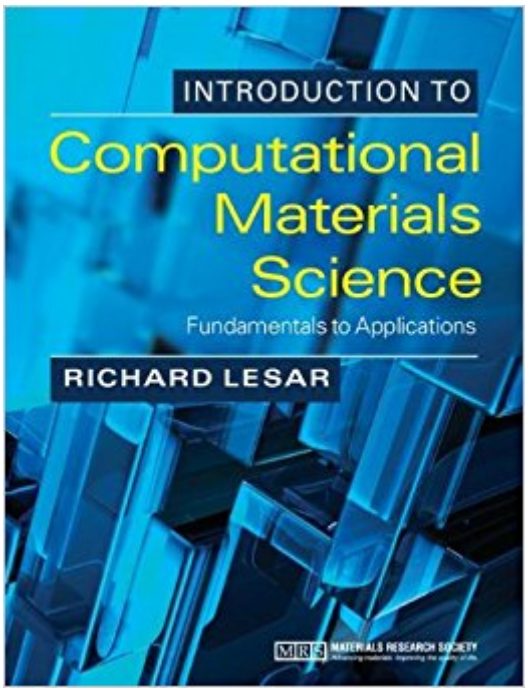
Introduction To Computational Materials Science: Fundamentals To Applications



Synopsis

Emphasising 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. Modeling is examined at a broad range of scales, from the atomic to the mesoscale, providing students with a solid foundation for future study and research. Detailed, accessible explanations of the fundamental equations underpinning materials modelling are presented, including a full chapter summarising essential mathematical background. Extensive appendices, including essential background on classical and quantum mechanics, electrostatics, statistical thermodynamics and linear elasticity, provide the background necessary to fully engage with the fundamentals of computational modelling. Exercises, worked examples, computer codes and discussions of practical implementations methods are all provided online giving students the hands-on experience they need.

Book Information

Hardcover: 427 pages

Publisher: Cambridge University Press; 1 edition (May 6, 2013)

Language: English

ISBN-10: 0521845874

ISBN-13: 978-0521845878

Product Dimensions: 7.4 x 0.9 x 9.7 inches

Shipping Weight: 2.3 pounds (View shipping rates and policies)

Average Customer Review: 4.2 out of 5 stars 6 customer reviews

Best Sellers Rank: #361,578 in Books (See Top 100 in Books) #20 inÃ Â Books > Engineering & Transportation > Engineering > Materials & Material Science > Extraction & Processing #120 inÃ Â Books > Science & Math > Chemistry > Physical & Theoretical > Physical Chemistry #339 inÃ Â Books > Engineering & Transportation > Engineering > Materials & Material Science > Materials Science

Customer Reviews

"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 Prof. 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"Prof. 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

Emphasising essential methods and universal principles, this textbook provides everything students need to understand the basics of simulating materials behaviour. Topics covered range from electronic structure methods to microstructural evolution, appendices provide crucial background material, and exercises, worked examples and computer codes are provided online to complete the teaching package.

+ Good selection of topics to give an overall overview of the field and its potential for development of innovative engineering practices.- More problems should be added at the end of each chapters.

Reference Book

Excellent book congratulations to the author

Good.

In the last 3-4 years a few Introduction to computational material science books have come out. Much of the earlier ones , although good, were more focused on specific length and time scales (i.e. either atomic, diffusive, continuum, etc.). This text attempts to be an intro style survey of the most relevant types of computational approaches in materials science and it does a great job at it. Dr.

Richard LeSar clearly and concisely covers the basics of electronic structure calculations, atomistics, and microstructure evolution using mesoscopic methods. I've reviewed "Computational Materials Science: An Introduction" by Dr. June Gune Lee which is an excellent book if your planning on using other codes/software to carry out your computational investigations (Also it only covers Molecular Dynamics and Density Functional Theory). This book differs in that it is targeted more towards understanding the techniques and being able to develop,implement, and code them on your own. For this reason I think this book is slightly more ideal for an undergraduate or 1st year graduate student who wants to learn about computational materials science.Pros:1. Well written and easy to read.2. Covers a good amount of topics.3. FANTASTIC Appendix.4. Available download resources are very nice.5. Good for someone who wants to establish a solid foundation in Comp.-MSECons:1. Could be less expensive (paperback edition?).2. Although the first edition; there a a decent amount of typos.

This is a review of the Matlab code only, not of the book. I only glanced at the book and cannot comment, and according to other reviewers, this should be an excellent textbook.Code, however, is not up to a standard. The author used Matlab, which I would say is a great choice, if I didn't look at the code. The author did say that intention was for the code to be easily transferable between languages, but this will mostly result in situations where students learn bad Matlab practices, while having less readable code at the same time.The code I would describe as a Matlab code that is written as a literal translation of a C or Fortran code. No operations on vectors or matrices, for-loops everywhere... As an example, the first exercise that would take 3-4 lines of clearly readable Matlab code were blown into 20+ lines of code across two functions (plus comments). Not to say anything about speed (as Matlab is kinda of an interpreted language).This said, there is a code and it is free, and that took some effort. Thus 2 stars, though I would encourage students to learn Matlab elsewhere and use supplied code as a last resort, or use the code as a black box, or use whatever programming language they are comfortable with.UPDATE: I would also like to comment on the exercises accompanying the book. Those are also available from the book's website. Exercises are nicely written and, in my opinion, have enough room for exploration by a student. They go from a relatively straightforward use of the accompanying code to harder ones that require an understanding of the material. The above review of the code still holds, though it cannot stand alone without also looking at the accompanying exercises, which I find well thought out. Thus, I am compeled to raise the review to 3 stars.PLEASE take into consideration, this is not a review of the book, but of the accompanying code.

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