Molecular Dynamics Techniques

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Molecular dynamics is a very important computational method which has been widely used for many years to investigate various properties of fluids and solids and phenomena in many areas of Physics, Chemistry and Materials Science. The main advantage of this method is that it provides a vivid and detailed microscopic picture of atomic motion. The macroscopic quantities can be extracted from these detailed microscopic quantities to compare with experiments or to predict possible phenomena occurring in a given system.

The molecular dynamics technique follows the time evolution of an ensemble of particles interacting *via* a given set of potentials by integrating Newton's equations of motion for all particles in the system. By this method, particles' trajectories can be observed directly; the basic quantities of motion such as velocities and positions can also be directly measured. Probably the most critical component of this technique is the knowledge of the interparticle or interatomic potential used in the calculation. It basically consists of a repulsive force (due to Pauli's exclusion principle) and an attractive force, which can consist of dipole-dipole and/or Coulombic interactions as well as higher-order interactions. Historically, the pairwise potential for rare-gas elements and ionic materials was the first developed, because these simplistic models can be easily treated mathematically. The adjustible parameters in the potentials are often compared with experimentally measured quantities such as compressibility and lattice constant. In the last decade many researchers have attempted to establish the interactions for semiconductors and metals. For semiconductors which have directional bonding, a three-body interaction is needed; for metals the method of treating conduction electrons as a cloud has been developed. These studies are motivated not only by the technological importance of these materials, but also by the understanding of material properties at the microscopic level that they provide; for example, the understanding of interface or surface properties is important in characterizing sputtering processes in thin-film media and fabrication of industrial devices.

Applications of molecular dynamics techniques are numerous in science

and engineering. Some of these studies center on comparing calculated quantities with experimental data such as compressibility, thermal expansion and thermal conduction. In a study of thermal expansion of rare-gas and ionic solids, Wu and Friauf obtained results in good agreement with experiment. Researchers at Argonne Laboratory have applied this method to investigate ionic motion and conduction mechanisms in superionic solids. These calculations deal mainly with equilibrium states; it is surprising that a quantitative measure for the equilibration of a system has been established only recently by Wu and Friauf.

In other areas, Amini and Hockney were probably among the first to investigate melting phenomena in ionic solids, while Corriet *et al* studied melting and dislocation in rare-gas solids. Recently, Phillpot, Yip and Wolf have used the technique to demonstrate the interplay between thermodynamics and kinetics during the melting process in silicon with a sophisticated interatomic potential for covalent bonds developed by Tersoff.

MD methods have also been used to explore more dynamic processes occurring in solids or surfaces due to external disturbance. For instance, the keV particle bombardment of solids is a technique used for fabrication of devices in the semiconductor industry, for mass measurements of biological compounds, and for structural determination of surface bonding arrangements. B. Garrison and others studied the ejection mechanisms and energy and angular distribution during the bombardment process. Wu, Friauf and Armstrong have used it to predict the possible damage to insulator surfaces from radiation-induced electrostatic disruption. These studies reveal a great deal of physical insight into dynamic processes at the atomic scale.

Very recently, MD techniques have been used to investigate the atomic mechanisms, energetics and dynamics underlying the interactions between two materials being brought together. Combined with atomic force microscopy techniques, these projects carried out by Landman *et al* significantly enhance our understanding of adhesion, contact formation, surface deformation, material elastic and plastic characteristics, microindentation, material hardness, friction and wear, and fracture. Wu at IBM is also using MD techniques to investigate interactions between head and disk surfaces for contact recording. Additionally, a group at Schlumberger-Doll (Ridgefield, CT) has applied MD to fluid dynamics, and their results examine fluid flows near solid boundaries. The method is also

used to study surface tension and wetting on surfaces.

The usual MD calculations solve the equations of Newtonian classical mechanics. They follow atomic motions for a single atomic state according to the Born-Oppenheimer approximation. Therefore, they cannot be used to determien the coupling between different electronic states. However, in the last three years, D. Ferry *et al* at the University of Arizona have developed quantum molecular dynamics techniques coupled with Monte Carlo methods to study electronic transport in semiconductors with very high electron density. The potential applications of MD simulations are so immense that AT&T and IBM have spent millions of dollars to develop special-purpose multiprocessors, which further spurs MD research both in materials applications and into the physics underlying these interesting phenomena.

I would like to dedicate this article to Dr. Armstrong, a great teacher, with my sincere appreciation for his teaching and constant support for my study. Congratulations on your fiftieth birthday.