dislocation cores and grain boundaries, to atomic force microscopies, which bring new meaning to experiments such as those on nanoindentation, all pose deep challenges in modeling the mechanics of materials. Each of these experiments calls for renewed efforts to establish the connection between defect mechanics and constitutive phenomenology that is relevant to the direct simulation of processes in the mechanics of materials. However, the link between the defects themselves and the observed macroscopic behavior is often a difficult one to forge theoretically and remains an active area of research.

The objective of this article is to review methods by which the classical boundary-value problems of continuum mechanics can be imbued with atomistic content. One of the difficulties that has stood in the way of efforts to forge the link alluded to above is the fact that, in some cases of interest, there is no natural separation of scales. Consideration of single defects in isolation is insufficient to yield relevant insights into material behavior, while the attempt to build up sufficient numbers of such defects to be of macroscopic relevance is computationally unfeasible and conceptually inelegant. In the present article, we first aim to review the strengths and weaknesses of the conventional microscopic and continuum perspectives. Our ambition in this respect is to identify the powerful features of both of these approaches with the aim of extracting those parts that are especially appealing in a way that permits a synthesis. This discussion is followed by an assessment of some of the ideas that seem particularly promising for effecting a linkage between understanding at the single-defect level and higher-level approaches.

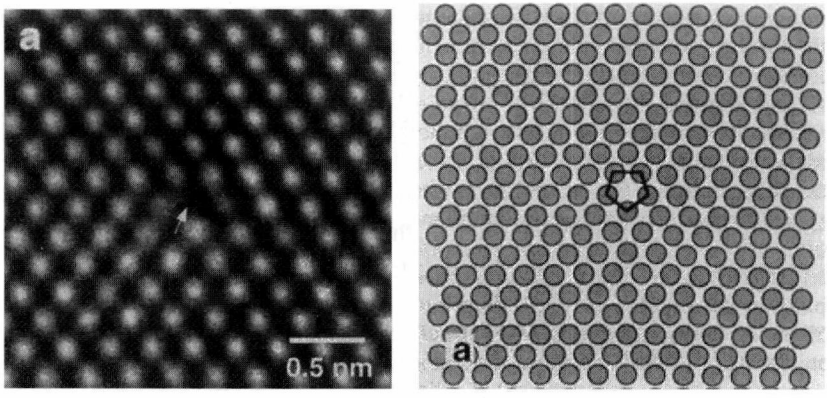
Microscopic modeling is founded on the fundamental assertion that beneath the details of observed macroscopic phenomenology there is a set of microscopic

processes which, when understood, rationalize the observed macroscopic behavior to the extent of enabling quantitative predictions. A microscopic simulation is one in which the relevant microscopic degrees of freedom and their evolution are treated explicitly. In this context, one may start with a prescription for computing the total energy. Given this prescription, a variety of tools are at hand to compute an energy-minimizing configuration—possibly metastable—for a given set of atoms. For example, if we interest ourselves in the geometry of a particular dislocation core, there are well-understood avenues for determining its structure on the basis of known interatomic interactions. For instance, given a high-resolution micrograph of a dislocation core such as shown in Figure 1, different structural alternatives may be evaluated by minimizing their respective energies and asking for that structure which is simultaneously lowest in energy and accounts for the observations. This process is carried out explicitly in Mills *et al.* (1994).

Continuum mechanics, on the other hand, is founded on the assumption that the spatial variations in a given field variable are sufficiently slow as to make possible the smearing out of the atomistic degrees of freedom upon which they are founded. In particular, there is an implicit mapping from the large set of atomistic degrees of freedom to a single vector field of displacements, namely,

$$\{\mathbf{r}_i\} \mapsto \mathbf{u}(\mathbf{x}). \tag{1}$$

One of the most significant virtues of the continuum approach is the considerable reduction it implies in the number of degrees of freedom that must be accounted



(a) (b)

FIG. 1. Lomer dislocation core in aluminum (Mills *et al.*, 1994). (a) High-resolution image of dislocation core; (b) Atomic positions in same dislocation core as obtained by energy minimization. Reprinted with permission of Elsevier Science.

for in a given model. By replacing the set of atomic coordinates $\{\mathbf{r}_i\}$ by a reckoning in terms of displacements, we pass from the realm of $3N$ discrete differential equations to a set of three coupled partial differential equations. We may then defer to powerful tools of analysis and approximation theory, such as the finite-element method, to examine their solutions.

