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PREDICTION OF TORSIONAL BUCKLING BEHAVIOR OF SINGLE-WALLED CARBON NANOTUBES VIA A MOLECULAR MECHANICS MODEL

Abstract

In the current study, torsional buckling analysis of chiral single-walled carbon nanotube (SWCNTs) is investigated using molecular mechanics modeling. To this end, the mechanical properties of a graphene sheet is first calculated on the basis of density functional theory (DFT) which leads to obtain force constants used in the molecular mechanics model. Then, based on the principle of molecular mechanics, the total potential energy of the system is calculated including bond stretching and bond angular variations and analytical solution is conducted to obtain the critical buckling shear strain corresponding to different types of chirality. The results of developed molecular mechanics model are compared with those of molecular dynamics simulation found in the literature and an excellent agreement is observed. However, in contrast to the molecular dynamics simulation, the present model has the capability to simulate large atoms systems with less computational time. According to the selected numerical results, it is observed that the value of critical buckling shear strain exhibit significant dependency on the type of chirality as armchair SWCNTs buckle at lower values of shear strain compared to zigzag one, especially for higher tube diameters. Numerical results indicate that the stability of the zigzag nanotubes is more than armchair ones with the same diameter. Also, it is found that among different type of chirality, the nanotubes correspond to (n,n/2) chiral vectors have the minimum critical buckling shear strain.