Scale Invariance and the Importance of 3D Effects in the Formation of Explosive Hot Spots

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ABSTRACT

Shock-induced collapse of voids with diameters in the 100-1000 nm range is thought to govern explosive initiation, but details of the hot spot formation process at this scale remain elusive to “full-physics” treatments based in all-atom molecular dynamics (MD). Using large-scale quasi-2D MD simulations, we predict the features of hot spots formed in a crystalline molecular explosive on multi-micron computational domains. Comparing a range of pore diameters and shock loading orientations shows a high degree of consistency in the hot spots formed at a given shock strength. A statistical test is developed that reveals rapid convergence and scale invariance in the predicted hot spot temperature fields for a given shock condition. Billion-atom scale MD simulations of hot spot formation with 3D spherical voids give direct evidence that widely adopted (quasi-)2D approximations significantly underestimate peak hot spot temperatures and reaction rates at shock initiation conditions. Prepared by LLNL under Contract DE-AC52-07NA27344. LLNL-ABS-855729.