One of the important recognitions that stands at the foundation of the approaches that we review in the present article is that, in some circumstances, progress can be made in linking the continuum and microscopic perspectives in a way that results in more theoretical power than either offers alone. One of the areas in which such models have had a significant impact is that of cohesive-zone theories, in which a conventional continuum mechanics statement of the boundary-value problem of interest is supplemented by constitutive laws governing interfacial slip and decohesion. The link to atomistics arises from the fact that, in many cases, atomic-level calculations can be used to inform the cohesive constitutive description. Alternative schemes have been devised in which parts of the body being modeled are treated explicitly via the tools of atomistic simulation, with a set of boundary conditions being specified which anchors the atomistic region to a conventional continuum. As a final example, the recently developed quasicontinuum method constructs a seamless connection between the two perspectives by explicitly taking advantage of atomistic constitutive insights throughout the body.

The remainder of the article is organized as follows. In Section II, we briefly review the foundations of atomistic modeling, including a discussion of the presently available approximations to the total energy. These approximations provide an important basis for many of the current efforts in nanomechanics. Section III addresses the development of patched atomistic/continuum models with special reference to cohesive-zone strategies, in which the constitutive nonlinearity is confined to particular planes. Section IV takes up an analysis of the insights offered into crystal elasticity by the atomistic perspective. This section culminates in a discussion of the way in which a range of microstructures arise by virtue of constitutive nonconvexity. Section V treats mixed atomistic and continuum computational schemes for effecting the atomistic/continuum linkage described in the preceding sections. The centerpiece of Section VI is the quasicontinuum method. This method makes possible large-scale atomistic analyses by systematically constraining the atomistic degrees of freedom through the application of finite-element discretization and interpolation. Finally, Section VII offers a perspective on the applications which have been made possible by mixed atomistic and continuum models.

It is important to note that the primary aim of this article is to recount our own involvement in efforts to imbue continuum boundary-value problems with atom-

istic content. As such, the present article should not be regarded as a systematic review of the literature, but rather as a personal account of modeling in the mechanics of materials.

II. Atomistic Models of Material Behavior

As stated above, there are circumstances in which the insights that are gleaned from atomistic analysis are indispensable. In this section, we provide an overview of how atomistics can inform higher-level continuum descriptions. We begin with a few illustrative examples for purposes of motivation, and follow with a description of precisely what it means to carry out an atomistic calculation. Finally, the section closes with more detailed examples of the use of atomistic analysis to link scales in the context of the mechanics of materials.

From a fundamental perspective, the microscopic simulation of materials is based on the evolution of degrees of freedom that are governed by the Schrödinger equation. Specifically, given a collection of atoms, each of which carries with it a set of electrons, the problem is to compute the total energy of the ensemble as a function of the relevant microscopic degrees of freedom, e.g., the positions of the nuclei and the electrons. Full-scale calculations such as just described are computationally intensive. The aim of the present discussion is to examine the various approximation strategies that have arisen from the desire to model such systems, with a view to characterizing precisely the compromises that are made in adopting such strategies.

We begin by considering an arbitrary collection of N atoms identified by some convenient labeling scheme $\mathcal{I}$, e.g., simple enumeration in an unstructured gas or Miller indices in a crystal (e.g., Hammond, 1990). Our objective is the determination of the total energy of this collection $E^{\text{tot}}(\{\mathbf{r}_i\})$. One immediate scheme is that presented by pair potential descriptions of the total energy in which E^{tot} is given by

$$E^{\text{tot}} = \frac{1}{2} \sum_{i,\, j \in \mathcal{I}} V^{\text{eff}}(r_{ij}), \tag{2}$$

where $r_{ij} = |\mathbf{r}_i - \mathbf{r}_j|$ is the distance between atoms $i,\ j \in \mathcal{I}$. It bears emphasis that in this description only the nuclear coordinates appear explicitly in the energy function and the electronic degrees of freedom have been condensed out, a situation which is hinted at in labeling the potential V^{eff}. Beyond these general restrictions, the choices of the energy function V available to the materials modeler are numerous.

