Enhanced Bursting Kinetics of Detonator-Integrated Nanobomb

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Nanobomb, which is a nitromethane (NM)-encapsulated carbon nanotube (CNT), is one of nano energetic material that has high chemical stability at ambient condition but exhibits enhanced explosive power at bursting. However, in order to be burst due to the stabilized NM inside the CNT, the nanobomb required compressively packed NM or high thermal-shock energy. In this study, to facilitate the reaction kinetics of nanobomb, we propose a detonator-integrated nanobomb, which was modelled by co-encapsulation of detonating molecule with NM inside the CNT. Considering the detonating pressure and velocity calculated via Kamlet-Jacobs equations, HMX and RDX were selected as candidates for detonator. By conducting non-equilibrium reactive molecular dynamics simulation with detonator-integrated nanobomb, detonator was found to exhibit faster decomposition than that of NM, and contribute to accelerated decomposition of NM by its radical intermediates. Nonetheless, overall bursting mechanism was not significantly affected by mixing with detonator. Through this study, we revealed that co-encapsulation of detonating molecules effectively improved reaction kinetics of nanobomb.