

Abstract Submitted
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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 $\sim 4,000$ atoms arranged in the equilibrium cg-N configuration equilibrated at $T = 250\text{K}$, $P = 1\text{ atm}$. 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.

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