Preface

Multiscale Materials Modeling for Nanomechanics is an interesting title for a book as the terms "nanomechanics" and "multiscale modeling" have different definitions and meaning to various scientific communities. Therefore, we feel it is important to inform the reader up front of our thoughts on this topic and why we chose to include the subjects discussed herein. We think of nanomechanics as the mechanics that occur at the smallest length scales in materials, down to nanometers. Thus, the study of nanomechanics should focus on materials where this regime of mechanics dominates or controls behavior, usually when a governing length scale is below a micron. In addition, it is our intent with a book on nanomechanics to focus equally on the materials as on the mechanics, because they are intrinsically linked at these size scales.

Multiscale modeling is also an intriguing term because of different ideas about what multiscale modeling encompasses. One might immediately assume that a book on multiscale modeling would focus on methods that couple scales or simulation methodologies, such as continuum and atomistic methods. While this is certainly part of multiscale modeling, this does leave out one other important way to conduct multiscale modeling: information passing between scales. The former is called *concurrent multiscale modeling* and the latter *hierarchical multiscale modeling*. In this book, we will cover both types of multiscale modeling approaches providing some breadth on the uses of the different types of multiscale modeling as applied to the mechanics of materials and structures at the nanoscale.

Finally, we would like to point out that our intent in writing this book was to cover a range of topics that span from fundamental methods to applications. The beginning of the book covers fundamental techniques like atomistic simulations, dislocation dynamics, continuum methods, and density functional theory calculations. These chapters are meant to provide the reader with a broad perspective on computational techniques that have been fundamental to materials modeling at various length and time scales. However, we realize that for those who are a completely unfamiliar with these techniques, the chapters in this book will provide a good introduction, but more detailed books will likely be needed to master the techniques. The self-containment of this book was sacrificed in order to allow for the later chapters of

the book that provide examples of both concurrent and hierarchical applications of multiscale modeling. We hope that the brevity of the first few chapters is accounted for by the number and depth of the applications provided later.

With this in mind, the book is organized in three parts. The first part, which contains Chaps. 1–4, covers what may be considered as fundamental or basic materials modeling methods. These chapters introduce the methods of molecular simulations, dislocation dynamics, continuum approximations, and electronic density functional theory calculations. These methods provide some of the basic modeling approaches that are used extensively in all of the chapters that follow and span from angstroms to meters in length scale. The second part, Chaps. 5–8, provides several more recently developed methods that are scale bridging including both length and time scales. The specific methods include the quasicontinuum method (Chap. 5), accelerated molecular dynamics (Chap. 6), the concurrent atomistic-continuum method (Chap. 8), and the "atoms to continuum" method. Chapter 6 is the only chapter that deals with time-scale bridging, while the rest of these chapters present length-scale bridging techniques which can be largely classified as concurrent multiscale techniques. It is important to note that there are many other length, and time-scale bridging methods, but our intent is to provide a few here that have been or can be used for modeling nanomechanics in materials. Chapters 9 and 10 provide methods to analyze and visualize the modeling results of particle systems (e.g., molecular simulations). This is of particular importance because the analysis and visualization of data are precisely what can be used to conduct more efficient multiscale modeling, either through concurrent schemes or hierarchical methods.

The third part, covering Chaps. 11–17, provides case studies in the use of multiscale materials modeling as applied to nanomechanics. The topics are diverse in the problems and how they solve them. The chapters include the study of the mechanical properties of nanowires and nanopillars made of metals by studying dislocation nucleation (Chap. 12) or dislocation motion of preexisting dislocations (Chap. 11) or their statistical nature in nano-grained materials using the quantized crystal plasticity method (Chap. 13). The rest of the chapters each deal with the mechanics of different systems including amorphous materials (Chap. 14), ferroelectric thin films (Chap. 15), silicon electrodes (Chap. 16), and thin liquid films (Chap. 17).

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