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On the molecular dynamics analysis of defect effect on mechanical properties and fracture behaviors of carbon nanotubes

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Summary

Due to the limitation of fabrication technologies nowadays, initial defects in carbon nanotubes (CNTs) are inevitably perceived particularly during the manufacturing process or chemical treatment. The investigation of the effects of initial defects existing in CNTs on their mechanical properties and fracture behaviors becomes essential for their potentiality in engineering applications.

In this study, the defect effects, including number in percentage, type, and location, are explored using the molecular dynamics (MD) simulation with Tersoff-Brenner potential. Results show that the mechanical properties, such as the elastic modulus, failure strength and strain, are strongly affected by the defects. Moreover, the distribution and the location of defects are also the factors to influence the mechanical properties of CNTs significantly. For example, with the same amount of defects, the elastic modulus and the failure strength both vary notably due to different defect locations of defects.

Not only their static/dynamic behaviors and material properties but also their fracture evolutions are discussed in this work. It turns out that the defected CNTs behave a brittle fracture characteristic. As a single bond is ruptured, the fracture will continue to propagate until all bonds around the circumference have failed. Additionally, based on the atomic-level stress distribution, it is also observed that the crack propagates along the maximum atomic-level stress region. As similar to the mechanical properties, the crack propagation path also depends on the location of initial defects considered.

In summary, according to the above results achieved, it can be reasonably explained that the large variation of mechanical properties often found in CNTs as reported in literature may result from the initial defects existing in CNTs.

keywords: Molecular Dynamics, Carbon Nanotube, Defect, Crack Propagation

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