Introduction to Computational Materials Science

Emphasizing essential methods and universal principles, this textbook provides everything students need to understand the basics of simulating materials behavior. All the key topics are covered, from electronic structure methods to microstructural evolution, appendices provide crucial background material, and a wealth of practical resources are available online to complete the teaching package.

- Examines modeling materials across a broad range of scales, from the atomic to the mesoscale, providing students with a solid foundation for future study and research.
- Presents detailed, accessible explanations of the fundamental equations underpinning materials modeling, and includes a full chapter summarizing essential mathematical background.
- Extensive appendices, including essential background on classical and quantum mechanics, electrostatics, statistical thermodynamics and linear elasticity, provide all the background necessary to fully engage with the fundamentals of computational modeling.
- Exercises, worked examples, computer codes and discussions of practical implementations methods are all provided online to give students the hands-on experience they need.

Richard LeSar is the Lynn Gleason Professor of Interdisciplinary Engineering in the Department of Materials Science and Engineering, Iowa State University, and the former Chair of the Materials Science and Engineering program. He is highly experienced in teaching the modeling and simulation of materials at both undergraduate and graduate levels, and has made extensive use of these methods throughout his own research.

"Finally, an introductory textbook on computational methods that addresses the breadth of materials science. Finally, an introductory textbook that emphasizes understanding the foundations of the subject. Kudos to Professor Richard LeSar for producing such a beautifully pedagogical introductory text that covers the major methods of the field, relates them to their underlying science, and provides links to accessible simulation codes. *Introduction to Computational Materials Science* is the perfect companion to a first-course on this rapidly growing segment of our field."

David J. Srolovitz, University of Pennsylvania

"Professor LeSar has written an elegant book on the methods that have been found to be useful for simulating materials. Unlike most texts, he has made the effort to give clear, straightforward explanations, so that readers can implement the models for themselves. He has also covered a wider range of techniques and length-/time-scales than typical textbooks that ignore anything coarser than the atom. This text will be useful for a wide range of materials scientists and engineers."

Anthony Rollett, Carnegie Mellon University

"Richard LeSar has successfully summarized the computational techniques that are most commonly used in Materials Science, with many examples that bring this field to life. I have been using drafts of this book in my Computational Materials course, with very positive student response. I am delighted to see the book in print – it will become a classic!"

Chris G. Van de Walle, University of California, Santa Barbara

Introduction to Computational Materials Science

Fundamentals to Applications

RICHARD LESAR
Iowa State University

MRS **MATERIALS RESEARCH SOCIETY**
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PREFACE

The goal of this book is to introduce the basic methods used in the computational modeling of materials. The text reflects many tradeoffs: breadth versus depth, pedagogy versus detail, topic versus topic. The intent was to provide a sufficient background in the theory of these methods that the student can begin to apply them to the study of materials. That said, it is not a "computation" book – details of how to implement these methods in specific computer languages are not discussed in the text itself, though they are available from an online resource, which will be described a bit later in this preface.

Modeling and simulation are becoming critical tools in the materials researcher's tool box. My hope is that this text will help attract and prepare the next generation of materials modelers, whether modeling is their principal focus or not.

Structure of the book

This book is intended to be used by upper-level undergraduates (having taken statistical thermodynamics and at least some classical and quantum mechanics) and graduate students. Reflecting the nature of materials research, this text covers a wide range of topics. It is thus broad, but not deep. References to more detailed texts and discussions are given so that the interested reader can probe more deeply. For those without a materials science background, a brief introduction to crystallography, defects, etc. is given in Appendix B.

This text covers a wide range of methods, covering a variety of time and length scales. The text is divided into parts, each with a specific focus. Part One, for example, introduces the basic methods used in essentially all simulations. The random-walk model in Chapter 2 illustrates some important concepts used throughout the text, including the stochastic nature of simulations. Since every method in this text involves representing the materials system on a lattice or grid, Chapter 3 focuses on how to sum quantities, such as the energy, on a lattice.

