Computational Materials Science:
A Scientific Revolution about to Materialize

White Paper

Materials Component

Strategic Simulation Initiative

March 5, 1999

Available at: http://cmpweb109.ameslab.gov/cmp/ccms/executive.html

I. Executive Summary

Preamble: From the Bronze Age to the silicon-driven Information Age, civilization has defined itself–and advanced itself–by mastering new materials. Advances in materials drive economic, social, and scientific progress and profoundly shape our everyday lives. Today, thanks to increasingly powerful computers, the materials science community finds itself on the verge of another revolution. In this new era, extensive computational modeling will complement and sometimes even replace traditional methods of trial-and-error experimentation. With simulation, scientists will guide advanced materials development and will comprehend how materials form, how they react under changing conditions, and how they can be optimized for better performance.

Overview: The terascale power envisioned for SSI represents an unprecedented opportunity to greatly increase the rate of discovery, reduce the time for development, and optimize processing routes to strategic materials vital for society and essential to DOE missions. This report addresses the importance of materials, the scientific challenges posed by materials research, the readiness of the community to use terascale computers to meet these challenges, and the opportunities to build collaborative efforts across disciplines. We offer a number of representative examples to give a flavor of both the excitement in the field and the promise that terascale computing affords. The examples provide nine different one-page color highlights, representing a cross section of computational materials science, each poised to exploit terascale computing. **READ THE EXAMPLES** to visualize what is ready now and what the future promises.

Societal Benefit: Materials underpin major industries, steer global markets, and are critical to national and economic security. Enhanced material performance and low-cost materials processing are essential to the DOE's mission for increased efficiency in energy production and consumption and for the successful deployment of environmentally benign products. Numerous federal studies highlight the widespread economic and strategic importance of materials, leading to support for basic materials research that complements focused industrial R&D.

Science: Scientists have a handle on the smallest length scale (relevant to materials), which cannot be seen with a microscope, and the largest length scale, which can be seen with the naked eye. In between is an intermediate length scale where there are particularly exciting new frontiers. The primary scientific challenge is to uncover the elusive connections in the hierarchy of time and length scales and to unravel the complexity of interactions that govern the properties and performance of materials. Terascale modeling and simulation makes this challenge achievable.

Readiness: In materials science, simulation has become as essential as experiment and theory. The 1998 Nobel Prize awarded to Prof. W. Kohn for the development of density functional theory is just one indication of the success and promise in this rapidly advancing field. Many of the tools to attack the scientific challenges are “terascale ready.” The newly created BES Center for Computational Materials Science establishes an infrastructure for bringing multidisciplinary teams together and will ensure that the community promptly assimilates new tools and new ideas.

Crosscutting Opportunities: The generic nature of the complexity of phenomena that exist over a large range of length and time scales, which are dynamic and which are not scale invariant, is a common theme throughout SSI. Specific synergies exist between the materials initiative and combustion, earth, life, and chemical sciences as well as fusion energy and ASCI materials programs. The needed advances in applied mathematics, computer science, and infrastructure are of a nature that would be broadly applicable in other disciplines.

II. Importance of Materials for Society and for the DOE Mission

Materials are so ubiquitous in our lives that we often overlook the revolutionary impact they have in shaping modern society. Materials not only directly touch us, but advanced materials play a crucial, enabling role underlying virtually all technologies. One need only consider the hallmark of the information age, the computer. Computational power has been compounding at an exponential rate for nearly 40 years, an achievement made possible by advances in silicon processing and fabrication at ever smaller length scales. Breakthroughs in control and fabrication of magnetic media have driven disk capacity to likewise grow exponentially. Innovation in materials can mean the discovery of a completely new material or, more commonly, the modification or replacement of a material to increase functionality or to reduce cost. Such innovations largely determine the pace of technological advance in many industries, which in turn greatly influences productivity, capital formation, the demand for labor, and the overall rate of economic development. Our standard of living today has been largely determined by past discoveries of "new" materials, and our future prosperity in large part will depend on the fruits of contemporary research into even newer materials and innovative processing routes.

Whereas the computer is possibly the most visible example of a high tech product that depends critically upon advanced materials, there are many other similar examples that also profoundly affect our lives. Within the areas of concern to the Department of Energy, consider energy efficiency in the aerospace and automotive industries. New lightweight alloys, polymers, and composites have substantially reduced weight while maintaining or even enhancing the durability and crashworthiness of vehicles. For a supersonic aircraft, lightweight alloys must be able to tolerate extremely high temperatures while retaining their superior strength. In the automotive industry, a 10 percent weight reduction results in a 5 percent increase in fuel economy and a corresponding decrease in CO_2 emissions. In fact, energy efficiency is paramount in the burning of all fossil fuels, which account for 80 percent of the electricity generated in the United States. Finding new cost effective ceramics that would allow the operating temperature of power plants to increase by just 100 degrees Celsius would raise their efficiency by two percent and reduce the amount of CO_2 emitted by 10 million metric tons. A few other materials contributing to higher efficiency and better performance include modern magnets, solar cells, and ionic conductors for batteries. Is there a common theme for many of these modern materials?

The four volume (~3000 page) *Encyclopedia of Advanced Materials* defines advanced materials as

> "those where first consideration is given to the systematic synthesis and control of the structure of the material in order to provide a precisely tailored set of properties for demanding applications."

This is a revealing characterization. No longer is mankind just using materials that come unchanged from nature (e.g., wood) or produced by elementary processing, such as heating (historically, ceramics and simple metals). Instead, materials scientists and engineers are now able, in the synthesis and processing of materials, to control material structure at the molecular, nano, meso, and macro scales. It is quite amazing that in the last decade biological materials and particularly genetically engineered materials are starting to fall within this definition of "advanced materials." Most of the Department of Energy's materials' basic research portfolio is devoted to discovering ways to control and characterize materials structure at all length scales, but particularly at the smallest dimensions, which determine fundamental bulk materials properties. For this purpose,

there are extraordinary new instruments and major new national facilities that are accelerating the development of increasingly advanced materials. The investments in large experimental facilities like the Advanced Photon Source, the Advanced Light Source, and the Spallation Neutron Source are spurring new techniques for probing materials on small length scales. These techniques can probe the precise length scale at which structural features, grains or microcrystallites, act to influence phenomena such as dislocation movement or the pinning of magnetic domains. These features and phenomena have a direct affect on a material's ductility and fracture strength or on the quality of permanent magnetic performance. An obstacle and opportunity arising from the large facilities and their modern instrumentation is the sheer volume of data produced and the nature of the data dealing with highly complex structures and phenomena. The problems associated with data volume, reduction, and visualization are issues being addressed with the help of experts in computer science. However, the difficulty of coping with the increased complexity of the phenomena under investigation is more basic and requires a marshaling of theoretical support. With the computational resources envisioned for SSI, the needed response will be forthcoming, including but not limited to synergistic partnerships with experimental colleagues for verification of advanced computational simulations, modeling, and predictions.

III. Opportunities for Computational Materials Science

The advent of quantum mechanics (less than 75 years ago) opened the door to understanding the fundamental interactions of the atomic constituents of matter and in turn to use that knowledge to design and control materials properties and processing. In practice, however, the solution of the quantum mechanical equations is intractable, except in relatively simple cases. Therefore, the control of materials structures at various length scales has necessarily progressed by intuition and by trial and error in the laboratory. This time-honored approach is not about to be replaced, but in many laboratories it is being supplemented if not supplanted by computer aided research and development. Today pharmaceutical companies routinely seek insight and guidance in the "design" of new drugs using computer simulations of molecular interactions. Similarly at the macroscopic scale, companies like Boeing and Ford use supercomputers to model airflow and other characteristics of design features before they actually build models for testing in wind tunnels or crashing into walls. It is many times cheaper to design on the computer.

The thousand-fold increase in computational power, resulting from new machines with massively parallel architecture, promises to change dramatically the use of simulation in aiding materials research. There are several reasons this will be revolutionary and not just evolutionary. Computing power is about to reach the level at which we can finally solve the quantum mechanical equations for large enough systems to be able to elucidate complex atomistic interactions occurring over length scales involving thousands of atoms. Scientists can envision a path that allows accurate simulations starting at this atomistic scale and proceeding to an intermediate length scale where many of the bulk materials properties, such as strength, are determined. Results from simulations at the intermediate length scale will naturally feed into continuum models to simulate the macroscopic engineering designs. The idea of accurate simulation capabilities at each of the length scales together with the possibility of overlapping the length scales is empowering. Young scientists will be trained to think and work from atoms to the bulk, and the divisions between disciplines (first principles theory to mechanical engineering) will start to dissolve. For this revolution to materialize, we must consolidate the progress made at various length scales and we must accelerate the development of the underlying science for bridging the scales.

