Lec 2 (2/8/02) **Survey of Simulation Techniques**

The Multiscale Materials Modeling Concept

During the past fifteen or so years, materials research has gained increasingly wide-spread recognition in the scientific community for its relevance to technological innovation and competitiveness. The advent of another powerful driver - high performance computing - has given rise, essentially in parallel, to intense interest in the computational approach to advanced materials research. The term *multiscale materials modeling* (MMM) has now taken on the meaning of theory and simulation of materials properties and behavior across length and time scales from the atomistic to the macroscopic. Although sometimes the importance of experiments is not explicitly acknowledged, it is nevertheless understood, at least by the more informed practitioners of materials simulation that selected experimental information will be indispensable to successful modeling, for providing appropriate database to determine the theoretical parameters and for validating the critical model assumptions.

The relevance of multiscale modeling is fundamentally predicated on the belief that such analysis and prediction will bring about better understanding and control of materials microstructures, which in turn are essential in the application areas of processing, performance evaluation, and ultimately the design of new materials. Because physics, chemistry, and various fields of engineering are all disciplines important to materials modeling, this emerging field has broad appeal to students with a diverse range of backgrounds. For basically the same reason, there is considerable impetus for different groups of research investigators at universities and research labs to team up to tackle grand-challenge type problems that lie beyond the expertise and capabilities of any single group.

As materials research expands 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. Even though computer-aided materials design has yet to achieve the success of computer-aided molecular (drug) design, there is impressive progress being made, especially in the area of functional materials for microelectronics, optical and magnetic applications. 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 blieved that the most promising approach to understanding and control of these phenomena is to effectively combine several simulation techniques, each one being suited for a particular length and time scale.

One can think of MMM as an open environment in which materials phenomena are described over a continuous distribution of length and time scales. The spirit of MMM is outward looking, intuitively logical, and flexible that it invites the investigtor to come up with his own interpretation. Yet despite the different ways of saying what is MMM, no general concensus on how to define the underlying concept has been established. Much like a good painting, it can have different meanings for different people, and in this way it maintains a certain freshness and contemporary appeal.

Simulation Techniques in Multiscale Materials Modeling

Returning to Fig. 1-1, shown at the last lecture, one sees that in materials processing the length scales span the range from 1 angstrom to about 1 m. The 10 decades go from nanotechnologies at the short end to system components and structures we normally associate with the macroscopic world. The order in which the topics themselves are arranged is interesting in that it begins with atomistic modeling which is one of the 4 characteristic length scales in MMM (see below) but not the smallest length scale. Several entries in this listing could be relevant to what we will be discussing later in the term, such as molecular dynamics/diffusion, phase equilibria/transformation, elasticity-plasticity, thermodynamics, thermomechanics, and deformation processing. Just these alone already give one the impression that materials processing involves a very wide range of physical phenomena, and this is only a partial list. We can regard this viewgraph as a reminder of the vastness of the material modeling landscape and the need to have a sense of direction in one's own research.

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 seeing it in real life, or it can be visualized (in our minds eye) 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.

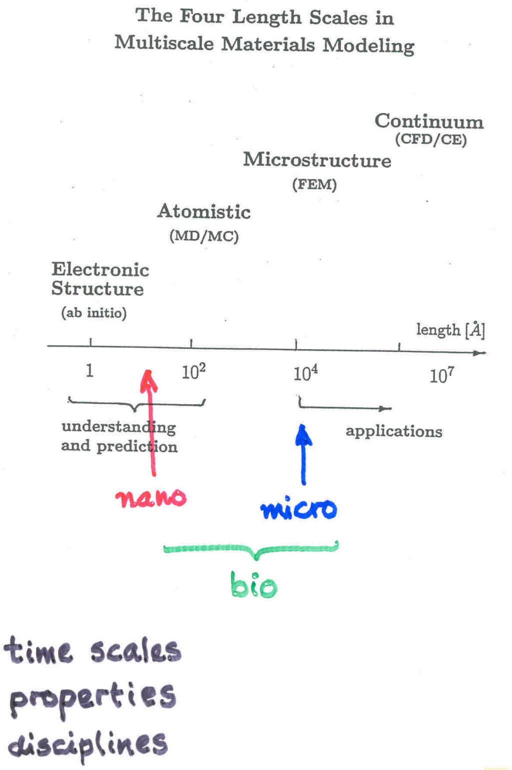


Fig. 2-1

For many materials problems one can identify four distinct length scales where different aspects of a physical phenomenon can be analyzed. As shown in Fig. 2-1 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, the current limit being about 300-400 atoms. The system being modeled at the electronic structure level is therefore a collection of atoms in the form of nuclei (or ions) and electrons, see Fig. 2-2.

