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Shock response of Ni/Al reactive inter-metallic composites[1]

MATHEW CHERUKARA, Purdue Univ, TIMOTHY GERMANN, EDWARD KOBER, Los Alamos National Laboratory, ALEJANDRO STRACHAN, Purdue Univ — Intermolecular reactive composites find diverse applications in defense, microelectronics and medicine, where strong, localized sources of heat are required. 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 inter-metallic composites, we present large scale (∼41 million atom) molecular dynamics simulations of shock-induced chemistry in porous, polycrystalline, lamellar Ni/Al nano-composites, which are designed to capture the microstructure that is obtained post milling. Shock propagation in these porous, lamellar materials is observed to be extremely diffuse, leading to substantial inhomogeneity in the local stress states of the material. We describe the importance of pores as sites of initiation, where local temperatures can rise to several thousands of degrees, and chemical mixing is accelerated by vortex formation and jetting in the pore. We also follow the evolution of the chemistry after the shock passage by allowing the sample to "cook" under the shock induced pressures and temperatures for up to 0.5 ns. Multiple "tendril-like" reaction fronts, born in the cauldron of the pores, propagate rapidly through the sample, consuming it within a nanosecond.

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