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Computational materials science and engineering (CMSE) is a relatively young field. The first-known case study of materials that used digital computers was made shortly after the Second World War. The legendary mathematician John von Neumann at the wartime Los Alamos National Laboratory is credited as being the first to seriously consider numerical methods and encourage using computing machines. Not surprisingly, early material simulations stemmed directly from the war efforts. One of the focuses of research at the time was on how irradiation of high-energy particles would change a material's structure and properties, an obviously urgent topic at the time. Nevertheless, the activities in this relatively obscure and small area remained dormant until the sixties when faster and more powerful digital computers became available. Now computational materials science is an active and fast-growing field. It covers many topics in nearly all branches of materials science and engineering. As its impact has grown, it has gained a reputation as being the third approach for scientific research and engineering, parallel to experiment and theory.

Compared to humans, computers are more efficient and less error-prone in handling repetitive or numerical tasks. For this reason, computers are used extensively in materials research (and other fields as well) to do such tedious work as data acquisition and data analysis. Computational materials science and engineering is, however, more ambitious in its objectives and much broader in its scope. Its aim is to understand and predict the structures-properties relationships of materials in various length scales, from not only the continuum (millimeters and up) level, but also from the mesoscopic (microns) and atomic (nanometers and Angstroms) levels. For instance, to materials scientists and engineers, the stress-strain relation is no longer the end in the pursuit of the mechanical properties of the materials. Now, using their understanding of stress-strain relations and microstructure, researchers seek to answer more complex questions such as how microstructures become what they are under different conditions, what dislocation cores look like, and how detailed interatomic interactions influence the microstructure and defect structures.

The efforts to answer these kinds of questions are the major motivation for the development of advanced instruments such as the transmission electron microscopy (TEM), atomic force microscopy (AFM) and various nanoscale testing equipment and scattering facilities. Our ability to acquire detailed information on material structure and process from these advanced tools allows us to more efficiently develop new materials and extend the life-cycles of their services. The same motivation is behind the development of computational materials science and engineering. Furthermore, the unique capability of computer simulations and modeling allows us to "see" materials not only better on smaller scales but also more quantitatively. With properly constructed models (Hamiltonian or interatomic interaction), one can simulate, or mimic, the entire physical process of the model materials, including microstructure evolution, deformation process, defect structure, or phase transitions. From the known constitutive relations, one can model a large number of material behaviors, ranging from mechanical deformation, magnetism, and chemical reaction, to piezoelectrics.

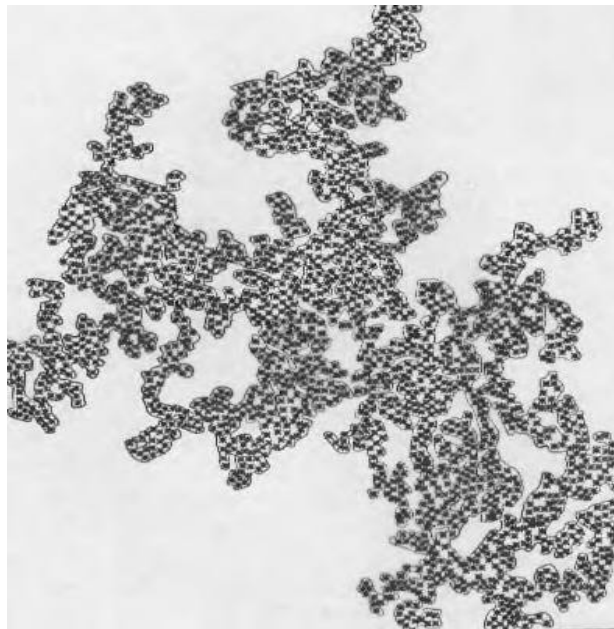
Several methods in computational materials science are widely used now, including molecular dynamics (MD), Monte Carlo (MC) method, and quantum mechanics (QM) calculations. MD takes the interatomic interactions between atoms as a major input. The trajectories of the atoms are obtained by numerically solving Newton's equation of motion. From the atomic positions and

velocities, physical properties can be obtained. MC methods use a stochastic approach to generate atomic positions, or configurations, of the material systems. Both methods have been used successfully in simulating structural, thermodynamic and transport phenomena of liquid, glass and crystalline materials. The quantum mechanic based calculations deal with both electrons and ions in materials. By numerically solving the Schrodinger's equations for these particles, detailed information on electronic band structures, magnetic and optical properties, and interatomic interactions can be gained. Since the calculation starts from the fundamental Schrodinger's equation, it could be performed with the input of the atomic numbers only. For this reason, the technique is often called the first-principles or *ab initio* method. In addition to the aforementioned techniques, there are model-based calculation methods for phase diagram calculations, phase-field modeling, and finite element methods.

Examples of the triumphs in computational materials science include the identification of the dislocation core structures using atomistic simulations and the award of the 1996 Nobel Prize to the development of the density functional theory in quantum calculations.

Remarkable progress has been made in computational materials science and engineering over the last four decades. Driven by our desire to know more and by the ever-increasing power in digital computer, new frontiers in materials modeling are constantly being explored using numerical methods. Among these new areas are simulations of nanoscale materials, glasses, soft and polymeric matters, granular matter, strongly disordered systems, non-equilibrium systems and driven phenomena. These topics pose new challenges that demand development of new simulation methods in mesoscopic scales, efficient platforms in hardware, and faster and efficient software to break the barrier of size and time limitations in atomistic and quantum simulations. Breakthroughs in these areas could finally bring the materials simulation and modeling to a new level where computational "experiments" could be conducted hand in hand with real experiments. The only difference one will notice is that the materials used in the experiment are digital materials, which are much cheaper and easier to make and pose no danger to our health or environment.

My research is in the area of atomistic, mesoscopic, and continuum simulation and modeling of materials and material process. I am currently conducting research on bulk metallic glasses, nanocrystalline materials, granular matter, magnetic materials. I am interested in understanding thermodynamics and phase transitions in undercooled liquid, defects and deformation process in metallic glasses, hysteresis and impurity effects on magnetization, granular flow, and dimensional effects on nanoscale materials. Using molecular dynamics simulation, my group recently observed highly inhomogeneous atomic density variation in undercooled liquids (See Figure). The result shed new light on how the glass transition occurs and why crystal embryos fail to grow. My group also engages in development of algorithms for mesoscopic microstructure simulations. The research projects in my group are supported by various funding agencies, including NSF, DOE, DARPA, Army Research Laboratory, Air Force, and Sandia National Laboratory.



The snap-shot of the atomic configuration of a undercooled liquid close to the glass transition temperature. The dark spots are atoms with low atomic density. The spongy configuration of the liquid regions can be seen clearly.

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