Shock Induced Phase Transitions in Polymeric Nitrogen

WILLIAM MATTSON, US Army Research Laboratory — The reported density functional molecular dynamics simulations are of a shock travelling through ~4,000 atoms arranged in the equilibrium cg-N configuration equilibrated at T = 250K, P = 1 atm. Atoms within a small segment of the material given an extra velocity consistent with various desired flyer plate impact velocity. The resulting atomic trajectories show a number of complex behaviors including a phase transition to a previously unseen phase, spontaneous defect formation, and chemical reactions. The stability of the shock and the unusual properties of the above phenomena will be discussed.