Effects of Structural Modification of Carbon Nanotube on Decomposition of Confined Nitromethane via Molecular Simulations

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Nitromethane (NM), the primary nitroalkane, is a typical explosive material and has been used in various engineering fields. Recently, researches have been carried out to utilize carbon nanotubes (CNTs) as nanocontainers for efficient use of NM. Even though the confinement effect of CNT and the interaction with encapsulated NM cannot be ignored, there are limited theoretical studies on the effect of structural modification of CNT to explosive properties of NM. In this regard, we modeled the NM-confined CNT and compared the difference of reaction characteristics and bursting mechanisms depending on the structural variation of CNT. In this study, reactive molecular dynamics (RMD) method was used to observe the nonequilibrium dynamics of decomposition reaction. Electromagnetic induction and corresponding amount of thermal shock were introduced to NM to initiate its decomposition, respectively. Also, to investigate the effects of structural changes of CNT on reaction properties, vacancy defect and nitrogen doping were introduced. The structural modification of CNT significantly altered the decomposition dynamics and bursting mechanism.