Molecular Dynamic Simulation of Torsion of Carbon Nanotubes

K G S Dilrukshi[1], M A N Dewapriya[2], U G A Puswewala[1], R K N D Rajapakse[2]

[1]*Department of Civil Engineering, University of Moratuwa, Sri Lanka*
[2]*Faculty of Applied Sciences, Simon Fraser University, Canada*

*Corresponding author: rajapakse@sfu.ca

Carbon nanotubes (CNTs) have attracted considerable attention due to their remarkable properties. Torsional oscillators based on CNTs have been fabricated. Fabrication of CNT-based nanomechanical devices has to be supported in parallel by theoretical/computational models.

It is recognized that modified continuum models that account for size-dependent behaviour are attractive in the analysis of nanomaterial systems. Constitutive properties such as Young's modulus, shear modulus and Poisson's ratio are essential in continuum modeling. This paper presents a comprehensive study of the torsional response of a CNT using MD simulations based on the REBO and AIREBO potentials. Numerical simulations are presented for different chiralities and diameters to understand the influence of potential function on size-dependency of the shear modulus. The size and potential function dependence of ultimate strength in torsion is also investigated. In addition, the mechanical response expressed in terms of the virial stress and the influence of vacancy defects are studied.

Acknowledgement: This study was supported by grants from the National Science Foundation of Sri Lanka and Natural Science and Engineering Research Council of Canada.

Keywords: Carbon nanotubes, Molecular dynamics simulation, Shear modulus, Stress, Torsion