In many contexts, and especially in cases involving large numbers of atoms within the molecular dynamics setting, it is often useful to resort to multibody expansions of the form

$$E^{\text{tot}} = \sum_{k=1}^{\infty} \left\{ \frac{1}{k!} \sum_{i_1,\ldots,i_k \in \mathcal{I}} V_k(\mathbf{r}_{i_1}, \ldots, \mathbf{r}_{i_k}) \right\}, \tag{3}$$

where the potential V_k accounts for k-body interactions. The term V_1 reduces to an inconsequential constant in the absence of external fields. In writing (3), the hope is that the expansion converges quickly and can be truncated after a few terms to a good approximation. The simplest such truncation scheme consists of keeping two-body interactions only, leading to the pairwise form of the energy:

$$E^{\text{tot}} \approx \frac{1}{2} \sum_{i,\, j \in \mathcal{I}} V_2(r_{ij}). \tag{4}$$

Here again we emphasize that, either phenomenologically or via explicit calculational strategies, the electronic degrees of freedom are implicitly subsumed in the effective pair potential. Once the pair potential has been identified, it is a straightforward matter to evaluate radial derivatives and the corresponding force fields. These force fields, in turn, provide the basis for lattice statics or molecular dynamics analyses of the problem of interest.

As an example of the state of the art in this regard, Figure II shows a sequence of temporal snapshots from a molecular dynamics simulation of dynamic fracture in an fcc crystal due to Abraham *et al.* (1997). One of the outcomes of this series of calculations is the observation of different fundamental mechanisms depending on the underlying crystal orientation. For the orientation shown in the figure, the generation of large amounts of dislocation activity at the crack tip in the form of dislocation loops is particularly noteworthy. It is immediately clear—even from casual inspection of the figure—that the short-range interactions between dislocations are a key part of the physics taking place in the crack tip region. A second key feature of the simulation concerns how to properly meld the boundary conditions of continuum mechanics and those that are *a fortiriori* used in the atomistic setting.

The interatomic interactions used in the example discussed above are of the pair potential variety and, in particular, of the Lennard–Jones form, namely,

$$V(r_{ij}) = \left(\frac{a}{r_{ij}}\right)^{12} - \left(\frac{b}{r_{ij}}\right)^{6}, \tag{5}$$

where the parameters a and b can be determined, e.g., by insisting that the crystal have the correct lattice parameter and cohesive energy. Using these highly sim-

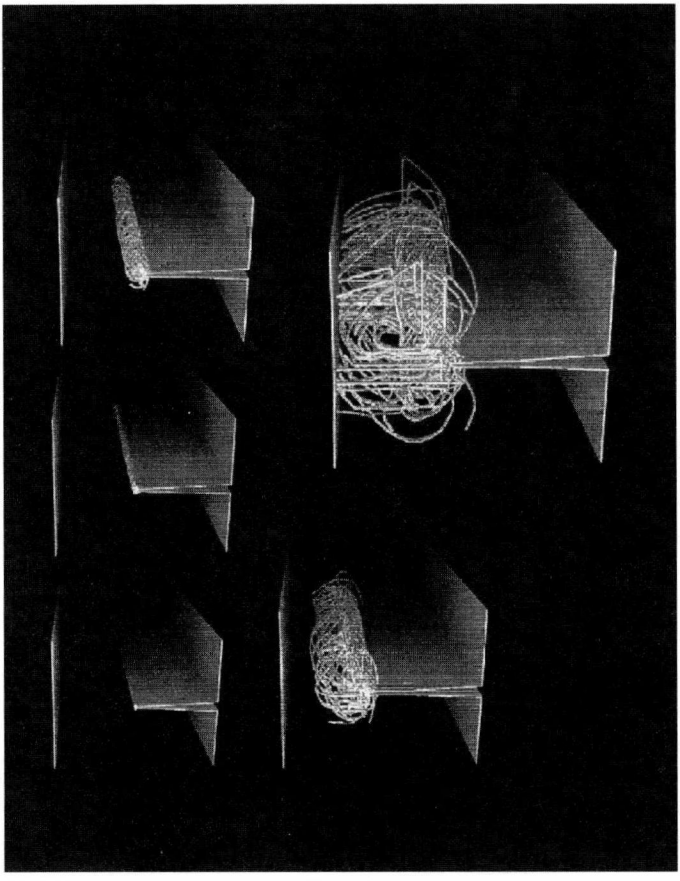


FIG. 2. Sequence of snapshots in deformation history for an FCC crystal undergoing fracture. Computations carried out using molecular dynamics (Courtesy of F. Abraham).