IV. Science:

A primary goal of a materials simulation initiative would be to develop a capability to reliably predict the properties of real materials. To achieve this far-reaching goal one must be able to realistically simulate physical phenomena over a vast range of time and length scales. For example, there is currently incomplete understanding of how the underlying structure, defects, or individual grains determine the mechanical or magnetic properties of real materials. Likewise, there is incomplete understanding of how the chemical composition and thermal history or other processing history determines the structure of the grains themselves. Today's mathematical models to describe materials physics (beyond the scale of electrons and atoms) are generally empirically based with phenomenological parameters. One important challenge is to determine those parameters entirely from first principles calculations. However, a much greater challenge is the simulation of essential properties that depend critically upon phenomena or processes at very different length and time scales. Table 1 shows a classification of characteristic ranges of time and length appropriate to materials. It is necessary to uncover the elusive connections in this hierarchy of quantum/molecular, atomistic/nano, mesoscopic, and macroscopic scales and to unravel the complexity of the interactions that govern the properties and performance of materials. Terascale modeling and simulation makes this challenge achievable.

Table 1. Classification of characteristic length and time scales appropriate to materials modeling.

Scale	Quantum/ Molecular	Atomistic/ Nano	Mesoscopic	Macroscopic
LENGTH (meters)	$10^{-11} – 10^{-8}$	$10^{-9} – 10^{-6}$	$10^{-6} – 10^{-3}$	$> 10^{-3}$
TIME (seconds)	$10^{-16} – 10^{-12}$	$10^{-13} – 10^{-10}$	$10^{-10} – 10^{-6}$	$> 10^{-6}$

Scientific issues abound in the rigorous translation of the nature of physical phenomena that govern the processing and the structure of complex materials into mathematical models that are both solvable and able to describe or predict the observable materials properties. Viewed at the smallest scale, the simple building blocks of materials are electrons and nuclei, which obey the quantum mechanical Schrödinger (or Dirac) equation and interact via Coulomb forces. The mathematical complexity arises from the fermion nature of electrons and the very difficult problems of describing many interacting particles. In principle, one could calculate all the properties and structures of any material from these known physical laws. However, it is impossible to simulate directly the huge number ($\sim 10^{23}$) of electrons and nuclei with an objective of predicting macroscopic properties. Moreover, even if the computer were large enough, such an approach would be unlikely to provide much insight into the essential physics governing the fundamental properties and structural features of materials.

Despite the difficulties mentioned above, all is not lost. As is typically the case with large systems, after suitable averaging or aggregating, the forces among the aggregated pieces can be accurately described by a new model with "renormalized" interactions. We refer to this as "coarse graining," because it arises from appropriate averaging or aggregating over many degrees of freedom at a finer scale. Nonetheless, subsumed in this statement is a very difficult scientific challenge. There

are no general paradigms for achieving this "coarse graining." In general, the next level mathematical model is determined heuristically and independently from the finer grain models. Oftentimes these models capture enough of the essential physics that, despite the absence of rigorous bridges connecting them to the finer grain mathematical models, substantial progress can be made. However, this generally comes at the expense of extensive fitting, tedious and expensive compilations of databases, and limited ability to extrapolate to systems where measurements have not been made.

SSI offers the genuine opportunity to eliminate the empiricism by using computer simulation and modeling to facilitate the development of "coarse grained" mathematical models and parameters from ever finer grained but more firmly grounded models. Such a development would allow us to move beyond qualitative, phenomenological connections between the scales to the creation of unified multiscale simulation tools. Figure 1 shows a schematic of this "coarse-graining" concept as it applies to the mechanical properties of materials.

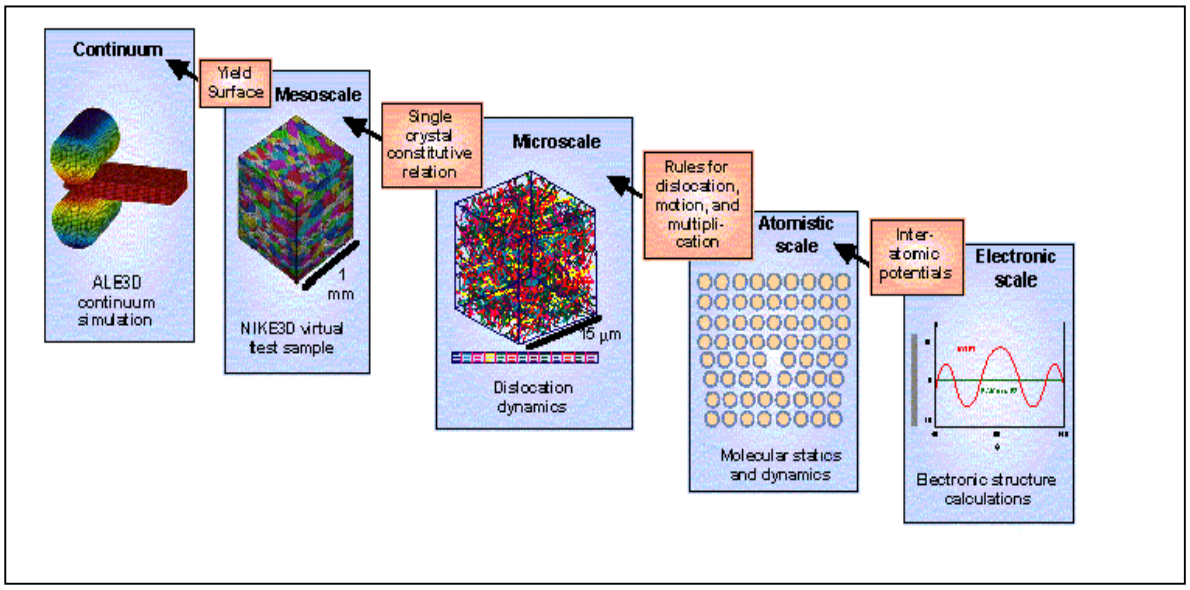


Figure. 1. A schematic of the multiscale challenge for mechanical properties of materials

The computational expense of a simulation will generally scale with the number of degrees of freedom, the complexity of the interactions between the effective degrees of freedom, and the number of simulation steps. Therefore, the simpler the mathematical model the more likely it will be feasible to translate it into efficient computational codes in order to extract useful information and the more likely it will provide new insights. This, of course, assumes that the model is neither too simple nor simply wrong. In the process of coarse graining, whether rigorously or heuristically, one moves up the length scales, so that one can simulate ever larger systems (while keeping the overall computational expense approximately constant) until one is simulating the macroscopic material.

The scientific challenges almost always involve determining mathematical models that have enough complexity to reliably capture the real physical processes, while not including excess complexity that precludes reaching a solution on the computer within a reasonable amount of time or

which obscures the dominant phenomena. Indeed, just a few short years ago, the mathematical models had to be so simplified for computational ease that their predictions often were no better than the intuition that went into constructing them. Terascale computing offers the opportunity to include the essential complexity.

Real materials have an abundance of "defects" including impurities and vacancies, dislocations (including misfit dislocations of interfaces) or other faults, grain boundaries, domain walls (in magnetic and ferroelectric materials), second phase precipitates, porosity, and so on. It is the structure of these defects, their interactions, and their thermodynamics that govern the macroscopic properties and performance of the real material. Some technologically relevant materials phenomena owe their unique desirable characteristics to the presence of natural or engineered defects (e.g., the pinning of superconducting vortices and magnetic domains, hardness, and strength). Other technologically relevant properties are limited in performance by the presence of the defects (corrosion resistance, some optoelectronics properties, fracture resistance). To complicate matters, it is often necessary to understand real materials response away from equilibrium, under conditions of high temperature, large strains, and time dependent external forces giving rise to irreversible processes (such as grain growth and recrystalization, stress development, plastic deformation, crack nucleation and growth).

