Abstract Submitted
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Shock-induced decomposition of high energy materials: A ReaxFF molecular dynamics study[1] SUBODH TIWARI, ANKIT MISHRA, KEN-ICHI NOMURA, RAJIV KALIA, AIICHIRO NAKANO, PRIYA VASHISHTA, University of Southern California — Atomistic simulations of shock-induced detonation provide critical information about high-energy (HE) materials such as sensitivity, crystallographic anisotropy, detonation velocity, and reaction pathways. However, first principles methods are unable to handle systems large enough to describe shock appropriately. We report reactive-force-field ReaxFF simulations of shock-induced decomposition of 1, 3, 5-triamino-2, 3, 6-trinitrobenzene (TATB) and 1,1-diamino 2-2-dinitroethane (FOX-7) crystal. A flyer acts as mechanical stimuli to introduce a shock, which in turn initiated chemical reactions. Our simulation showed a shock speed of 9.8 km/s and 8.23 km/s for TATB and FOX-7, respectively. Reactivity analysis proves that FOX-7 is more reactive than TATB. Chemical reaction pathways analysis revealed similar pathways for the formation of N_2 and H_2O in both TATB and FOX-7. However, abundance of NH_3 formation is specific to FOX-7. Large clusters formed during the reactions also shows different compositions between TATB and FOX-7. Carbon soot formation is much more pronounced in TATB. Overall, this study provides a detailed comparison between shock induced reaction pathway between FOX-7 and TATB.

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