Atomistic Modeling of Materials Failure

Markus J. Buehler

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To my wife, for inspiration and loving support

Preface

This book has evolved from lecture notes of undergraduate and graduate level subjects as well as review articles and journal papers. The book provides a review of atomistic modeling techniques that successfully link atomistic and continuum mechanical methods. It intended to be a reference for engineers, materials scientists, and researchers in academia and industry. The writing of this book was motivated by the desire to develop a coherent set of notes that provides an introduction and an overview into the field of atomistic-based computational solid mechanics, with a focus on fracture and size effects.

The book covers computational methods and techniques operating at the atomic scale, and describes how these techniques can be used to model the dynamics of cracks and other deformation mechanisms. A description of molecular dynamics as a numerical modeling tool covers the use of interatomic potentials (pair potentials such as the Lennard-Jones model, embedded atom method (EAM), bond order potentials such as Tersoff's and Brenner's force fields, as well as the first principles based ReaxFF Reactive force field) in addition to the general philosophies of model building, simulation, interpretation, and analysis of simulation results. Example applications for specific materials (such as silicon, nickel, copper, carbon nanotubes) are provided as case studies for each of the techniques, areas, and problems discussed. Readers will find a physics-motivated discussion of the numerical techniques along with a review of mathematical concepts and code implementation issues. Using specific examples such as investigations of crack dynamics in brittle materials or deformation mechanics of nanomaterials, this volume conveys how atomistic studies have helped to advance developing new theories, or provided insight into the molecular deformation mechanisms, explaining or supplementing experimental results. Many of the examples are adapted from studies carried out by the author of this book, and some of the discussion should therefore not be considered as a comprehensive and inclusive review with respect to the wider range of available results. Rather, they represent a set of specific examples to illustrate the application of the atomistic simulation techniques reviewed here.

Completing this book would not have been possible without the help and support of numerous people. The author is most greatly indebted to all who have contributed to this book in some way. In particular, sincere gratitude goes to those individuals from whom he had the opportunity to learn from over the years, in particular his graduate advisor Huajian Gao and postdoctoral advisor William A. Goddard III. The author is deeply humbled by the many contributions that have pioneered the development of this research field over the past decades. The author would also like to thank the Editor Mrs. Elaine Tham of Springer and her staff for the continuous support for this project. The efforts by the reviewers of the manuscript are greatly acknowledged, as they provided valuable suggestions for revisions in the final manuscript.

The study of materials failure using atomistic simulation has been a rewarding journey that continues to bring so much joy, excitement, and inspiration. The author hopes to convey some of the excitement about this research field in this book.

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Markus J. Buehler

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