Extended defects such as dislocations and grain boundaries most directly affect the mechanical properties of a material, including ductility and fracture resistance. Interactions of extended and point defects determine fundamental mechanisms of solid-solution hardening. The structure and thermodynamics of domain walls and their interactions with lattice defects are fundamental to determining the quality of permanent magnets. Some of the most fundamental issues concerning the interactions of defects remain unexplored even though qualitative descriptions of many of these interactions have been around for decades. The reason is that the defects are too "big" to belong to the microscale, where the mathematical models are fairly mature, yet too "small" to be modeled on the macroscale, where again the mathematical models are quite mature.

In general, simulation at the intermediate scale (the mesoscale) is limited by insufficient molecular scale understanding of the nature of inhomogeneities in the material, i.e., of the underlying interfacial processes and microscopic mechanisms that govern essential aspects that determine the evolution of the microstructure. Phenomenological theories are only applicable to highly simplified microstructural models, with essentially no information on a variety of crucial phenomena that can only be determined from realistic atomistic simulations. Terascale computing affords the opportunity to identify those critical processes and mechanisms with microscale simulations. The insights and parameters extractable from such simulations become the inputs for both the development and parameterization of mathematical models for mesoscale simulations. It is fair to say that there is substantially incomplete understanding of how the microstructure determines the properties and performance of real materials, but that terascale computing can provide the needed capability to start filling in the science gaps.

There are at least five different simulation modes that are prerequisites to building a capability for reliably and accurately predicting a wide range of materials phenomena and properties. The five modes are

- discovering new relations and paradigms for complex behavior,
- providing benchmarks to test the forms of the mathematical models,

- directly calculating parameter input for mathematical models,
- ultimately validating models by careful comparison with experiments, and
- predicting difficult to observe behavior of complex materials processes and phenomena.

A suitable term for, perhaps, the most far-reaching use for terascale computing is the *discovery* mode, a mode of uncovering new constructs for phenomena in materials that leads to the development of new mathematical models firmly grounded in known science. It has always taken a great deal of creativity and innovation to uncover the appropriate collective or aggregate degrees of freedom and the laws for effective interactions at the coarser level. Simulation can provide information that is difficult or even impossible to obtain by experiment and yields new insights for this creative endeavor. Simulations can serve as a powerful laboratory through which one makes discoveries until a fundamental understanding of elusive phenomena emerges.

A second role for simulations is to perform *benchmark* calculations that provide critical tests of the faithfulness of models. The physics of the aggregated modes and their interactions at a coarser scale must be compatible with simulations from theories and models at the finer scale. Ultimately models must be consistent with the shortest length and time scales, the realm of electrons and nuclei. At each scale, benchmarks using the most advanced computation possible are crucial for establishing the ultimate reliability of the multiscale simulations.

With the establishment of faithful models coupled with increasing computational power, the third role for simulation emerges. In the *calculation* mode simulations at a finer scale directly provide the needed input to models at a coarser scale. There are many already identified examples where such input is critical to the goal of predicting the properties of materials. For example, electronic structure calculations often determine the interatomic force field that is the input for large-scale molecular dynamics simulations involving many millions of atoms. In turn, these molecular dynamics calculations can provide information on defect structures and their interactions, which becomes the input for the next coarser level, involving simulations of grain boundary and dislocation dynamics. Another example comes from magnetism. At the finest scale, the fundamental quantities are magnetic moments, exchange interactions, anisotropy energies, etc. Such quantities, calculated near interfaces or defects, are necessary inputs for the coarser scale calculations that ultimately are capable of evaluating and predicting technologically relevant magnetic properties of materials, such as saturation magnetization, permeability, coercivity, and remanence.

The *validation* mode uses computation to simulate complex phenomena with such realism that comparison with controlled experiments can provide definitive validation of the underlying assumptions and algorithms. With new methods and computational power, one can iterate among laboratory and computer experiments (with exquisite and rapid control on the variables) and theoretical model development. This has the potential to revolutionize the way science proceeds by having computational science as a full partner to laboratory experimental science.

The fifth *predictive* mode is essentially the final goal. Once sufficiently validated, computer simulation can perform "virtual" experiments that would be either too time consuming or difficult to execute in the laboratory. Computer simulation can rapidly explore parameter space, such as variations in composition, or conditions not easily available in the laboratory (e.g., ultrahigh temperature and pressure) to explore new and interesting resulting properties. For "virtual" materials

that exhibit potentially useful behavior, the simulations can explore pathways to producing the candidate material. This is an exciting, far-reaching and in certain cases achievable goal.

Combining the five modes, simulation becomes a powerful, revolutionary tool to accelerate conceptual advances, thereby providing a critical component in developing environmentally benign new materials, processes and technologies for energy generation, storage, and utilization. Properly used it has the possibility to substantially shorten the time from discovery of a new phenomenon to its technological use in products that positively affect everyday life. It is often this "development" time, and its attendant cost, that is the arbiter of success in the marketplace.

V. Readiness

The scientific challenges are not to be underestimated. However, the materials research community has the tools to attack the challenges head-on. The award in 1998 of a Nobel prize to Professor Walter Kohn for his development of Density Functional Theory (DFT), which provides the theoretical foundation for modern first principles quantum calculations of materials, is just one indication of the success and promise of this rapidly advancing field. It is now standard for modern materials modeling and simulation to be used to interpret experiments, to investigate phenomena, to predict properties, and to test mathematical models. Simulations using sophisticated models and efficient algorithms are already being applied to solve materials problems at the characteristic length scales, from atomic to macroscopic dimensions. For many of the initially relevant materials codes, efficient parallelization and verification has taken place on architectures similar to those planned for the SSI machines. In addition, the required computational time of many of these codes scale optimally, i.e., linearly with system size. Furthermore, these codes will scale up to the multi terascale machines. Hence, the computational materials community will be able to use the SSI facilities immediately as they become available. The need to solve complex multiscale problems is acute. Many advanced algorithms used to address them already exploit the most advanced computer resources available. Several essential materials simulation codes are already achieving remarkable performance in real applications. Through the newly formed Center for Computational Materials Science (CCMS), the computational materials science community is rapidly building the necessary infrastructure to support the move to terascale computing.

Over the last three decades materials physicists/scientists have been in the vanguard of exploiting successive generations of computer hardware – scalar, vector, parallel – as these machines have become available to basic science. For example, first generation electronic structure codes developed in the late sixties and seventies on IBM and CDC scalar machines were ported to Cray vector machines in the eighties and were some of the most efficient codes running on these machines. Beginning in the late eighties many of these codes were ported to parallel – Cray X/MP and Y/MP – and massively parallel – Intel ISP2, ISPC860, NCUBE, Thinking Machines CM1, CM2–architectures, with the result that several major DFT based electronic structure codes are now running on the most advanced parallel machines – Intel Paragon, IBM SP2, Cray T3E, ASCI Red, ASCI Blue Mountain, ASCI Blue Pacific. Indeed, they are among the most efficient massively parallel codes from any discipline. Currently, near terascale simulations using first principles quantum mechanics can model electronic structure to accurately compute properties (crystal structures, formation energies, magnetic structure, thermal expansion coefficients) for ideal crystals and for non-crystalline systems containing up to several hundred atoms. Other quantum mechanical

methods, which sacrifice some accuracy and reliability by using parameters derived from fits to first principles results or experiment, are able to simulate systems containing thousands of atoms on these same machines. Similar progress has occurred at the nanoscale where classical molecular dynamics is currently able to simulate systems containing a billion atoms. At the mesoscale a complex Potts model code is able to study systems with tens of millions of sites. At the continuum level, simulations using finite element methods and experimentally derived constitutive and elasticity equations are able to model macroscopic physical structures with element sizes that approach the interface with mesoscale models.

Overall, computation at each length scale is making rapid progress that roughly scales with increases in computer power. A major contribution to this favorable scaling results from new theoretical and algorithmic developments. First principles DFT methods traditionally scale as the third power of the system size, N. Previously, this scaling limited applications of these powerful techniques to systems containing a few tens of atoms using generally available computer resources. Recently developed techniques have been pushing the asymptotic cubic scaling to larger N. At the same time, new algorithms are striving for asymptotic linear scaling. For system sizes of up to a thousand electrons, ab initio plane wave electronic structure codes now effectively scale as $N^2 \log N$. Developments using a local representation are close to achieving linear scaling for very large systems. In molecular dynamics simulations, advances in fast multipole methods reduce the scaling from N^2 to N, for potentials that have long ranged Coulomb interactions. In addition, HyperMD has the potential to substantially increase the time over which the system evolves.