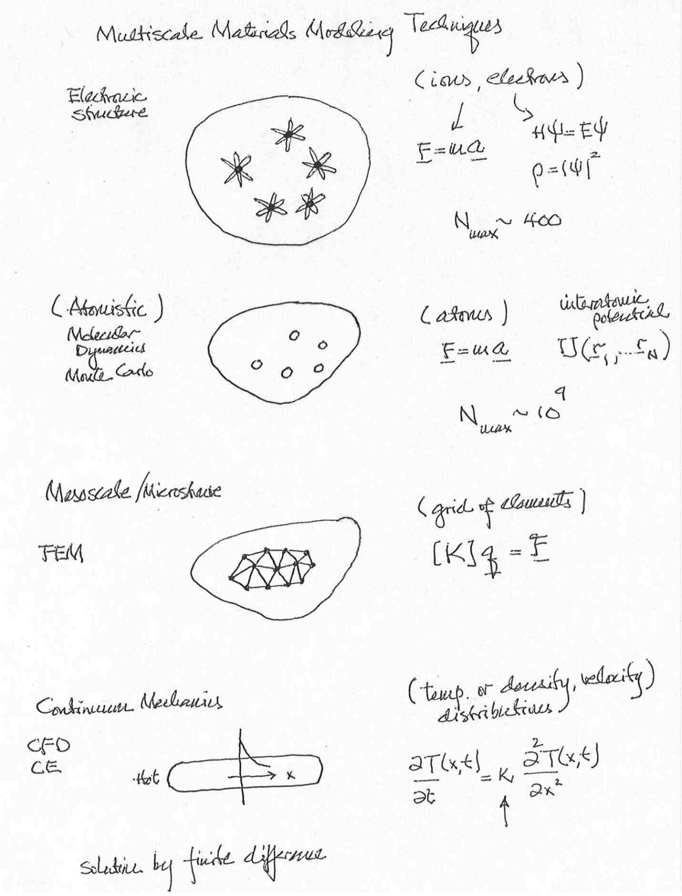


Fig. 2-2

Sometimes the electrons are further separated into core and valence electrons. The ions are described classically using Newton's equations of motion, $\underline{F} = m\underline{a}$, while the electrons are governed by the Schroedinger equation, $Hy = Ey$. The computationally intensive part of the calculation lies in the solving the Schroedinger equation. Once the wave function y is determined, we then know the electron charge distribution in the system, $r = |y|^2$, which tells us about the bonding between atoms, a very fundamental and useful piece of information.

The next scale in Fig. 2-1, spanning hundreds of angstroms, is called atomistic. Here the system is represented a collection of atoms. The appropriate simulation techniques are called molecular dynamics (MD) and Monte Carlo (MC); they are quite well developed and will be discussed in detail in Weeks 3 and 4 respectively. Such methods require the knowledge of an interatomic potential function $U(\underline{r}_1, \ldots, \underline{r}_N)$ (recall Lec 1) which are often obtained empirically by fitting a functional form with several parameters to experimental data. By not treating the electrons explicitly, atomistic simulation is computationally much simpler than electronic structure calculations, which means that one can treat a much larger number of particles, the limit being about 10^9 at the present time. The equations to be solved in the case of molecular dynamics is again Newton's equation of motion, while in the case of Monte Carlo one does not solve any equations of motion but instead sample a certain distribution of positions. With either simulation the essential input is the same, the potential function U. The goodness of a simulation therefore depends on how accurately do we know U for the material of interest. Because the electronic structure effects are ignored, atomistic simulations are not as reliable as ab initio calculations. This is especially true in situations where chemical bonds are broken as in fracture or rearranged as in chemical reactions. On the other hand, one has the advantage of being able to simulate much larger systems over much longer times. This in turn means one can study more physical properties and behavior of the material.

