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Multi-scale molecular dynamics simulations of steady shock waves in Lennard-Jones and nitromethane EVAN REED, Lawrence Livermore National Laboratory, LAURENCE FRIED, M. MANAA, WILLIAM HENSHAW, CRAIG TARVER, Lawrence Livermore National Laboratory — We compare spatial profiles of steady shock waves using our multi-scale simulation technique (Phys. Rev. Lett. 90, 235503 (2003)) and direct simulation techniques and find good agreement. Multi-scale simulations of shocked amorphous Lennard-Jones are in good agreement with NEMD simulations and multi-scale simulations of shock waves in analytical equations of state of explosives are in good agreement with hydrodynamic simulations. In both cases, agreement improves with distance behind the shock front. We have applied the multi-scale technique to the study of chemically reactive shock waves in condensed nitromethane (CH3NO2) using the density-functional tight-binding (DFTB) method. We study shock waves with speeds ranging from 5.5 km/s to 8 km/s for durations up to 0.5 ns behind the shock front. We believe these are the longest duration tight-binding simulations of shocked matter ever performed.

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