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Nano-scale spinning detonation in condensed phase energetic materials VASILY ZHAKHOVSKY, MIKALAI BUDZEVICH, AARON LANDERVILLE, University of South Florida, CARTER WHITE, Naval Research Laboratory, IVAN OLEYNIK, University of South Florida — Single- and multi-headed spinning detonation waves are observed in molecular dynamics simulations of a condensed phase detonation of an energetic material (EM) confined in round tubes of different radii. The EM is modeled using a modified AB Reactive Empirical Bond Order potential. The thermochemistry and reactive equation of state are varied by adjusting the barrier height for the exothermic reaction AB+B $\rightarrow$ A+BB. This allows us to study the evolution of the detonation-wave structure as a function of physico-chemical properties of the AB explosive. The detonation wave is found to exhibit a pulsating planar front in a tube of 8 nm radius, which later collapses due to the development of longitudinal perturbations. Upon increase of the tube's radius to 16 nm, the detonation wave structure is stabilized through the development of a single-headed spinning detonation. The spinning detonation displays a *four-wave* configuration, including incident, oblique, transverse, and contact shock waves. The contact shock generated by a contact discontinuity is observed for the first time in our MD simulations. A multi-headed turbulent-like detonation structure develops within tubes of larger radii, and exhibit features similar to those observed in gases.

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