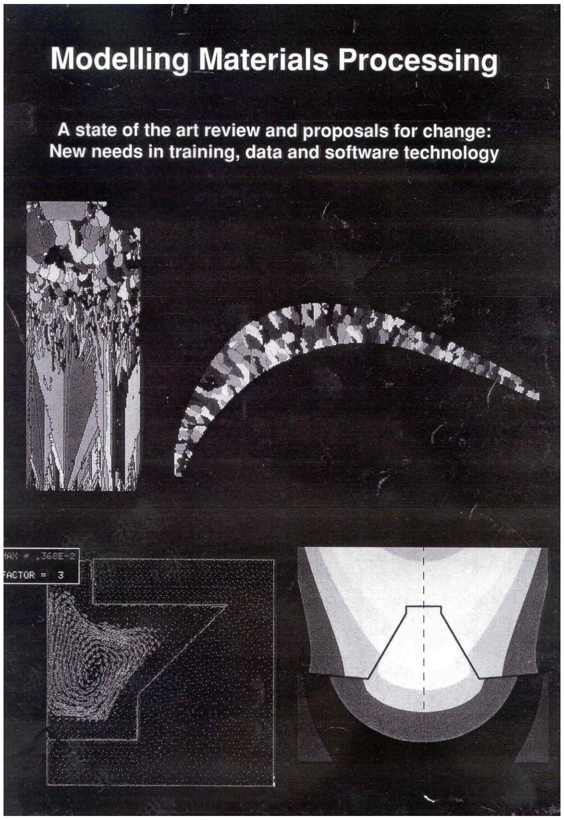
The length scale above atomistic is sometimes called the mesoscale, the characteristic length being a micron (10^4 angstrom). Here the simulation technique commonly in use is the finite-element method (FEM), where the system is represented by a grid of elements, triangles in 2 dimensions, cubes or tetrahedra in 3 dimensions, for example. The equations to be solved describe force balance on each element, the output being the nodal displacements of the specified grid. Typically, the grid is chosen to be fine enough to represent idealized microstructural features of micron size, which makes this method well suited for the simulation of materials microstructure in many applications. Notice, however, for FEM calculation one needs to specify the force acting on an element due to its neighbor, and this kind of mterials property has to be provided either from experiment, if available, or from studies at the atomistic or ab initio level.

Beyond the mesoscale one has the macroscale where the material is represented as a continuum described by distributions which vary rather smoothly on the scale of mm and larger. As an example we can imagine the temperature distribution in a rod that is heated at one end. The equation describing this system is the time-dependent heat conduction equation (Fig. 2-2), with k denoting the thermal conductivity of the material. Like the FEM simulation, the materials properties needed for simulation at the continuum level have to be supplied externally. In this case the conductivity is a quantity that one measure experimentally, or calculate by means of atomistic simulation.

We can see why it is important to couple the different length scales. For practical design calculations, either continuum or finite-element methods are the most useful. However, these methods require parameter or property specifications that cannot be generated internally, nor can they provide the electronic structure or atomic-level understanding of mechanisms that are essential for prediction and design. It is only when the different methods are effectively integrated that one can expect materials modeling to give fundamental insight, or reliable predictions on the appropriate length scale. Once this is achieved, then materials modeling can justifiably claim to be a valuable complement to experiment and theory.

In Fig. 2-1 we also indicate the regions where nanoscience and technology would operate, in contrast what is previously the microscale. With regard to biological science at the cellular levl, the range spans from the nanoscale up to tens or even hundreds of microns. The presnet length scale classification has counterparts in time scales. Moreover, one can discuss various physical properties that manifest on the different length-time scales, and finally one can even roughly associate different disciplines with each level of scales. For example, electronic structure would be the domain of quantum chemistry and condensed matter physics, atomistic and microstructural levels would be materials science and engineering, and continuum level would be the domain of engineering.