In Part Two, the text focuses on modeling of systems of atoms and molecules, starting with Chapter 4, which describes the fundamental methods used to calculate the electronic structure of materials. To extend length scales beyond what can be done with such methods, analytic descriptions of the interaction potentials between atoms are discussed for a variety of materials types in Chapter 5. Molecular dynamics methods, in which Newton's equations are solved to monitor the motion of atoms, are presented in Chapter 6, enabling the modeling of the thermodynamic and dynamic properties of materials. The Monte Carlo method of Chapter 7 is thermodynamically driven, with great flexibility to be applied not only to systems of atoms but also to any models for which there is an expression for the energy in terms of a set of

variables. The final chapter of this part of the text, Chapter 8, discusses how to extend these ideas to molecular systems.

One of the most important distinctions between how materials scientists view materials and how many of those in other fields do so is the materials scientist's focus on defects and defect distributions, which involve a range of length and time scales intermediate between the atomic scale and the continuum scale of everyday objects. This range of length and times is often referred to as the mesoscale. Recognizing this distinction, Part Three extends the discussion to methods used in modeling the physics of materials at the mesoscale. Chapter 9 introduces the kinetic Monte Carlo method, which evolves a system based on the rates of its underlying processes. Standard Monte Carlo is revisited in Chapter 10, with a focus on a common approach used to model microstructural evolution. Cellular automata are rule-based methods with great flexibility, and some limitations, and are discussed in Chapter 11. One of the fastest-growing, and most powerful, methods in materials computation is the phase-field method, which is based on thermodynamics. The presentation in Chapter 12 is basic, using relatively simple examples of applications of the phase-field method. In the final chapter of this part of the text, Chapter 13, a set of methods is introduced that are based on what I call mesodynamics – the application of standard dynamical methods to systems of collective variables that represent, generally, defects in a material.

The single chapter of Part Four summarizes and integrates many of the ideas brought forth in the previous text. Chapter 14 is couched in the ideas of *Integrated Computational Materials Engineering* (ICME), a new field that integrates experiment with computation to accelerate materials development. The basic ideas behind *materials informatics* are introduced and their important role in ICME is discussed.

A series of appendices provide background material to the text, covering such diverse topics as classical mechanics, electronic structure, statistical thermodynamics, rate theory, and elasticity.

The text does not present any continuum-level modeling, such as the finite element method, heat or fluid flow, etc. It is not that these topics are not interesting or that they are unimportant in materials science and engineering – there simply was not sufficient space in the text.

Computation

Both the development of materials models as well as how one can utilize models in a computer-based calculation are covered in this text. A variety of numerical methods used in such calculations are presented. Understanding the limitations of the methods discussed in the text will require a working knowledge of those methods.

That said, this is not a computer programming text and details of the implementation of the methods and algorithms into a computer program are not discussed. Sample applications are, however, available on the web at http://www.cambridge.org/lesar, in which the implementation of the methods is discussed in some detail. These codes are based on the commercial platforms MATLAB® and Mathematica®, which are commonly available in many universities. These platforms are powerful enough to use for the examples in this book, yet straightforward enough so that programming is understandable. The graphics capabilities needed for the examples

are typically built into them. Note that the sample applications may not be well-optimized computer codes – they were written to be clear not efficient. Students who want a more extensive experience are urged to create their own codes based on the algorithms in the text.

Computational modeling is best learned by doing. I encourage the use of the computer codes available at http://www.cambridge.org/lesar. Not only is doing these types of simulations essential for understanding the methods, I generally find that students enjoy running calculations more than reading about them.

Acknowledgments

A number of people have read parts of this text over time, giving excellent advice on how to improve it. I particularly want to thank Chris Van de Walle, Tony Rollett, Simon Phillpot, Robin Grimes, Scott Beckman, Jeff Rickman, and Alan Constant for critically reading chapters of the text. Their comments helped me greatly. Any remaining errors and inadequacies in the text are, of course, my own.

This text originated in a course on computational modeling that I taught in the Department of Materials at the University of California Santa Barbara while I was a member of the technical staff at the Los Alamos National Laboratory. I want to thank Professor David Clarke, who, as then Chair of the Department of Materials at UCSB, invited me to share with him, and then teach, a course on computational modeling. I also want to thank my managers at Los Alamos, who tolerated my periodic disappearances off to Santa Barbara. The members of the Department of Materials Science and Engineering at Iowa State University also deserve thanks for putting up with a distracted Chair as I finished this project. All of these people contributed to the rather twisted path I followed to create this book and I thank them.