Books

Also This Month

Crystals, Defects and Microstructures: Modeling across Scales

Rob Phillips

Cambridge U. Press, New York, 2001. $130.00, $47.95 paper (780 pp.). ISBN 0-521-79005-0, ISBN 0-521-79357-2 paper

Although nanoscience gets all the publicity, many of its thornier intellectual issues actually concern multiscale modeling. Indeed, this is one of the foci of the recent NSF program solicitation for nanoscale science and engineering. Modeling across scales goes to the heart of how we do physics, connecting different levels of description economically, faithfully, and above all, predictably. Some concrete examples: Can we make continuum models of real materials, simultaneously capturing the elastic properties at long scales and the atomic forces that seem to govern the motion of crack tips? Can we make predictive models for microstructure formation that take into account mechanisms of heat transport on long length scales and the details of atomic attachment kinetics at short scales? And how does microscopic disorder determine the large-scale mechanical properties of materials? These are all difficult questions, because many different length scales need to be treated or resolved simultaneously. In the ideal world, there would be a single protocol capable of incorporating the level of description and degree of resolution appropriate for each point or region in space. Hence, almost any theoretical framework hinges on the notion of adaptivity: In the context of numerical calculations, this means adaptive mesh refinement of one sort or another.

It was thus with some trepidation that I opened *Crystals, Defects and Microstructures: Modeling Across Scales*, by Rob Phillips. The last I had heard, the title topics were still open problems. What, I wondered, had I overlooked during the last few years, while I was somewhat preoccupied with changing my children's diapers? Had the dust settled to such an extent that people were now writing textbooks about these subjects? Eager to find the answer, I flipped to the last page--page 755, no less. There my eye lit upon the following sentence: "On the other hand, after the long journey of writing a book such as this, I am also struck at the mismatch between what I had hoped this book would become and what it actually is." Phew! In fact, only in the last 107-page chapter does Phillips actually discuss ways to bridge length scales. This discussion is an exercise in consciousness-raising, which many readers will find rather thought-provoking. It is packed with examples of multiscale modeling at work, ranging from Newton's realization that the gravitational field of Earth can be treated as originating from a point, to modern research topics, including hyperdynamics methods for accelerating time-dependent simulations, mesoscopic dislocation dynamics, solidification processes, and the author's own pioneering work on linking atomistic simulations to finite element simulations. One of the nice things about this chapter is that, in places, it acts as a sort of reinterpretation of much that has gone before it--for example, the discussion on linear elasticity theory and density functional theory.

Unfortunately, I finished this chapter wishing that the author had provided much more detail about the techniques. After all, one wants the readers to come away being able to do computations that they couldn't previously do; having the right

philosophy is only half the battle. In particular, I would have wished to see a more complete description of the different techniques for implementing adaptive mesh refinement ideas (disclosure: I do indeed work on this topic, and my work is appropriately reproduced and cited) and perhaps a more practical description of renormalization group ideas, and their relation to effective theory construction, with actual examples.

The preceding 648 pages present a nicely-written, self-contained course on materials physics. There is a tasteful blend of the theoretical physicist's view of the material and the material scientist's more empirical, data-informed view. Many courses on solid-state physics are closely based around the classic *Solid State Physics* by Neil W. Ashcroft and N. David Mermin (Holt, Rinehart, and Winston, 1976), which mainly focuses on the properties of ideal materials, an appropriate focus for the sorts of experiment that physicists prefer to do. Phillips's book, by contrast, is much more focused on the interesting, but unpleasant, phenomena that plague real materials, such as how defects determine mechanical properties; nonequilibrium effects, such as microstructure evolution; the role of long-range forces, such as stress fields; and the more complex features of materials phase diagrams. By the time readers have reached page 648, they should have an appreciation of the absolute necessity of being able to handle different scales. Thus, I would be tempted to use selected parts of this book in a first-semester graduate course on solid-state physics, in order to make the readings more relevant to the interesting and crucial materials problems that are the focus of modern research.

In summary, this book has appeared at a useful time--if not slightly too early. Nevertheless, I would recommend it to anyone wishing to get both a broad overview of the intersection of theoretical condensed matter physics with modern materials science, and some good pointers toward future research directions.

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