In as much as the advantages of linking simulation and modeling techniques across different length scales are quite apparent, actual implementation of coupling the different levels of description is highly nontrivial. It is fair to say that no single research group thus far has fully succeeded in demonstrating such a capability, so there are still many opportunities for original research. To emphasize this point we return to Fig. 1-3 which describes a research program currently on-going at the Lawrence Livermore National Laboratory with the goal of understanding dislocation dynamics for applications in high strain-rate deformation. The idea is to take a bottoms-up approach of linking atomistic simulation of dislocation interactions and mobility with mesoscale simulation of single crystal and polycrystal plastic deformation to arrive at appropriate constitutive relations which then may be incorporated into design codes at the continuum level. This is presently one of the most comprehensive efforts to solve a critical materials problems. Its success will go a long way in demonstrating the unique power of the MMM approach to materals research.



Modelling Materials Processing

A state of the art review and proposals for change:
New needs in training, data and software technology

Fig. 2-3

Fig. 2-3 shows several examples of FEM simulations in materials processing. One sees (counter clockwise) the grain microstructure in a turbine blade and a block undergoing directional solidification, the flow pattern or velocity plot in a casting where solid and melt zones begin to separate, and the thermal profile or temperature zones in a directionally chilled continuous casting. The results demonstrate the usefulness of modeling microstructure in materials technology.

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Fig. 2-4

Fig. 2-4 is a cover of a journal devoted to computer-aided materials design, showing a composite of simulation results at different length scales. Starting at the bottom one has the charge distributions in crystalline silicon given by electronic-structure method of density functional theory. As we have mentioned, such information cannot be obtained by any of the other methods in Fig. 2-1. Going up on the left side, one has a molecular dynamics simulation of a crack tip in a two-dimensional crystal under uniaxial tension. The crack (dark region), while moving upward, has started to branch out to take on a jagged appearance which is also seen in laboratory measurement. In Fig. 2-5 we see the same simulation in greater details, the individual atoms in the simulation are now visible. The sequence of six snapshots begins on the left from the top down. The two colors denote the two opposing directions of strain. The fact that the strain directions start to mix as the simulation proceeds means that the state of strain is no longer simple once the crack moves further into the crystal. This simulation involves about 30 million atoms, quite large by present standards. If one were to show all the particles in some kind of color

