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Mesoscale Modeling of Shock Wave Propagation and Dynamic Failure in Metallic Systems AVINASH DONGARE, Chemical, Materials & Biomolecular Engineering, University of Connecticut — The response of materials under conditions of thermomechanical extremes is very complex and involves damage creation and propagation, phase transformation, heat generation and transfer, etc. A principal challenge in predictive modeling of failure behavior is presented by the gap between the atomistic description of micromechanisms of the relevant processes and the macoscale response in continuum simulations/experiments. This difficulty can be approached through the development of a robust mesoscopic computational model that retains the relevant physics and is capable of representing the material behavior at time- and length-scales intermediate between the atomistic or continuum levels. Mesoscale models typically reduce a group of atoms by a mesoparticle system with much smaller number of collective degrees of freedom, and hence are often difficult to apply for problems such as heat transfer, phase transformation, and dissipation of mechanical energy during wave propagation. To achieve this goal, a novel mesoscopic model is being developed based on the idea of coarse-graining with the energetics defined for the particles based on interatomic potentials used in molecular dynamics (MD) simulations. The coarse-grained molecular dynamics simulations (CGMD) allows larger size systems and improved time-steps for simulations and thus able to extend the capabilities of MD simulations to model materials behavior at mesoscales. The successful application of the CGMD method is demonstrated by prediction of the phase-transformation, heat generation and wave-propagation behavior under the conditions of shock loading, as would be predicted using MD simulations.

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