

22.106 Neutron Interactions and Applications (Spring 2005)
Lecture 14 (4/21/05)

Multiscale Materials Modeling

References --

S. Yip, "Synergistic Science", *Nature Materials* **2**, 3 (2003). A pdf file of this commentary is attached immediately following

Introduction – Emergence of Materials Modeling

The increasing need for new materials in various technological enterprises in our society has brought about the realization that successful materials design requires a holistic approach, where understanding of the fundamental materials properties and behavior is integrated with innovations in synthesis and processing methods, and further combined with performance analysis, lifecycle predictions, environmental concerns, and economic studies. The highly interdisciplinary nature of materials design makes it imperative that the different sectors of the scientific and engineering community establish effective communication with each other and that they work across traditional boundaries.

In each of the distinct areas encompassed by materials design, remarkable progress driven by the exploitation of computation is being made, as indicated by such developments as the quantitative understanding of electronic properties of semiconductor materials through first-principles total energy calculations, and the improvement in design of injection-molding processing through modeling of rheological behavior of polymers. As scientific computing and visualization grow in power and accessibility, the role of modeling in materials design will become even more pervasive, not only for simulation, analysis, and prediction, but also for database generation and virtual testing.

Materials research has become an extremely active and highly interdisciplinary field of scientific research and technological development [1]. Scientists and engineers in universities, industrial and government research laboratories all play an important part in the evolution of this field, as witnessed by the explosive growth of the Materials Research Society meetings. Other indications are a number of new journals, such as *Journal of Computer-Aided Design* [2] and *Modelling and Simulation in Materials Science and Engineering* [3], and conferences, such as the Workshop on Modeling Industrial Materials: Connecting Atomistics and Continuum, held at the Institute for Theoretical Physics, University of California at Santa Barbara, January 1996 [4].

Still another factor which contributes to the growing importance of materials modeling is the realization on the part of government agencies that simulation and modeling are becoming sufficiently reliable that they can begin to replace physical testing. Several programs in the Department of Defense involve the development and implementation of

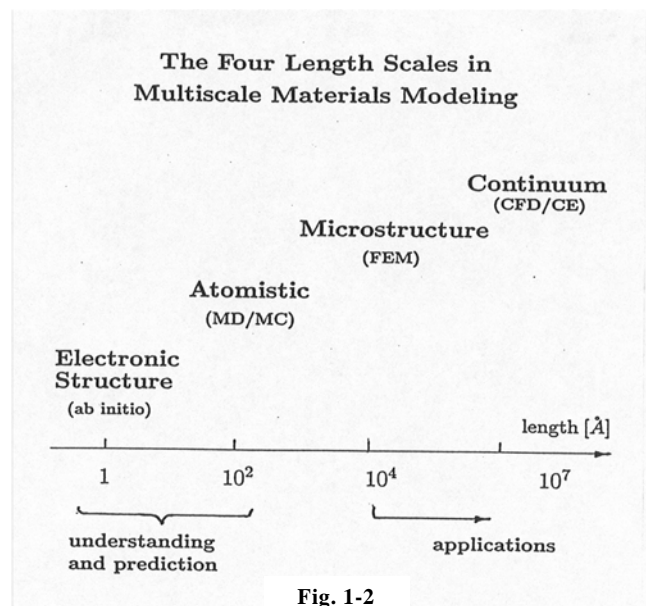
high performance computing as a means of achieving mission objectives with greater efficiency and at lower cost (sometimes personnel safety is also an issue). Examples of this trend are the High Performance Computing Modernization Program [5] and the Accelerated Strategic Computing Initiative which is closely coupled to the Science-Based Stockpile Stewardship, itself a national program of unprecedented scope and commitment [6].

