Molecular Dynamics Simulations of Flame Propagation of Monopropellant PETN Embedded with Carbon Nanotubes

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1 Overview

Carbon-based nanomaterials could act as a thermal energy conduit transferring heat from the reaction zone to the unburned fuel, resulting faster flame propagation and faster burning rate. They may also potentially change deflagration to detonation transition and shock sensitivity of propellants. Recently, Choi et al. [1] discovered a phenomenon called "big power from tiny wire". In their experiment, vertically aligned multi-wall carbon nanotubes (MWCNTs) were coated with an annular shell of cyclotrimethylene trinitramine (TNA), which was then ignited at one end. A combustion wave was found to propagate along the tube while the carbon nanotubes were intact. This wave propagated much faster than the theoretical flame speed of TNA and created a strong electric current that could be harnessed for nanoscale energy systems. Andrei Khlobystov pointed out in a review article [2] that nanotubes are much more than just passive containers, and the confinement at nanoscale can dramatically change the pathways of chemical reactions, often leading to unexpected products. Additionally, heat transfer, an important mechanism in combustion processes which largely affects how fast flame can propagate, is quite different at nanoscale from that in macroscale as a result of size effects on the phonon and electron transport [3].

These discoveries motivated us to investigate the flame propagation process of PETN (Pentaerythritol Tetranitrate) on CNTs using reactive molecular dynamics simulations. The simulations were performed using LAMMPS and the interactions between atoms were calculated using ReaxFF reactive force field. From our preliminary simulations we found that the computed flame propagation speed of PETN on CNT is indeed much faster than that of pure PETN (137 vs. 80 m/s) at an external hydrostatic pressure of 3GPa. This enhancement is attributed to faster heat propagation in CNT via phonon transport than in PETN, which elevates the temperature of unburned PETN, causing flame speed to increase. This particular case was run with 35,235 PETN molecules and the CNT consist of 3800 carbon atoms. The main goal of this work is to determine both qualitatively and qualitatively the effect of the CNT loading on the burning speed and flame ignition of PETN. We expect a parabolic trend between the CNT loading and the flame speed. Lower CNT loading should approach the pure PETN flame speed. Furthermore, increasing the CNT loading above a threshold value will eventually decrease the flame temperature, resulting in lower flame speed, ultimately reaching the flammability limit. The CNT loading will also have a strong effect on the flame ignition, as higher effective thermal

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conductivity of the composite will make ignition more difficult. In addition, the effect of pressure and the use of the MWCNTs on the flame speed will also be considered.

References

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