 Proceedings of ICCES'08, pp.1353-1353

Multimillion to Billion Atom Simulations of Nanostructured Materials under Extreme Conditions

Priya Vashishta[1,2], Rajiv K. Kalia[1,3] and Aiichiro Nakano[1,4]

Summary

Molecular dynamics (MD) simulations are performed to investigate critical issues in the area of structural and dynamical correlations and reactive processes in nanostructured materials under extreme conditions. Scalable space-time multiresolution algorithms implemented on multi-teraflop to petaflop computers enable large-scale MD simulations involving multimillion to multibillion atoms. We report the results of MD simulations of: (1) CdSe nanorods undergoing forward and reverse structural phase transformation under hydrostatic pressure; (2) initiation, growth and healing of wing cracks in confined silica glass under dynamic compression; (3) hypervelocity projectile impact damage in aluminum nitride and strong interplay between shock-induced structural phase transformation, plastic deformation and brittle cracks; (4) interaction of nanovoids in silica glass under hydrostatic tension; (5) initiation of chemical reactions at shock fronts prior to detonation and dynamic transition in the shock structure of an energetic material (RDX); and (6) exploding nano particles - explosive burning of aluminium nanoparticles. We are also implementing Lattice Boltzmann scheme for a mesoscale description of fluids on PS3 cluster.

[1]Collaboratory for Advanced Computing and Simulations (CACS), Departments of Chemical Engineering & Materials Science, Physics & Astronomy, and Computer Science, University of Southern California, Los Angeles, CA 90089-0242, USA

[2]Email: priyav@usc.edu

[3]Email: rkalia@usc.edu

[4]Email: anakano@usc.edu