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Molecular Dynamics Simulation of Shock Waves Interacting with Nano-structures AHMAD ALQANANWAH, JOEL KOPLIK, YIANNIS ANDREOPOULOS — Typical theoretical treatments of shock wave interactions are based on a continuum approach, which cannot resolve the spatial variations in solids with nano-scale porous structure. To investigate such interactions we have developed a molecular dynamics simulation model, based on Lennard-Jones interactions. A piston, modeled as a uni-directional repulsive force field translating at a prescribed velocity, impinges on a region of gas which is compressed to form a shock, which in turn is driven against an atomistic solid wall. Periodic boundary conditions are used in the directions orthogonal to the piston motion, and we have considered solids based on either atoms tethered to lattice sites by stiff springs, or on embedded atom potentials. Velocity, temperature and stress fields are computed locally in both gas and solid regions, and displacements within the solid are interpreted in terms of its elastic constants. In this talk we present preliminary results, and the longer-term goal of this work is to understand energy transport and absorption in porous materials.

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