

## Lec 1 (2/6/02) Overview of Modeling Concepts

We begin by considering several simple questions.

### 1. Why Modeling and Simulation ?

This is a fundamental and quantitative way to understand complex systems/phenomena which is complementary to the traditional approaches of theory and experiment. Modeling and Simulation (Mod/Sim) are concerned with powerful methods of analysis designed to exploit high performance computing. This approach is becoming increasingly widespread in basic research and advanced technological applications, cross cutting the fields of physics, chemistry, mechanics, engineering, and biology.

### 2. Why teach Mod/Sim at the UG level ?

Mod/Sim studies are mostly being carried out at the graduate and postgraduate levels. But there is no reason why the undergraduates cannot participate in a meaningful way and benefit from the physical insights and technical know-how that it can provide. We believe that engaging the undergrads broadly across the Institute through a team of multidisciplinary faculty, as instructors and mentors, can succeed at MIT, providing the students with a broader academic exposure than what they would normally encounter within their own departments.

### 3. What are the goals of Mod/Sim ?

The students should gain a significant appreciation of the broad use of modeling in several fields of science and engineering, acquire hands-on experience with simulation, ranging from basic use of computers to advanced techniques, and develop communication skills by working with practicing professionals. Additional benefits could come from further interactions with the faculty afterwards, such as mentoring, UROPs, thesis supervision, etc.

### Why Modeling and Simulation ?

*Fundamental and quantitative way to understand and analyze complex systems and phenomena*

*Complement to Theory and Experiment, and often Integrate them*

*Becoming widespread in:  
Computational physics, chemistry, mechanics, materials, ..., biology*

## Why teach Mod/Sim at UG level ?

*Undergrads can be junior partners in what is going on at the grad and postgrad levels.*

*Broad exposure to new ways to learn:*

*Applied Math  
Thermodynamics  
Statistical Mechanics  
Quantum Mechanics  
Solid and Fluid Mechanics  
Materials Science*

*Interact with a team of Instructors and Mentors across the Institute*

## What are the goals of Mod/Sim ?

*Appreciation of broad use of modeling*

*Hands-on experience with simulation techniques*

*Develop communication skills working with practicing professionals*

**Subject is taught in two parts  
(see Lecture Schedule)**

4. Subject is taught in two parts (see **Lecture Schedule**)

Part One: simulation methods lectures, HW

Part Two: term project, applications lectures/demos, presentation

In both parts students have an opportunity to learn concepts in thermodynamics, statistical mechanics, quantum mechanics, solid and fluid mechanics, materials science, condensed matter physics, chemical physics, etc. through a modeling and simulation applications context.

In this, our first meeting, we will discuss briefly what we mean by modeling and give several examples.

Model ∪ a **simplified** description of an actual system, useful for studying the system behavior. Models are used in every branch of science; they are tools for dealing with

complex systems and the interactions of their constituent parts. Scientists and engineers have long used models to better understand the systems they are studying, for analysis and quantification, performance prediction and design.

**Types of models** -- a physical system can be described at different levels:

- (a) a collection of nuclei and electrons (**electronic-structure** level)
- (b) a collection of atoms and molecules (**atomistic** or molecular)
- (c) a set of coupled structural elements (**finite-element**)
- (d) a medium described by fields and distributions (**continuum**)

In terms of details, (a) has the most details (note we are not considering the protons and neutrons that make up a nucleus, that would take us into the domain of nuclear physics). At each level one can construct a model that can be used to analyze the system properties and behavior.

**When is a model useful?** When a complex system can be simplified (reduced) to a tractable level that makes clear the essential structure of system and how the internal constituents interact with each other.

**Key to a good model** lies in what and how simplification is introduced; it is very important to understand what aspects of the system the model is intended to describe, and what are the model's limitations as a result of the simplification.

Suppose we are interested studying a Cu crystal at the atomistic level. This means our model is a collection of  $N$  Cu atoms which interact with each other through a potential energy  $U(r_1, r_2, \dots, r_N)$ , where  $r_1, r_2, \dots, r_N$  denote the positions of atoms 1, 2, ...,  $N$  respectively. At this level  $U$  is a given function. Knowing  $U$  and the system structure we can use the model to calculate the various properties of Cu crystal. How? The process that allows us to do this is **simulation**.

We continue our introductory discussion by showing a few brief examples of materials problems that can be addressed by modeling and simulation. Fig. 1-1 shows a list of topics compiled by the Materials Processing Center at MIT, an organization linking the research activities at the Institute with industrial companies with an interest in materials technology. This list shows the variety of problems that involve one form of modeling research or another in producing materials all kinds of technologies. Notice that atomistic modeling is at the top of the list - this is a technique we will come back to discuss in some detail. While Fig. 1-1 may be impressive in its technological variety, it may be easier to see what is materials modeling by thinking about only one kind of materials property such as the strength of material.

Fig. 1-2 shows 3 high-speed photographs of a shape charge where a metal is pushed through an orifice by an explosive, the molten metal then expands as in a plume once it clears the orifice in about 12 microseconds. This process is of interest to the scientists at the Lawrence Livermore National Laboratory in connection with its program on (nuclear) stockpile stewardship. This is work for the Department of Energy to ensure the safety and reliability of our existing nuclear weapons stockpile. What this figure

conveys is that a fundamental process of metal being deformed at very high pressure and strain rate actually has important practical applications, in this case a matter of national security and defense. The relevance of the shape charge to modeling of strength of materials is indicated in Fig. 1-3, showing a sequence of models which takes the basic understanding gained from modeling the behavior of dislocations (a line defect in crystals) at the atomistic scale through first the behavior of a single crystal under stress (on the micron scale, then the behavior of a polycrystal, a collection of single crystals (on the mm scale), and finally to the actual shape charge specimen. This is an example of multiscale modeling about which we will say more in the next lecture.