To illustrate further the state of readiness of the computational materials science community to effectively utilize terascale computing, it is useful to consider the state of development of some specific codes:

- Plane-wave DFT pseudopotential codes have become the workhorse for performing first principles calculations of structure and bonding. Coupled with molecular dynamics algorithms they are now being extended to direct simulation of dynamical processes. One of these codes, used to simulate properties of semiconductors, runs at 105 Gigaops on the 512 processor SGI/Cray T3E900 at NERSC. A related Gaussian based code, used to simulate a variety of materials systems from molecules to amorphous alloys, achieved 605 Gigaops accurately simulating 3072 atoms of bulk silicon in three hours on the 9112 processor ASCI Red machine.
- A multiple scattering code being developed to study non-equilibrium and finite temperature properties of magnetic materials was awarded the 1998 Gordon Bell Prize for "Best Performance of a Supercomputer Application." The code yielded a performance of 265 Gigaops at NERSC and 658 Gigaops on a 1024 processor T3E1200 system at another government site. A subsequent run on a 1458 processor T3E at SGI-Cray was the first to achieve Teraops performance for a full application code. Interestingly, the Gaussian pseudopotential referred to above was the runner-up in the 1998 Gordon Bell Prize competition.
- A one billion atom molecular dynamics simulation using a Lennard-Jones potential at a liquid density (2.5 σ cutoff) runs in six seconds per time step on 3600 nodes (in dual processor mode) on the ASCI Red machine. A 100 million atoms runs in 0.75 sec per timestep in single-processor mode on all 4500 nodes

- A Potts model mesoscale code, used for simulating grain growth in materials and for investigating the effects of impurities and their interactions with cracks on grain growth, runs in 326 (563) seconds on 1000 (512) processors of ASCI Red for Q=100 Potts states, 64 million sites on the lattice, and 1000 sweeps.
- Finally, to run microstructure level PZT shock response simulations with 30 million finite elements would take about 43 seconds per time step on 3240 nodes of ASCI Red.

All these codes will easily scale up for use on multi-terascale computers and will allow the effective use of SSI capabilities immediately as they become available.

Although conceived independent of SSI, an important contributor to readiness is the recently formed Center for Computational Materials Science (CCMS). This virtual center is sponsored by the DOE-Office of Science (OSC), Office of Basic Energy Sciences (BES), Division of Materials Science (DMS). The CCMS provides a formal structure for promoting collaborative computational projects in materials science. These projects are of a kind that cannot be undertaken by single investigator groups and involve collaborations among multiple DOE Laboratories, Universities, other Governmental Laboratories, and Industry. Many of these projects will require computer resources of the capacity provided by SSI. The collaborative aspects of CCMS projects are fostered through "coupling money" provided by BES-DMS to support partnering, investigator exchange, special workshops and travel. By construction CCMS projects are multi-disciplinary. Selection of CCMS projects follow focused workshops and peer-review. The relevance of CCMS to SSI is that it can provide a formal structure identifying, promoting and sanctioning large-scale computational materials science projects that are of national importance and are relevant to DOE missions in basic science. Thus, those CCMS projects that require computer resources of the type provided by SSI will naturally fit within the scope of SSI.

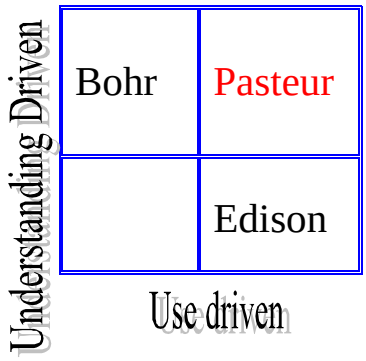


Figure 2. Pasteur's Quadrant

The materials science community has the initial codes and the infrastructure to take advantage of the immense resources envisioned for SSI. Moreover, the materials science community is on the verge of a paradigm shift in the way it does science with the promise of building a sturdy bridge across the "valley of death" between basic science and technological impact. A useful construct for thinking about this potential paradigm is "Pasteur's Quadrant." (Reference: Pasteur's Quadrant, Basic Science and Technological Innovation, D. E. Stokes, The Brookings Institution, Washington D.C., 1997; See Figure 2). Due to the complexity of materials systems, progress has necessarily proceeded either within the Bohr quadrant (experiment and theory done on model systems) or Edison's quadrant (research and development by trial and error). Realistic simulation is the vehicle for moving materials research firmly into Pasteur's quadrant.

VI. Examples

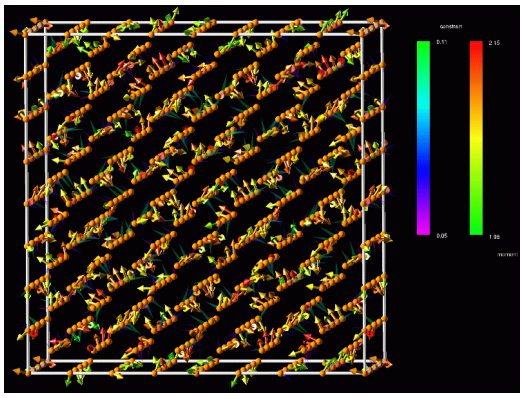
As we have stressed throughout this document, terascale simulation will enable multiscale modeling and thereby promote science-based understanding of the properties of complex materials and phenomena. Multiscale modeling of mechanical properties and multiscale modeling of magnetic materials are two obvious large scale, high impact problems that could form SSI foci. However, rather than fully develop some limited subset of preordained SSI problems, we present in the next section a smorgasbord of representative examples that illustrate materials simulation and modeling, pushing into Pasteur's Quadrant. The examples are chosen to represent, by today's standards, large scale simulations, but more important they hint at what could be done with increased computational power. They also sample each of the length scales (see Table 1 or Figure 1) and a wide range of material classes and issues.

The magnetism example (VI.A) demonstrates a sophisticated quantum scale calculation. The researchers are anxious to meet the multi-scale challenge by collaborating with scientists working at larger length scales using micromagnetics algorithms. The melting of diamond (VI.B) is an example with thousands of atoms. It pushes the quantum regime, albeit with some simplifying approximations into the nanoscale. The calculation illustrates that it is possible to explore materials in extreme environments where it would be difficult to do experiments. The martensitic phase transformation example (VI.C) illustrates significant progress toward understanding of an important microstructural phenomenon by combining first principle calculations with large-scale atomistic simulations. The fourth example (VI.D) uses a billion atom molecular dynamics simulation with a highly simplified classical potential for a prototypical ductile metal extending the atomic scale towards the mesoscale. In this example, the simulation allows the investigation of the materials behavior near the tip of a propagating crack. The grain sliding in aluminum example (VI.E) uses a simplified model of metals to investigate plastic deformation at high pressures and high stress, again in a regime that experiment is unable to explore. Polymers, particularly complex but ubiquitous material systems, are the subject matter of the sixth example (VI.F). To simulate these systems not all the atoms can be treated explicitly. Some are aggregated together for computational feasibility. The polymer example demonstrates that the long time scales for modeling phase transformations are not out of reach. The seventh example (VI.G) investigates radiation damage in materials. This is extremely important to aging fission reactors and future fusion reactors and involves complex materials issues far from equilibrium. Such extreme conditions are nearly impossible to access experimentally. The eighth example (VI.H) confronts complex phenomena in solidification. This example illustrates a major step in bridging from the microscale to the macroscale, albeit using a phenomenological model (empirically fit with parameters that are notoriously difficult to measure). Here there is a need to inform these calculations with input from accurate and reliable simulations at a finer scale. The final example (VI.I) involves simulating the processing of alloys for the control of microstructural features in order to optimize properties. This work is a bridge between mesoscale models that consider the intermediate length scale of micron size grains and interfaces to the larger scale continuum models, which take the final microstructural characteristics and evaluate bulk materials properties for applications.

Taken together, these nine examples illustrate current projects for various length scales and provide a glimpse of approaches that can be suitably combined and further developed to achieve integrated multiscale modeling that will facilitate the design and development of advanced materials.