As the capabilities of materials modeling expand in both breadth and depth, molecular engineering of materials becomes more of a reality. This is the long-held dream of every materials scientist and engineer where new materials can be created with such benefits as enhanced performance, extended service life, and acceptable environmental impact, not to mention cost reduction. Although computer-aided materials design is still lagging behind computer-aided molecular (drug) design, impressive progress is being made, especially in the area of functional materials for microelectronics, optical and magnetic applications [7]. In contrast, for structural materials the complexities of mechanical, thermal, chemical (alloying, corrosion, etc.) phenomena continue to pose formidable challenges to reliable and predictive modeling. As a result, it is becoming recognized that the most promising approach to the understanding and control of these phenomena is to effectively combine several modeling techniques, each one being suited for a particular length and time scale. This concept is now known as multiscale materials modeling.

Length/Time Scales in Materials Modeling

In many fields of scientific inquiry, it is commonly recognized that a single physical phenomenon can be examined at several levels or length (time) scales. For example, the complicated motion of a ocean wave as it washes onto a beach can be observed by watching a movie, or it can be visualized in terms of the individual movements of the water molecules which make up the wave. Depending on the scale of interest, the relevant dynamics requires quite different ways of analysis - in this case, continuum fluid dynamics to describe waves breaking on a beach and discrete-particle molecular dynamics to describe the atomic motions of the molecules.

For many materials problems one can identify four distinct length scales where different aspects of a physical phenomenon can be analyzed. As shown in the figure below these



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 can deal with the individual electrons of an atom.

The appropriate method for modeling relevant processes is called density functional theory or first-principles (ab initio) calculation; being fully quantum mechanical, it is the most computationally demanding of all the techniques, and as a result it can be applied only to small simulation systems, no more than 300 atoms.

The next scale, spanning hundreds of angstroms, is called atomistic. Here discrete particle simulation techniques of molecular dynamics and Monte Carlo are well developed. Such methods require the specification of an interatomic potential function which are usually developed empirically by fitting a functional form with several parameters to experimental data. The usefulness of atomistic simulation is that one can now study a system of N atoms, where at present N can be as large as 10^7 . On the other hand, by ignoring the electrons atomistic simulations are not as reliable as ab initio calculations.

At the level above atomistic, the relevant length scale is a micron (10^4 angstrom). Here the simulation technique common in use is finite-element calculations. Because many useful properties of materials are governed by the microstructure, this is perhaps the most critical level for materials design. Notice, however, that the information required to carry out such calculations (for example, the stiffness matrix, or any material-specific physical parameters in the calculation) has to be provided either from experiment, if available, or from studies at the atomistic or ab initio level. To a large extent, the same can be said for the continuum level, namely, the parameters needed to perform the calculations have to be supplied externally.

We now see why the different techniques of simulation need to be linked. For practical design calculations, either continuum or finite-element methods are most appropriate. Since they require parameter or property specifications which cannot be generated within these methods, and nor can they provide the atomic-level insights which are essential for design, atomistic and ab initio methods are needed. It is only when the different methods are effectively integrated that one can expect materials modeling to give fundamental insight as well as reliable predictions on the appropriate length scale. Once this is achieved, then materials modeling can claim to be a valuable complement to experiment and theory.

In as much as the advantages of linking simulation and modeling techniques across different length scales are readily apparent, the actual implementation is highly nontrivial. It is fair to say that no single research group has successfully demonstrated such a capability. At a recent workshop where this issue was raised and discussed, the conclusion was that one should focus on specific problems and work on a case by case basis in order to gain some much-needed experience [8]. Given that this is a recognized

critical issue facing the materials modeling community, one can expect significant progress will be achieved in the near future.

The field of computational materials modeling is continuing to expand rapidly and attracting participants from all the related fields of computational physics, chemistry, mechanics, and materials science (and even computational biology). As the community becomes every larger so is the literature. A Handbook of Materials Modeling will be published in the summer of 2005 [9]. This largish work, a collection of some 150 articles and 40 perspectives, provides a current view of an exciting field still in its infancy.

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