Fig. 1-3 shows another aspect of the strength of materials problem, that of stress-strain behavior of a Cu crystal. The plot shows the variation of stress with strain; this kind of information is very useful in analyzing the strength and deformation of a material. If one wants to understand the various features of plastic deformation, starting a strain of 0.01 (stage I) and extending to larger strains, then one has to consider how the underlying defects, particularly dislocations, are behaving. This is a current challenge to the research community. On the right of Fig. 1-3 two TEM pictures show the patterns of dislocation structures. It is not yet possible to explain these features fully from basic theory or simulation.

We conclude this short discussion with Fig. 1-4 showing how one can study a small crack, with dimension of a few nanometers, using a combination of three models, TB refers to a quantum mechanical calculation which is very computationally intensive and is therefore applied only at the most critical region (the crack tip), MD refers to atomistic calculation which is applied to the region surrounding the crack tip, and finally FE (FEM in the next lecture) is applied sufficiently far from the crack where the material is not subjected to any stress concentration and therefore can be treated more approximately.

Remainder of class discussion is a short talk by Professor Gerd Ceder on his current research on modeling materials for batteries using first-principles (quantum mechanical) calculations.

Fig. 1-1 MPC Modeling List

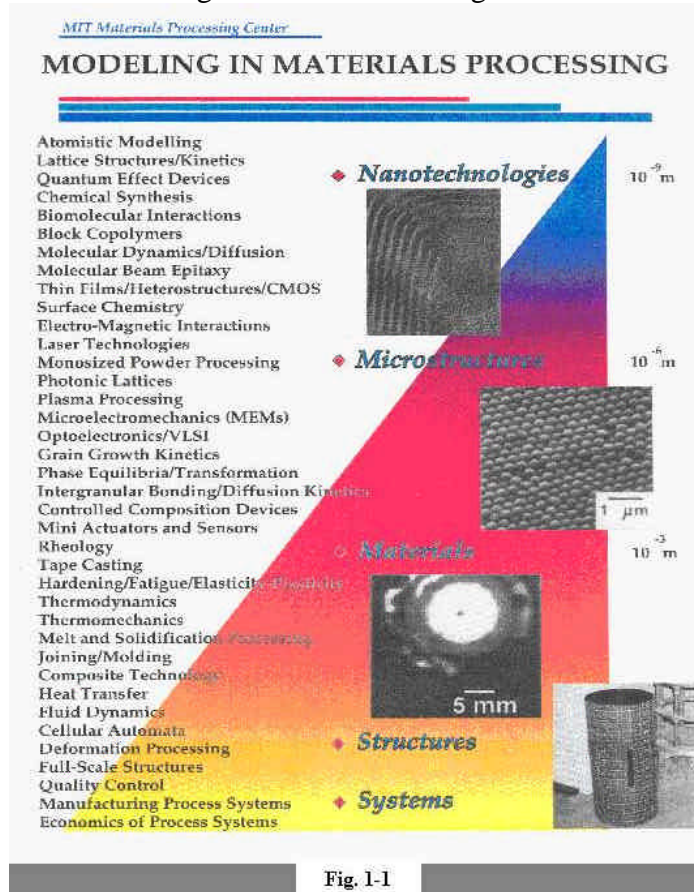


Fig. 1-1

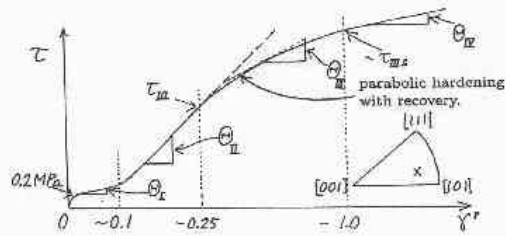
Fig. 1-2 Shape Charge (LLNL)

**Understanding high deformation rates in metals is essential**

**To predict these integrated and complex phenomena, we must understand the underlying microscopic physical processes; i.e., dislocation dynamics**

Fig. 1-3 Stress-Strain Curve (Cu)

TENSILE STRESS/STRAIN CURVES OF COPPER  
AT ROOM TEMPERATURE  
(Seeger, 1957)



Underlying Microstructures?

Dislocations:

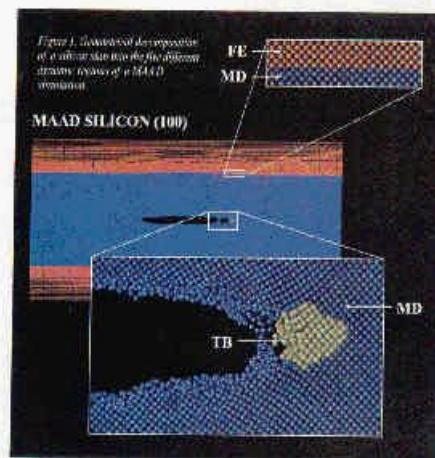
density, mobility, patterning

atomic-level processes

governing dislocation microstructures?

Fig. 1-5

Fig. 1-4 Crack Simulation Multiscale



### Spanning the Length Scales in Dynamic Simulation

Farid E. Abraham,  
Jeremy Q. Broughton,  
Noam Bernstein, and  
Efthimos Kaxiras

*A computational approach to the simulation of crack propagation in silicon seamlessly unites quantum, atomistic, and continuum descriptions of matter*