Electric field induced bursting mechanism of nanobomb by physicochemical modifications on CNT

전우철, 이정현, 김진철, 정상현[1], 조수경[1], 곽상규†
울산과학기술원; [1]국방과학연구소
(skkwak@unist.ac.kr†)

Application of high-energy materials (HEMs) has been studied until now due to their excellent performance. Especially, several studies have been conducted to control the explosion characteristics of HEMs employing carbon nanotubes (CNTs), but these studies did not consider the structural effects of CNTs on reaction characteristics under electric field. Thus, in this study, decomposition of nanobomb, where nitromethane (NM) is confined inside the modified CNT, under electric-field was investigated using non-equilibrium reactive molecular dynamics (NERMD) simulation. Three types of modifications (i.e., chirality, nitrogen-doping and vacancy defect) were applied to the CNT, and intensity and frequency of the electric field were tuned to simulate each electric spark and electromagnetic induction. From in-depth analysis of explosion characteristics, nanobomb with vacancy defect on CNT showed superior performance. Also, the frequency, which corresponds to C-N stretch of NM in electric-field, brought much rapid decomposition of nanobomb. Consequently, the variation of modifications on CNT and electric field could have major impact on the decomposition of system.