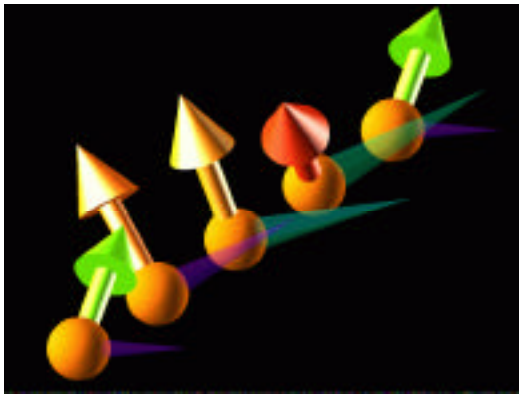
VI.A First Principles Studies of Finite Temperature Magnetism

Introduction: Understanding and predicting the properties of magnetic materials is essential for optimizing the design of power generators, motors, and essentially all devices containing permanent magnets. New magnetic materials have made lightweight tiny motors (for cameras, car windows, and electric pencil sharpeners) a part of everyday life. Yet magnet performance is far from reaching known theoretical limits. There has been no method for using the quantum mechanical (QM) interactions governing magnetism at the atomic level to predict practical properties. Recently, new approaches have been developed that permit full QM treatment of thousands of magnetic atoms at finite temperature. The illustration at left shows atomic magnetic moments at high temperature. At low temperatures, the moments are aligned. The magnitudes of the moments and the fields can now be precisely evaluated for complicated situations.



Magnetic moments and local magnetic fields for a model of Iron at high temperature

Calculational Notes: Calculations were performed using the Locally Self-consistent Multiple Scattering (LSMS) method. The calculation shown is for a 512 atom per unit cell array of moments and was performed on the 512 node SGI-Cray T3E at NERSC. The research won the 1998 Gordon Bell Prize for "Best Performance of a Supercomputer Application."



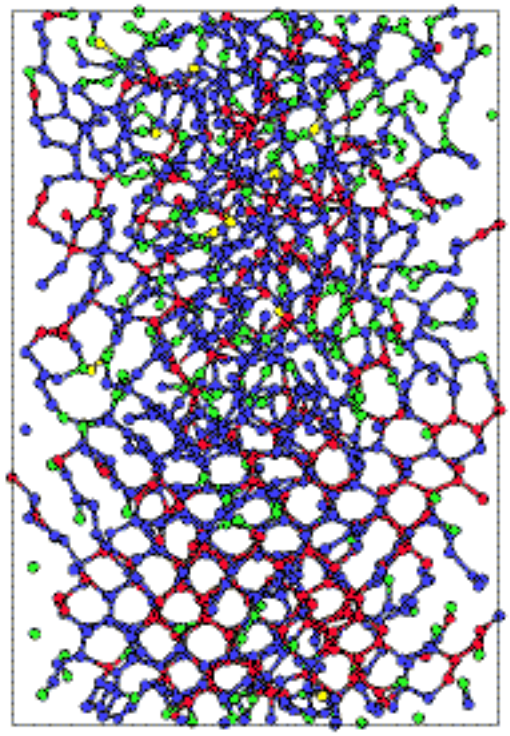
Detail taken from upper illustration showing relationship between magnetic moments and magnetic fields

Results: The upper illustration is a snapshot of the results of calculations of the magnetic moments (arrows) and forcing fields (translucent spikes) for a model of iron above its magnetic ordering temperature. In the calculation, the magnetic moments and resulting forcing fields are obtained entirely from first principles calculations (i.e., using no empirical parameters). The lower illustration is a blowup of a few of the sites in the upper illustration, allowing a better view of the detailed relationship between moments and forcing fields.

Significance: The ability to accurately treat a large number of magnetic atoms will allow detailed evaluation of the interactions among moments near defects. The defects can pin the magnetic moments in a good permanent magnet and keep them from changing direction. Understanding of these interactions will provide needed information for micromagnetic modeling tools so that scientists will finally be able to understand the detailed relationship between a material's microstructure and its bulk magnetic properties. SSI levels of computing power are essential to consider extended defects, which are known to enhance permanent magnet performance and for integrating with micromagnetics.

VI.B Melting A Diamond Crystal with Tight Binding Molecular Dynamics

Introduction: Well beyond its value for jewelry, diamond is invaluable as the hardest known substance. Fine diamond particles are the ultimate abrasive, and wear resistant diamond coatings are used on tools from saw blades to surgical instruments. But who would consider melting diamond? Materials scientists and engineers who are searching for cheaper and more robust processing routes to the synthesis of diamond coatings could use the thermodynamic phase diagram of carbon as a guide. The conditions that it takes to melt diamond are too extreme for careful laboratory experimentation. Melting diamond on a computer, however, makes it possible to determine the complete pressure-temperature phase diagram.



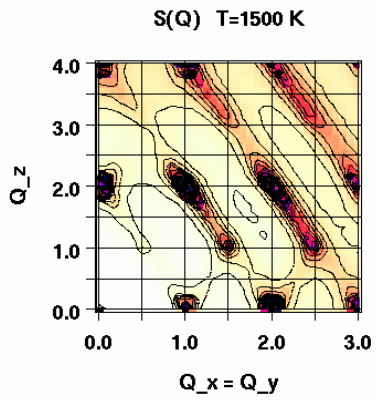
Calculational Notes: Quantum mechanical tight binding (TB) molecular dynamics calculations were run with a parallel code and an algorithm that scales linearly with the system size, for large systems. A highly efficient implementation permits the calculation of the electronic structure and forces for systems of up to 10,000 atoms on the 1024 node Paragon XP/S 150 at ORNL. The empirical parameters for the TB code were determined by fits to the results from extensive first principles calculations for many static geometries.

Results: The figure shows a snapshot of 2000 carbon atoms (T>6000 K) with the lower half in a diamond lattice and the upper half in a liquid phase. Red atoms indicate four-fold bonded (diamond-like) atoms; the blue atoms indicate three-fold (graphitic) bonded atoms; and there exist some two-fold and five-fold coordinated atoms. The large number of three-fold atoms is an indication that the liquid phase is less dense than the four-fold diamond phase. By changing temperature and/or pressure, the interface between the solid and liquid will move (e.g., the solid fraction increases below the melting point). Such simulations permit the accurate determination of the melting temperature of diamond as a function of pressure.

Significance: Molecular dynamics simulations can lead to new insights for understanding natural and artificial diamond synthesis. Experiments that are difficult, expensive, or impossible in the laboratory, can be accurately simulated on modern computers. By including the essential quantum nature of the electrons and their chemical bonds, the tight binding calculations form a natural bridge leading from first principles electronic structure calculations to the mesoscopic regime. This eliminates the need to develop new force fields or other more simplified interactions among atoms in complex environments. SSI resources will permit the extension of the quantum mechanical treatment to even larger numbers of atoms in order to investigate more complex nanoscale phenomena involving extended defects. This would illuminate the fundamental relationship between microstructure and important macroscopic materials properties.

VI.C Atomistic Simulations of Martensitic Transformations

Introduction: The formation of a martensitic phase controls the strength and hardness of carbon steels. The martensitic transformation is a diffusionless, cooperative movement of atoms resulting in a unique microstructure. Martensitic transformations are also responsible for shape memory effects in "smart materials" [e.g., NiTi-alloys]. Materials scientists are studying the formation of martensite in order to understand more about the complexities of how it forms to enable the design of specialized alloys and smart materials. Some important clues in understanding martensite formation come from x-ray studies at high temperatures. These experiments exhibit an unusual streaking pattern which suggest that there is an instability in the material that precedes the actual formation of martensite. The details of the cause of the streaking have been a puzzle for decades. Zirconium was chosen as a model material since, as an element, its martensitic transformation (at 1133 K) is uncomplicated by alloying effects.



Calculated scattering in the < 110> plane

Calculational Notes: The calculations involved molecular dynamics simulations for a model of zirconium with up to 200,000 atoms per unit cell and up to 80,000 time steps for extracting anharmonic lattice dynamics. They used classical embedded atom potentials fit to extensive first principles electronic structure calculations. The calculations ran on the 1024-node Intel Paragon XP/S-150 at ORNL-CCS.

Results: In the figure shown above the calculated x-ray scattering of the high-temperature bcc phase shows a characteristic streaking in the x-ray patterns as observed in experiments. Examination of the x-ray scattering as a function of time shows that the streaking is due to coherent atomic fluctuations toward the low temperature hcp martensitic phase. The picture shown to the left illustrates the microstructure after quenching to below the transformation temperature, with blue atoms separating the three orientationally different types of domains of transformed material.

