

Extending Non-Equilibrium Molecular Dynamics Simulation Methods

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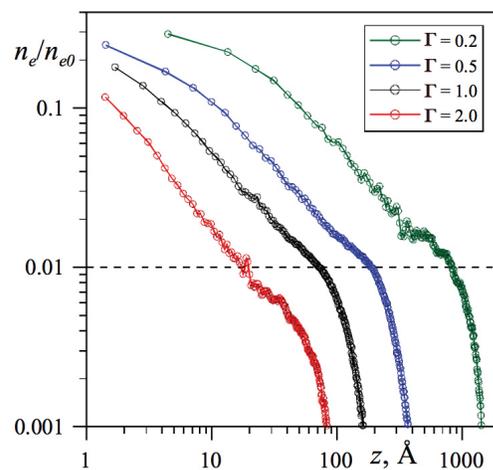
Project Description

Novel nonequilibrium molecular dynamics (NEMD) simulation methods are being extended and applied in four areas of mutual interest to Sandia and Joint Institute for High Temperatures, Russian Academy of Sciences (JIHT RAS). NEMD is being applied to (1) understanding relaxation and equilibration in non-ideal, nondegenerate plasmas; (2) characterizing melting or cavitation of condensed matter systems that are super-heated or under hydrostatic tension; (3) devising classical interaction potentials that can represent changing bonding character as a system evolves; and (4) investigating the mechanisms of shock-induced plasticity and fracture in metals.

Three tasks were performed in CY06:

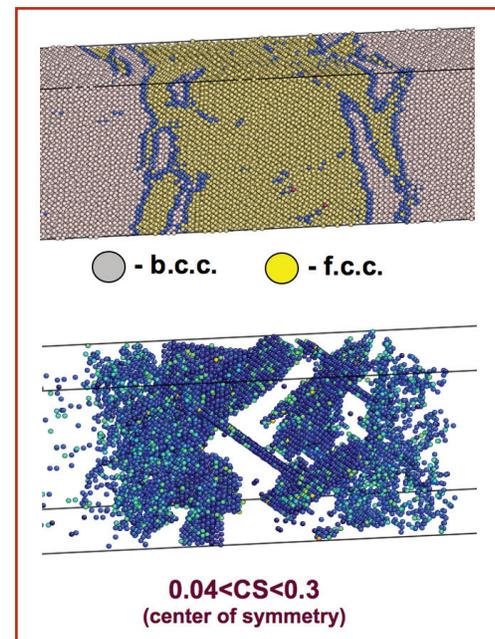
- Investigation of interacting, drifting, nonideal plasmas;
- Investigation of melting in super-heated condensed matter;
- Development of reactive potentials for material interfaces using the Cluster Multi-Range Interpolation (CMRI) scheme.

Follow-on work in each of the four areas is being pursued in CY07. In the area of nonideal plasmas, JIHT is studying the role of bound, high energy, quasi-classical electron-ion pairs on the relaxation of nonideal plasmas. Algorithms are being developed for identifying such bound states in MD simulations. The fraction of the bound states, their energies, and lifetimes will be studied for the nonideal plasmas simulated in CY06. The formation process for the bound states will be determined, and the recombination time will be compared with characteristic times of the different relaxation processes observed in the CY06 simulations. JIHT will also compare the results from CY06 with existing continuum models of plasma equilibration to assess the agreement in various regimes defined by the set of values of nonideality parameter; ion and electron temperatures; and ion mass and charge. Finally, JIHT is developing a new simulation technique for more accurate treatment of close particle collisions. The approach being used is to separate the interaction potential into short-ranged cluster binding models and long-ranged classical pair-wise force field. The antisymmetrized wave packet MD will be used to describe the



Formation of the Double Layer-Relaxed density profiles of electrons depending on the plasma nonideality.

Structural changes in the rarefaction wave in an initially BCC single crystal.



0.04 < CS < 0.3
(center of symmetry)

particle collisions or bound states of a small number of electrons and ions for the cluster model. The CMRI scheme will be applied to combine individual cluster binding models and long-ranged force field into a single set of dynamic equations for electrons and ions. In the area of highly nonequilibrium condensed matter, JIHT will study cold crystal lattice stability in the presence of "hot" electrons (~ 10 eV) using *ab initio* MD based on the finite temperature density functional theory. The *ab initio* simulations will be used to validate the quality of the description of interatomic interactions in the two-temperature states considered by classical (many-body) potentials. A procedure will be proposed for development of temperature dependent classical potentials suitable for describing the two-temperature systems considered.

JIHT is using the CMRI scheme to fit empirical potential parameters to quantum chemistry (QC) data. In particular, they are pursuing development of an automated procedure for construction of combined potentials: fitting the parameters of two functionally different empirical potentials in different atom environments and fitting the CMRI-specific interpolation parameters to the QC data in the transition between the two empirical potentials.

JIHT is also pursuing several related tasks in the area of shock-induced plasticity and fracture. This includes investigating the mechanisms of structural transformations, spall, and fracture in solids under high rate impulse loading. They are developing a kinetic nucleation-and-growth model to represent the results obtained from the NEMD simulations in hydrodynamic simulations of shock wave spall experiments. Lastly, they will attempt to use the CMRI scheme to construct an interatomic potential that switches smoothly between fast nonreactive potential and the more accurate, computationally demanding reactive potential ReaxFF developed by van Duin and Goddard.

Technical Purpose and Benefits

This project will enhance both our understanding and our capabilities for investigating the dynamic response of multiple types and states of materials under a variety of loading conditions. This understanding finds application in weapons performance, weapons effects, ICF, high energy density physics (HEDP), and advanced nuclear energy reactors.

Possible future applications of the more accurate treatment of close particle collisions in nonideal plasma simulation are plasmas at low temperatures, mixtures of molecules, atoms and multiple charged ions.

The interpolated, combined force fields should find useful application in simulating nonequilibrium systems of atoms. The demonstration simulation will treat graphite oxidation reactions. The hybrid force field incorporating ReaxFF will be demonstrated in simulating cracking in silicon and, if that is successful, applied to study spontaneous decay of distended silicon near its stability boundary.

Understanding the mechanisms of shock-induced plasticity and fracture in metals is a long time, outstanding problem in shock wave physics. JIHT's innovative approaches stand to make significant contributions in this area.



Signing the agreement. Clockwise from left: Ms. Patty Jojola (SNL buyer), Dr. John Aidun (SNL PI), Dr. Genri Norman (JIHT PI), and Dr. Vladimir Zeigarnik (JIHT).

JIHT

*Collaboration between Sandia National Laboratories, Albuquerque, NM, USA, and
JIHT RAS (Joint Institute for High Temperatures, Russian Academy
of Sciences), Moscow*

