INTRODUCTION

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The way a scientist looks at the materials world is changing dramatically. Advances in the synthesis of nanostructures and in high-resolution microscopy are allowing us to create and probe assemblies of atoms and molecules at a level that was unimagined only a short time ago – the prospect of manipulating materials for device applications, one atom at a time, is no longer a fantasy. Being able to see and touch the materials up close means that we are more interested than ever in understanding their properties and behavior at the atomic level. Another factor which contributes to the present state of affairs is the advent of large-scale computation, once a rare and highly sophisticated resource accessible only to a few privileged scientists. In the past few years *materials modeling*, in the broad sense of theory and simulation in integration with experiments, has emerged as a field of research with unique capabilities, most notably the ability to analyze and predict a very wide range of physical structures and phenomena. Some would now say the modeling approach is becoming an equal partner to theory and experiment, the traditional methods of scientific inquiry.

There are certain problems in the fundamental description of matter, previously regarded as intractable, now are amenable to simulation and analysis. The *ab initio* calculation of solid-state properties using electronic-structure methods and the direct estimation of free energies based on statistical mechanical formulations are just two examples where predictions are being made without input from experiments. Because materials modeling draws from all the disciplines in science and engineering, it greatly benefits from cross fertilization within a multidisciplinary community. There is recognition that *Computational Materials* is just as much a field as Computational Physics or Chemistry; it offers a robust framework for focused scientific studies and exchanges, from the introduction of new university curricula to the formation of centers for collaborative research among academia, corporate and government laboratories. A basic appeal to all members of the growing community

S. Yip (ed.),
Handbook of Materials Modeling, 1–5.

is the challenge and opportunity of solving problems that are fundamental in nature and yet have great technological impact, problems spanning the disciplines of physics, chemistry, engineering and biology.

Multiscale modeling has come to symbolize the emerging field of computational materials research. The idea is to link simulation models and techniques across the micro-to-macro length and time scales, with the goal of analyzing and eventually controlling the outcome of critical materials processes. Invariably these are highly nonlinear, inhomogeneous, or non-equilibrium phenomena in nature. In this paradigm, electronic structure would be treated by quantum mechanical calculations, atomistic processes by molecular dynamics or Monte Carlo simulations, mesoscale microstructure evolution by methods such as finite-element, dislocation dynamics, or kinetic Monte Carlo, and continuum behavior by field equations central to continuum elasticity and computational fluid dynamics. The vision of multiscale modeling is that by combining these different methods, one can deal with complex problems in a much more comprehensive manner than when the methods are used individually [1].

> "*Modeling* is the physicalization of a concept,
> *simulation* is its computational realization."

This is an oversimplified statement. On the other hand, it is a way to articulate the intellectual character of the present volume. This *Handbook* is certainly about modeling and simulation. Many would agree that conceptually the process of modeling ought to be distinguished from the act of simulation. Yet there seems to be no consensus on how the two terms should be used to show that each plays an essential role in computational research. Here we suggest a brief *all-purpose* definition (admittedly lacking specificity). By concept we have in mind an idea, an idealization, or a picture of a system (a scenario of a process) which has the connotation of functionality. For an example consider the subway map of Boston. Although it gives no information about the city streets, its purpose is to display the *connectivity* of the stations – few would dispute that for the given purpose it is a superb physical construct enabling any person to navigate from point A to point B [2]. So it is with our two-part definition; it is first a thoughtfully simplified representation of an object to be studied, a phenomenon, or a process (modeling), then it is the means with which to investigate the model (simulation). Notice also that when used together modeling and simulation implies an element of coordination between *what* is to be studied and *how* the study is to be conducted.

Length/Time Scales in Materials Modeling

Many physical phenomena have significant manifestations on more than one level of length or time scale. For example, wave propagation and

attenuation in a fluid can be described at the continuum level using the equations of fluid dynamics, while the determination of shear viscosity and thermal conductivity is best treated at the level of molecular dynamics. While each level has its own set of relevant phenomena, an even more powerful description would result if the microscopic treatment of transport could be integrated into the calculation of macroscopic flows. Generally speaking, one can identify four distinct length (and corresponding time) scales where materials phenomena are typically studied. As illustrated in Fig. 1, the four regions may be referred to as electronic structure, atomistic, microstructure, and continuum. Imagine a piece of material, say a crystalline solid. The smallest length scale of interest is about a few angstroms (10^{-8} cm). On this scale one deals directly with the electrons in the system which are governed by the Schrödinger equation of quantum mechanics. The techniques that have been developed for solving this equation are extremely computationally intensive, as a result they can be applied only to small simulation systems, at present no more than about 300 atoms. On the other hand, these calculations are theoretically the most rigorous; they are particularly valuable for developing and validating more approximate but computationally more efficient descriptions.