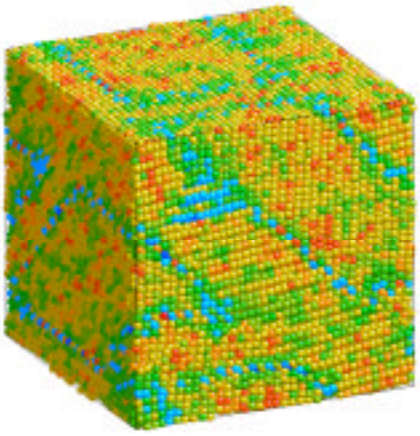
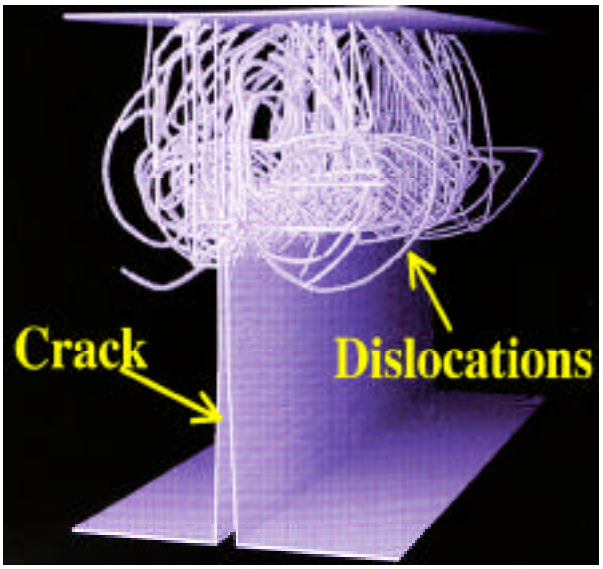


Image of microstructure formation in cubic simulation cell

Significance: This computational exploration demonstrates the potential of realistic atomistic simulations for understanding complex dynamical phenomena; in this case the calculations explained a long outstanding problem in experimental metallurgy. The ability to model phase transformation in metals and alloys, such as the martensite transformation, will enable materials scientists to control the microstructural properties of alloys. The increased computational power of terascale computers will allow detailed studies on more complicated and technologically relevant multi component alloys.

VI.D Computational Simulations of Crack Propagation

Introduction: Cracks happen! Fracture of materials causes structural damage, loss of productivity, and at times, loss of life. However, predicting how and when a material or structure will fail is a difficult task for scientists. Why and how things break involve complex fundamental processes and phenomena occurring on a wide range of length and time scales. Scientists are turning to the largest computers available in order to uncover new clues in solving the mystery of catastrophic materials failure. Laboratory testing of materials can reveal fracture strengths and explore the macroscopic reasons for fracture, but material scientists know that, ultimately, fracture involves breaking bonds between the atoms that make up the solid. Computers are ideal for studying these local, atomistic processes.



Atomistic model of crack propagation in ductile metal

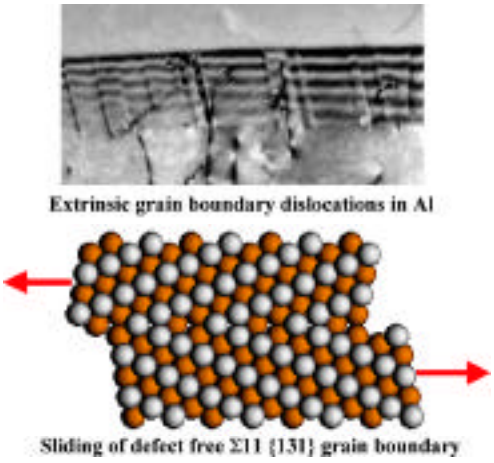
Calculational Notes: A simplified model of a metal utilizes Lennard-Jones (LJ) interaction potentials. The figure on the left shows a schematic of a molecular dynamics simulation of an atomistic LJ model with parameters representative of a prototypical ductile fcc structure. The actual calculation contained one billion atoms.

Results: The simulation illustrates some of the complex events that occur as a crack moves in a ductile metal. At first, the crack moves very rapidly and local bonds break in a "brittle" manner, but at some point the crack-tip begins to emit dislocations (the tangles in the picture) and stops propagating. One refers to such a crack as blunted. A blunted crack can cause intense local deformation, but it does not cause failure. Cracks that can emit dislocations usually stop before complete structural failure occurs. However, when the material is unable to emit dislocations, crack propagation does not terminate, which eventually leads to failure and irreversible damage of the material. The fundamental phenomena that determine whether a material is able to emit the beneficial dislocations are yet to be elucidated.

Significance: Materials scientists have been studying fracture of metals, alloys, and ceramics for many years. They are still unable to accurately predict when a particular structure may fail. It is possible with large-scale computations, such as the one shown here, to gain new insights into this complex phenomenon. A computer simulation of fracture is able to reveal details at the atomistic scale that cannot directly be observed in experiments. With SSI resources, materials scientists will be able to include needed realism and essential complexity in the fundamental interactions. This will lead to unraveling of the intricate processes that occur as materials catastrophically fail.

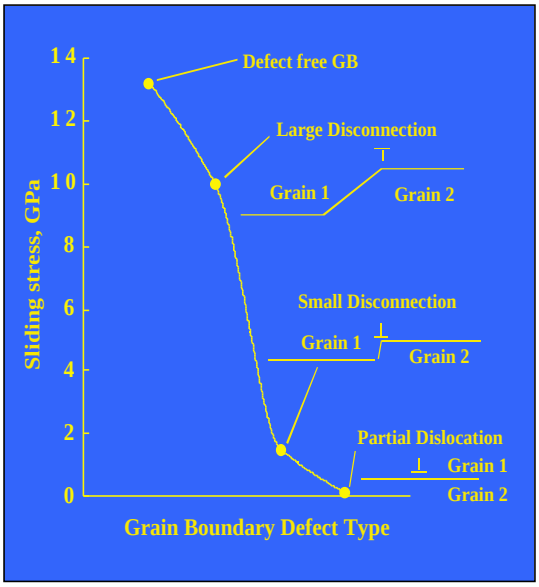
VI.E Grain Sliding for Superplastic Deformation of Aluminum

Introduction: The fuel efficiency of the automobile increases as the weight of the automobile decreases. This simple relationship is driving a large nationwide effort to develop new low cost, robust, lightweight alloys for multiple uses on the car. However, until the cost of processing can become competitive with sheet steels, the cost to produce automobiles using significant amounts of aluminum is prohibitive. To reduce the cost of processing, it is necessary to rapidly form the alloy. Rapid forming is possible with aluminum because, under the right conditions, it "superplastically" deforms. Superplastic deformation involves low-stress sliding along grain boundaries, a complex process of which material scientists have limited knowledge. Experimentalists are not able to directly measure the force or stress required to slide the aluminum along a grain boundary. Therefore, it is necessary to rely on realistic simulations to provide a measure of this invaluable material property.



Computer model of grain boundary sliding

Calculational Notes: The calculations involve molecular dynamics relaxations using the embedded atom potential for Al. It simulates 2,000 movable atoms with flexible borders for 2,000 relaxation steps to minimize the energy. The calculation is done at 0°K with up to 20,000 atoms for a chain-of-states method to analyze the energy barrier to grain sliding. The simulation ran on a HP C-160 workstation.



Computed sliding stress for various boundary defects

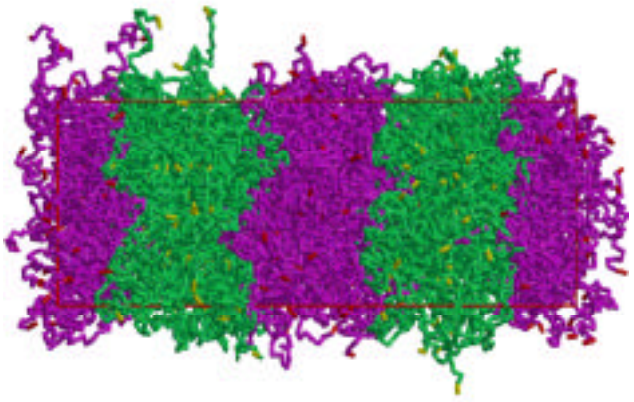
Results: Simulating the atoms in a chunk of aluminum provides opportunities for gaining understanding of the mechanisms underlying sliding processes. The figure to the left shows the calculated stress that is necessary to slide a grain boundary in aluminum. The simulations also analyze and provide information about the energy barriers to the grain sliding.

