Abstract Submitted
for the SHOCK15 Meeting of
The American Physical Society

Quasi-Coarse-Grained Dynamics (QCGD): Modeling of Defect/Damage Evolution at Mesoscales using Atomic Scale Interatomic Potentials AVINASH DONGARE, KAROON MACKENCHERY, GARVIT AGARWAL, RAMAKRISHNA VALISETTY, ARUNACHALAM RAJENDRAN, RAJU NAMBURU, Department of Materials Science and Engineering and Institute of Materials Science, University of Connecticut — A computationally efficient modeling method called "quasi-coarse-grained dynamics" (QCGD) is developed to expand the capabilities of molecular dynamics (MD) simulations to model behavior of metallic materials at the mesoscales. This mesoscale method is based on solving the equations of motion for a chosen set of representative atoms from an atomistic microstructure and retaining the energetics of these atoms as would be predicted in MD simulations through scaling relationships for the interatomic potentials. The success of the mesoscale method is demonstrated by the prediction of the high temperature thermodynamics, deformation behavior of interfaces, phase-transformation behavior, heat generation during plastic deformation as well as the wave-propagation behavior in metallic systems under various conditions, as would be predicted using MD simulations. The reduced number of atoms and the improved time-steps allow the modeling of metallic materials at the mesoscale in extreme environments. The applicability of the QCGD simulations to predict the evolution of defect structures and the microstructure during deformation and failure in FCC metals at the mesoscales will be discussed.

Avinash Dongare
Department of Materials Science and Engineering and
Institute of Materials Science, University of Connecticut

Date submitted: 30 Jan 2015 Electronic form version 1.4