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Critical velocities for deflagration and detonation in a REBO high explosive S. DAVIS HERRING, TIMOTHY C. GERMANN, Los Alamos National Laboratory, NIELS G. JENSEN, University of California, Davis — The effects of circular voids on the shock sensitivity of a two-dimensional model high explosive crystal are considered. We simulate a piston impact using molecular dynamics and a Reactive Empirical Bond Order (REBO) model potential for a sub-micron, sub-ns exothermic reaction in a diatomic molecular solid. The probability of initiating chemical reactions is found to rise more suddenly with the piston velocity for larger voids that collapse more deterministically than smaller voids. A void of only 10 nm radius reduces the minimum initiating velocity by a factor of 4. The shock-to-detonation transition at larger velocities is also studied using a micron-long sample containing a single void (and its periodic images). The reaction yield during the shock traversal increases rapidly with velocity, then becomes a prompt, reliable detonation. A void of radius 2.5 nm reduces the critical velocity by 10% from the perfect crystal. A Pop plot of the time-to-detonation at higher velocities shows a characteristic pressure dependence.

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