Significance: These simulations are providing essential input needed for the rational design of improved aluminum alloys. The ability to analyze the sliding resistance of a single grain boundary with and without various defects is an example of a new way of doing science. With SSI resources, it will become possible to provide increasing guidance in the development of new, more formable alloys instead of relying on trial and error.

VI.F Interfacial Behavior of Symmetric Diblock Copolymers

Introduction: Polymers are one of the 20th century miracle materials. Light weight, high strength, ease of formability, and other desirable properties have led to a vast array of new and improved products. Polymer systems are notably complex materials in which both the local chemical interactions and the conformations of the polymer chains play important roles in determining properties. The range of characteristic length and time scales span many decades. The properties and phenomena exhibited by a single chain in a dilute solution are markedly different from an entangled polymer melt or a cross-linked network. Increasingly, computer simulations are playing an important role in testing the basic assumptions of theoretical models and interpreting experimental results. Studies of phase transformations provide an illustrative example.

Calculational Notes: The calculations involve molecular dynamics simulations of polymer melts and networks of 50,000 to 1,000,000 monomers and up to 200 million time steps. The classical interaction potentials are either explicit or united atom for short chains and coarse- grained bead-spring models for long chains. The calculations run on systems from workstations to both shared memory and distributed memory clusters.



Lamellar phanse in a symmetric diblock copolymer system

Results: The figure shows a snapshot of a diblock copolymer system in the ordered lamellar phase. The two incompatible halves of each chain are jointed at one point. To determine the dynamic properties, it is necessary to simulate for very long times to properly allow for diffusion of the chains parallel and perpendicular to the interface. For temperatures above the order-disorder transition, the polymers form a disordered phase. However at low temperatures, various complex ordered phases form. The nature of the ordered phase depends on the relative amounts of the two components. In the symmetric case, shown here, the ordered phase is lamellar. The yellow and dark red indicate the ends of the chain. As the temperature increases the interface between the two phases becomes more disordered.

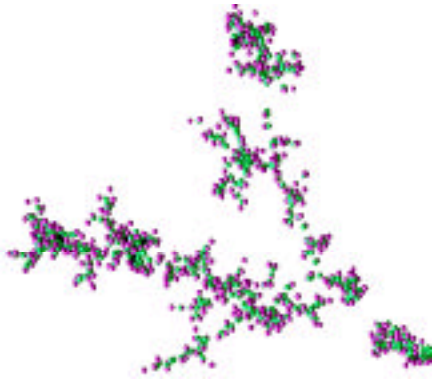
Significance: The ability to model a variety of homopolymer systems, from melts to cross linked networks or rubbers, has led to new insight into the mechanisms that control the complex dynamical and relaxation processes. As computational power has increased over the past few years, there has been rapid progress in bringing new insights to a number of important technological issues, including how to strengthen the interface between incompatible polymers. The simulations are able to provide essential features of the phase diagram of immiscible polymer blends. New terascale computers provide the opportunity to build accurate models of polymers at interfaces. More accurate models are a necessary prerequisite to a better understanding of complicated phenomena such as adhesion and failure and to a study of polymers under shear, which is a critical element in the technological process of polymer extrusion.

VI.G Atomistic Simulations of Radiation Damage in Metals

Introduction: High-energy neutrons, which are necessarily produced in nuclear reactors, can damage the materials used to contain the core. Not only is this a serious problem affecting the life and safety of present fission reactors, but it will present a major hurdle for future fusion reactors. The primary form of damage is atomic displacement. This occurs when energetic neutrons hit atoms in the solid, giving them enough energy to create a series, or cascade, of further displaced atoms. Under the right conditions, these displaced atoms collect at internal surfaces creating voids and causing a significant overall dimensional change. The figure to the left illustrates this swelling. It shows a comparison of originally identical samples after irradiation of one of them. Although the swelling occurs rather slowly, after large radiation doses and long times, the dimensional changes are quite extraordinary. Material scientists are using computer simulation to try to gain further insight into the detailed mechanisms of radiation damage. The goals are to predict problems over long periods of time (reactor aging) and to design new materials that are less sensitive to radiation damage.

Swelling of irradiated steel

Calculational Notes: Molecular dynamics simulations model the initial displacement of atoms caused by a single high-energy neutron. "Monte Carlo" simulation techniques model the random motion of thousands of such displaced atoms diffusing over long times. To simulate cascades requires models containing millions of interacting atoms. Gathering adequate statistics requires multiple realizations (runs).



Portion of a high-energy displacement cascade in copper

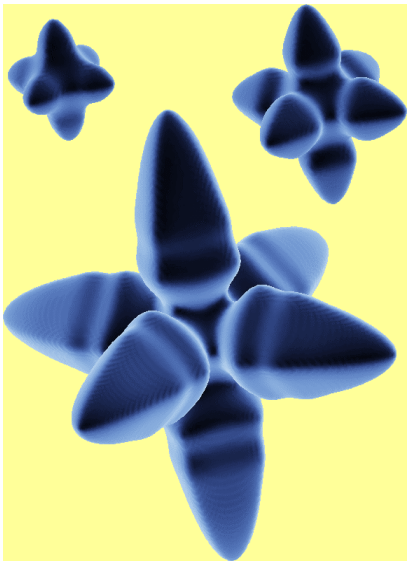
Results: The lower figure shows the results of a computer simulation of a single high-energy neutron striking a piece of copper. The small spheres represent the defects produced in the otherwise regular arrangement of atoms in the crystal structure. The green spheres represent vacant crystal lattice sites from which atoms have been displaced, and the magenta spheres represent the displaced atoms that have been pushed into places not usually occupied by atoms.

Significance: This initial work provides a detailed map of the atomic displacements. Knowing the structure is the first step to understanding the properties induced. SSI resources will permit the accumulation of thousands of events for improved statistics. It will also permit the extension to complex structural alloys, which exist in aging reactors, as well as to the development of new radiation-resistant alloys for future fission and fusion reactors. Simulation will play a particularly important role since experiments are extremely time consuming, expensive, and in some cases, impossible.

VI.H Simulations of Three-Dimensional Solidification: Dendritic Structures

Introduction: Dendritic (snow-flake like) growth is a complex pattern formation process that takes place during the solidification of engineering materials ranging from Al-based alloys for the automotive industry to Ni-based superalloys for the aircraft industry. The growth morphology of dendrites determines the microstructure of these materials. Thus, the ability to accurately model this growth is of fundamental importance for predicting essential mechanical properties controlled by the microstructure, such as strength and durability. Yet, the prediction of the microstructure remains often qualitative and unreliable in a variety of industrial processes (including welding, casting, sintering, etc.). There are two major obstacles. First, microstructures form via the motion of anisotropic interfaces (solid-liquid, solid-solid, and grain boundaries). Thus, one is faced with the difficulty of tracking the time evolution of two-dimensional surfaces of arbitrary complex shapes. Second, fast atomic scale processes determine the thermodynamic and kinetic properties, which in turn govern the response of an interface to a driving force (diffusion flux, stress, etc.). However, the macroscopic length and time scales on which the microstructure evolves are several orders of magnitude larger than the atomic scales. Reliably bridging the gap between these microscopic and macroscopic scales has remained a computational challenge.

Results: A major advance in coping with both difficulties has occurred recently in solidification modeling. The figure illustrates the first fully quantitative simulation of the growth of a three-dimensional dendrite, which is the fundamental building block of alloy microstructures. In this example, bridging the micro-macro gap has involved treating scales ranging from a nanometer capillary length to a millimeter diffusion length. It was found that a weak anisotropy in surface energy has a profound influence on the growth morphology of dendrites and thus the properties of cast products.



