Mechanistic study of decomposition of Nitro Methane encapsulated in CNT Nanocontainer via Reactive Molecular Dynamics

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Nitro Methane (NM) is the simplest type of nitro compound in high explosive energetic material (HE), which finds explosion-related applications. Decomposition mechanism of the confined NM inside the isolated capped carbon nanotube (CNT) container was studied through reactive molecular dynamics simulation. Initial densities of NM and thermal shock conditions were expected to give a major impact on the decomposition pathway of NM -CNT container. The five systems at different densities (i.e. 1.137, 1.2, 1.3, 1.5, and 1.7 g/cc) with four initial shock temperatures (i.e. 2500, 3000, 3500, and 4000 K) were considered in this study. Each system was run with NVE MD simulations after introducing fast heat-up procedure with NVT MD simulation. Cascading release of the potential energy from decomposed NM resulted in the elevation of the reaction temperature, which stimulated the accelerated decomposition reaction, while reaction mechanism was traced by generated intermediates and products. Finally, the NM-CNT container was burst at the final stage of the reaction. The explosive decomposition of confined NM, which has never been reported, was first introduced in this study.