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Shock induced chemistry in granular Ni/Al nanocomposites

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Intermolecular reactive composites find diverse applications in defense, microelectronics and medicine, where strong, localized sources of heat are required. However, fundamental questions of the initiation and propagation mechanisms on the nanoscale remain to be addressed, which is a roadblock to their widespread application. Motivated by experimental work which has shown that high-energy ball milling can significantly improve the reactivity as well as the ease of ignition of Ni/Al intermetallic composites, we present large scale ($\sim$ 41 million atom) molecular dynamics simulations of shock-induced chemistry in granular Ni/Al nano-composites, which are designed to capture the microstructure that is obtained post milling. Shock propagation in these granular composites is observed to be extremely diffuse at low piston velocities, leading to a large inhomogeneity in the local stress states of the material. At higher piston velocities, the shock front is more homogeneous as a consequence of a change in the compaction mechanism; from plastic deformation mediated pore collapse at low piston velocities, to fluid filling of the pores at higher impact velocities. The flow of molten ejecta into the pores subsequently leads to the formation of vortices, where the reaction progresses much faster than in the bulk.

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