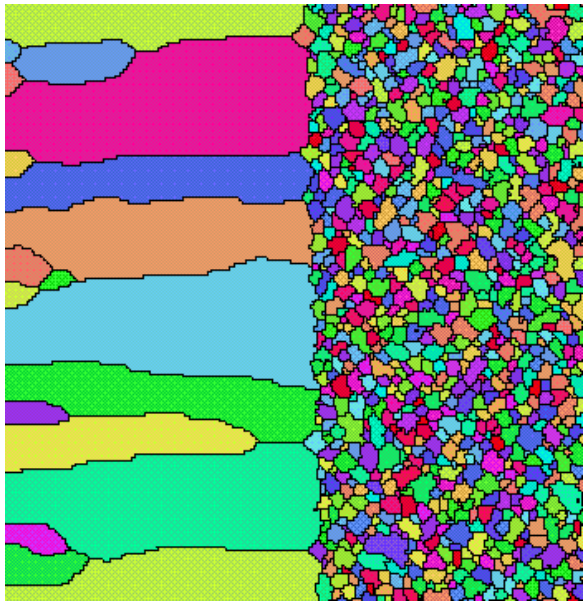
Three snapshots of dendritic growth

Calculational Notes: These calculations were made possible by developing a computationally efficient phase-field model that allows tracking an arbitrarily complex interface shape in three dimensions. The work required massively parallel implementation on the Cray T3E at NERSC. Three snapshots of the solid-liquid interface are shown following the morphological instability of a spherical nucleus. One second of real time corresponds to 100 hours of CPU time using 64 processors of the Cray T3E.

Significance: This work represents one of the earliest successful efforts to bridge the micro-macro gap. The surface energy anisotropy is an input parameter of the model that presently needs to be determined experimentally, which is not yet feasible in metallic systems. Therefore, atomic scale first principles calculations must predict the required critical parameter (the surface energy anisotropy) independent of experiment. The computing power available with SSI should also permit extension of this work to incorporate the convection (fluid motion) that is universally present in castings and strongly influences the microstructure. Thus, we are on the verge of realistically modeling one of the most technically important and most basic of materials processing phenomena.

VI.I Materials Process Modeling for Microstructure Optimization

Introduction: The processing of a material can be the determining factor in it's cost and it's performance. Often a material's strength, reliability, and other properties are sensitive to details of processing. In order to reduce costs and to optimize a material's performance, materials scientists must gain a better understanding of the relationship between processing conditions and the resulting microstructure. Nearly all materials forming processes (forging, rolling, extrusion, welding, powder processing) include high-temperature excursions during which grain structure evolves, whether intentional (annealing) or inadvertent (heat affected zone in welds). Microstructural evolution can take many forms during these processes: e.g., grain growth, recrystallization, precipitation, and coarsening. These microstructural changes introduced by forming largely determine the final material properties.



Columnar grain development in zone annealing.

Calculational Notes: The calculation uses the Monte Carlo Potts model to simulate the annealing of a polycrystalline grain structure. The simulations in two dimensions involve 40,000 sites and take a day to run on a fast workstation. A prototype three-dimensional algorithm includes 64 million sites, runs on 1000 processors of ASCI-Red, and a run takes 326 seconds.

Results: The top figure shows a zone annealing simulation of a gas turbine blade alloy. The grain size in the initial, randomly oriented, microstructure is about ten microns. The figure shows the development of a creep resistant columnar grain structure, which results when the material is pulled through a highly localized hot zone (a narrow vertical region at the middle of the figure). Simulations allow determination of process parameters (pull speed, hot zone temperature) that optimize the grain aspect ratio (length and width). As another practical application, the lower figure shows the recrystallized grain structure in an incandescent lamp filament. Related simulations revealed process parameters that influence development of the creep-resistant grain structure.

Recrystallization of a tungsten lamp filament.

Significance: Simulations provide a flexible tool for probing the dependence of microstructure on a range of processing conditions. The model's reliability can be enhanced by accurate input parameters from smaller length scale models (atomic, interface, dislocation), while the model's output can be directly utilized by larger scale continuum simulations for the prediction of material performance. These microstructural evolution models will play a critical role in forging the links from materials composition to processing and from processing to performance.

VII. Cross Cutting

The modeling and simulation of key phenomena spanning several orders of magnitude over multiple time and length scales is central to significant advances in virtually all of the scientific disciplines. A common goal across disciplines is to enable major advances in predictive capabilities that will be more reliable and markedly superior to empirical phenomenological modeling and extrapolation. The nature of complexity of phenomena that exist over a large range of length and time scales, which are dynamic, and which are not scale invariant, is a common theme throughout SSI. While we are not so naïve as to suggest that there is one generic approach independent of the nature of the specific complexities, we are confident that there will be commonality in paradigms for uncovering the nature of the essential complexity as the scales change. We would also suggest that, on a case by case basis, a given complex system in one discipline has some analogy to another complex system in a different discipline. Since real material systems are as complex as any interacting system, advances in bridging scales and methodologies for building those bridges will have impact on other disciplines. Similar advances in other disciplines can likewise impact materials science.

For example, the nature and complexity of long range interactions is ubiquitous in materials science (poorly screened Coulomb potentials, dipole-dipole interactions, stress fields, etc.) and common in biology, earth sciences, cosmology, fusion, etc. Oftentimes, there is no obvious connection from the science, but once the science is translated into a mathematical model, the model is virtually the same as that derived for some entirely different discipline and system. The parameters may mean something very distinct, the parameter range itself may be very different, and the scales may be very dissimilar, but nonetheless the mathematics may be quite similar. In such cases, much can be learned by exploiting analogy. An example that doesn't stray beyond materials physics, but illustrates the point, is the recent success of techniques for manipulation of light in photonic materials using many of the concepts learned from the nature of electrons in semiconductors and insulators.

Besides the opportunity for advances from analogies between disciplines, there are numerous examples where materials research directly overlaps with other disciplines. For example,

- Rigorous models for understanding surface degradation/corrosion, and the adhesion of thermal barrier coatings are applicable to the combustion initiative. These are fundamentally multiscale materials science problems.
- Understanding and optimizing new catalysts for NO_x abatement in lean burn internal combustion engines is critical to the success of a combustion initiative. Here first principles electronic structure methods that would form an integral part of any materials multiscale modeling initiative are immediately relevant.
- Plasma surface interactions and radiation damage of materials is central to the fusion initiative. Indeed, much of the development of materials for future fusion reactors will be, of necessity, virtual and based on simulations and modeling techniques developed in materials science. This is because only (extremely) limited facilities will be available for experimentation under conditions relevant to fusion reactors, independent of the nature of reactor design.

- In biology, the determination of the free energy of binding of substrates to enzymes requires precisely the same tools and similar developments as envisioned for a materials initiative. These involve accurate quantum simulations of local processes and construction of interaction potentials for larger classical molecular dynamics simulations.
- Similar tools are applicable to the interaction of fluids with minerals, relevant to geosciences, ground water flow, and environmental remediation.
- Since materials problems abound in science based stockpile stewardship, there would be synergy between multi-scale modeling capabilities developed by ASCI and SSI. It is natural for projects envisioned in a SSI initiative to include elements closer to basic science and general theoretical and algorithmic development, whereas the ASCI effort is more closely tied to engineering imperatives.

The advances in materials science envisioned from a SSI initiative will have broad implications to industry. Industry would benefit greatly from the improved mathematical models and simplified engineering tools that would emerge from a materials SSI initiative, especially for treating multiscale phenomena. Industrial researchers are anxious to take advantage of computational developments. However, existing algorithm and modeling capabilities are too limited to justify investment by industry of terascale computing facilities. The basic research and the initial development needs to be undertaken by DOE research teams. Ideally this will be in partnership with industrial colleagues to help ensure a clear path to relevance.

It almost goes without saying that success of a materials component of SSI depends on effective partnering with applied mathematicians and computer scientists. There are numerous examples where advances in applied mathematics or computer science will directly impact a materials initiative. For example, finite element techniques are used to treat nonlinear problems such as plasticity and crack tip analysis. Boundary integral methods are effective for treating linear problems through reduction of dimension. This is especially advantageous for situations where the domain evolves in time (e.g., crack propagation and void evolution), because rediscretizing becomes considerably easier. The level set method is a powerful alternative to traditional front tracking techniques, because it is capable of following discontinuous changes in topology, splitting or merging of surfaces, and singularities (cusp formation). Boundary integral methods have the capability of handling complicated geometries, but the calculations are expensive. The fast multipole method provides a highly effective technique for significantly reducing the computational cost for large scale problems. General advances in nonlinear optimization including genetic algorithms, efficient and robust methods for solving stochastic differential equations, methods for handling stiff systems, and ideas regarding extracting long time behavior would all have broad impact. Robust sparse matrix routines, parallel BLAS and highly optimized FFT's are ground zero, as are tools for parallel programming, visualization, integrated software design, handling distributed data sets, aiding portability of codes, and collaboration.

All of these areas of interactions among computational materials scientists, applied mathematicians and computer scientists are critical to the development of multiscale modeling. Success will enable the computational materials science revolution to materialize.