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Shock-induced Reactions in Pentaerythritol Tetranitrate Studied by Molecular Dynamics Simulation[1] JOANNE BUDZIEN, AIDAN P. THOMPSON, Sandia National Laboratories, SERGEY V. ZYBIN, California Institute of Technology — Molecular dynamics simulations were performed using the reactive force field, ReaxFF, as implemented in the General Reactive Atomistic Simulation Program code for systems consisting of a single crystal of PETN with not fewer than 237000 atoms. The crystals were shocked along the [100] direction using two different piston velocities. The resulting chemical reactions were tracked in an attempt to elucidate short-time initiation mechanisms. Here, we present the primary, secondary, and intermediate products as a function of time and position behind the shock front.

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