The scale at the next level, spanning from tens to about a thousand angstroms, is called atomistic. Here discrete particle simulation techniques, molecular dynamics (MD) and Monte Carlo (MC), are well developed,

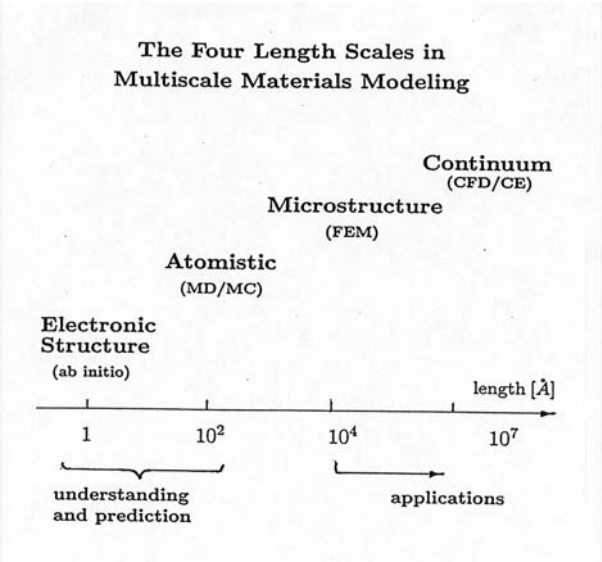

Figure 1. Length scales in materials modeling showing that many applications in our physical world take place on the micron scale and higher, while our basic understanding and predictive ability lie at the microscopic levels.

requiring the specification of an empirical classical interatomic potential function with parameters fitted to experimental data and electronic-structure calculations. The most important feature of atomistic simulation is that one can now study a system of large number of atoms, at present as many as 10^9. On the other hand, because the electrons are ignored atomistic simulations are not as reliable as *ab initio* calculations.

Above the atomistic level the relevant length scale is a micron (10^4 angstroms). Whether this level should be called microscale or mesoscale is a matter for which convention has not been clearly established. The simulation technique commonly in use is finite-element calculations (FEM). Because many useful properties of materials are governed by the microstructure in the system, this is perhaps the most critical level for materials design. However, the information required to carry out such calculations, for example, the stiffness matrix, or any material-specific physical parameters, has to be provided from either experiment or calculations at the atomistic or *ab initio* level. To a large extend, the same can be said for the continuum-level methods, such as computational fluid dynamics (CFD) and continuum elasticity (CE). The parameters needed to perform these calculations have to be supplied externally.

There are definite benefits when simulation techniques at different scales can be linked. Continuum or finite-element methods are often most practical for design calculations. They require parameters or properties which cannot be generated within the methods themselves. Also they cannot provide the atomic-level insights needed for design. For these reasons continuum and finite element calculations should be coupled to atomistic and *ab initio* methods. It is only when methods at different scales are effectively integrated that one can expect materials modeling to give fundamental insight as well as reliable predictions across the scales. The efficient bridging of the scales in Fig. 1 is a significant challenge in the further development of multiscale modeling.

The classification of materials modeling and simulation in terms of length and time scales is but one way of approaching the subject. The point of Fig. 1 is to emphasize the theoretical and computational methods that have been developed to describe the properties and behavior of physical systems, but it does not address other equally important issues, those of applications. One might imagine discussing materials modeling through a matrix of methods and applications which could be useful for displaying their connection and particular suitability. This would be quite difficult to carry out at present because there are not enough clear-cut case studies in the literature to make the construction of such a matrix meaningful. From the standpoint of knowing what methods are best suited for certain problems, materials modeling is a field still in its infancy.

An Overview of the *Handbook*

The *Handbook* is laid out in 9 chapters, dealing with modeling and simulation methods (Part A) and models for specific areas of studies (Part B). In Part A the first three chapters describe modeling concepts and simulation techniques at the electronic (Chapter 1), atomistic (Chapter 2), and mesoscale (Chapter 3) levels, in the spirit of Fig. 1. In contrast Chapter 4 describes a variety of methods based on mathematical analysis. The chapters in Part B focus on systems in which basic studies have been carried out. Chapter 5 treats rate processes where time-scale problems are just as important and challenging as length-scale problems. The next four chapters cover a range of physical structures, crystal defects (Chapter 6) and microstructure (Chapter 7) in solids, various models and methods for fluid simulation (Chapter 8), and models of polymer and soft matter (Chapter 9). In each chapter there are other significant topics which have not been included; for these we recommend the readers consult the references given in each article. Each chapter begins with an introduction which serves to connect the individual articles in the chapter with the broad themes that are relevant to our growing community. While no single chapter attempts to be inclusive in treating the many important aspects of materials modeling, even with restrictions to fundamental methods and models, hopefully, the entire *Handbook* is a first step in that direction.

The Handbook also has a special section which we call Plenary Perspectives. This is a collection of commentaries by recognized authorities in the materials modeling or related fields. Each author was invited to write briefly on a topic that would give the readers, especially the students, insight on different issues in materials modeling. Together with the 9 chapters these perspectives are meant to inform the future workers coming into this exciting field.

References

[1] S. Yip, "Synergistic science," *Nature Mater.*, 3, 1–3, 2003.
[2] M. Ashby, "Modelling of materials problems," *J. Comput.-Aided Mater. Des.*, 3, 95–99, 1996.