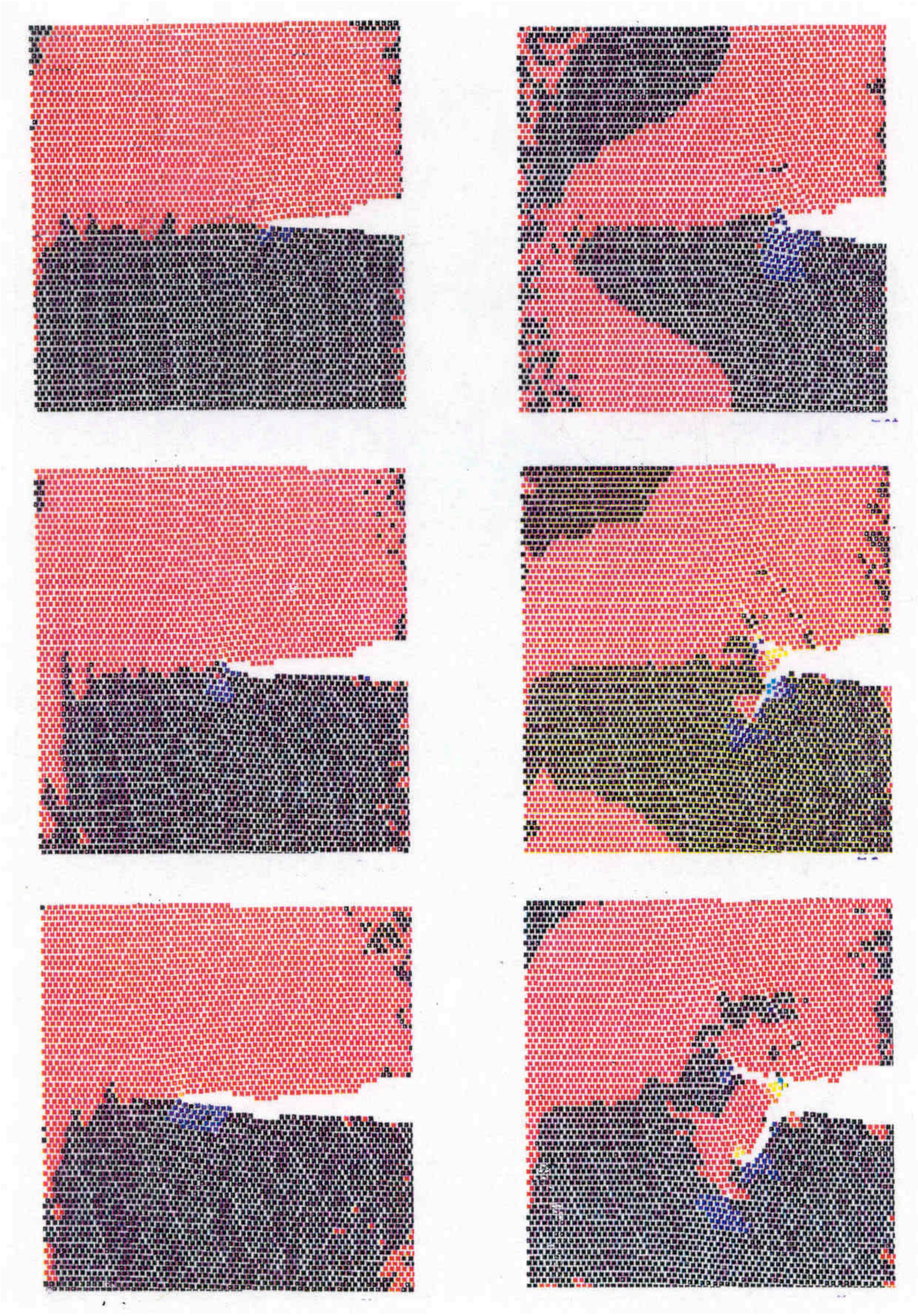

Fig. 2-5

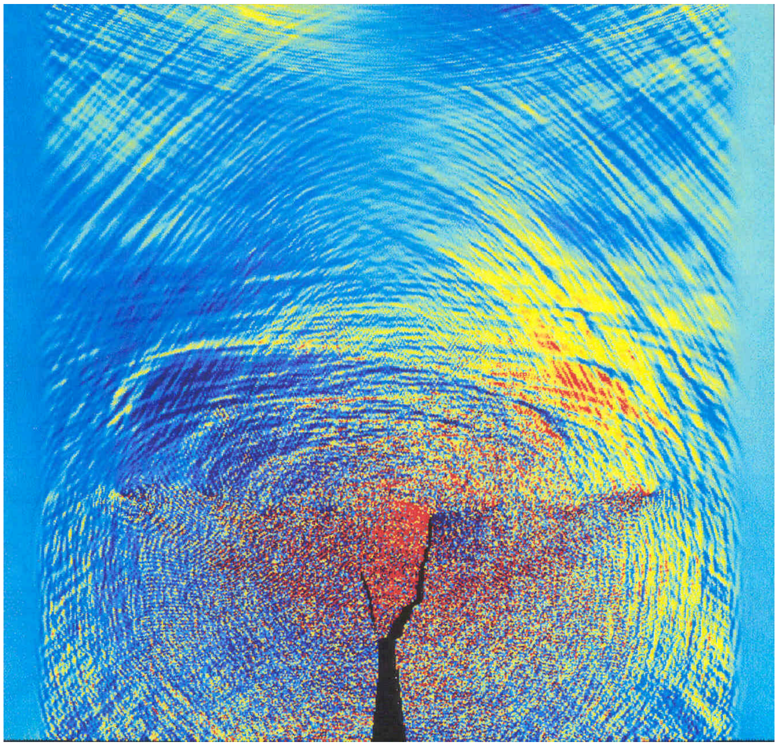

Fig. 2-6

coding scheme, as in Fig. 2-6, one would lose the discreteness of the simulation and the system starts to look like a continuum, including the stress waves that are reflected from the fixed borders of the simulation cell (reminiscent of ripples on the surface of a lake). This is an illustration of how one level of simulation can merge into the next level. The impression we would like to leave here is that atomistic simulation can reveal very local details of how the material is tearing apart, a level of microscopic information that experiments at present cannot provide. The challenge is to understand this kind of complexity and use the knowledge to design materials that would be more resistant to failure.