Molecular Dynamics Analysis on

Buckling of Embedded Carbon Nanotubes Using Materials Studio

D.D.T.K Kulathunga, A/Prof Ang Kok Keng

(Department of Civil and Environmental Engineering)

Carbon nanotube (CNT) has been identified as an excellent fiber in reinforcing nanocomposites. Buckling in CNTs embedded in composites has been observed experimentally and has been identified as a major mode of failure of composites. Hence, it is important to know the buckling properties of CNTs embedded in matrices. Having identified this importance, several studies have been devoted to study the buckling of embedded CNTs. However, these studies are based on continuum mechanics modeling owing to the high computational time demanded by the molecular dynamics simulations. However, it is necessary to verify the accuracy of these continuum mechanics models and hence the molecular dynamics studies are essential in studying buckling of embedded CNTs. Therefore, in the present study, a detailed molecular dynamics analysis is conducted on embedded single-walled CNTs.

Molecular dynamics is the widely accepted tool in analyzing mechanical behavior of CNTs because at the nanoscale, atomic interactions are expected to have a significant effect on mechanical behavior of CNTs. However, molecular dynamics is considered as a computationally expensive method especially for systems with higher number of atoms. Several computationally efficient software such as Materials Studio, Discovery Studio, DL-POLY, LAMMPS, TINKER and GROMACS are now available to conduct molecular dynamics simulations. Some of these software enable parallel computation and
hence molecular dynamics simulations on large atomic systems are now possible within considerably lower time periods.

In the present study we employ Materials Studio software by Accelrys. Materials Studio software facilitates molecular dynamics simulations based on several forcefields. We employ COMPASS forcefield for our simulations as this forcefield has been proven by several researchers as a suitable forcefield for CNTs. Materials Studio consists of several tools which are called modules to facilitate various molecular modeling tasks. Out of those modules, we employ Forcite module for molecular dynamics calculations and Amorphous module for the packing of CNT in a polymer matrix. In order to submit the jobs to HPC servers, input files for both the modules mentioned above are written in Perl language.

In the present study, single-walled CNTs with various diameters and lengths embedded in polyethylene (PE) matrix are subjected to the analysis. Effect of boundary condition and volume fraction of composite on the buckling properties of the embedded SWNTs is investigated here. Our results suggest periodic boundary condition as the most suitable boundary condition in the analysis of buckling of embedded CNTs. Non-periodic boundary condition is found to produce erroneous results despite the considerably lower computational time demanded by the non-periodic boundary condition compared to the periodic boundary condition. Moreover, a considerable effect of the volume fraction is found on the buckling properties of embedded CNTs especially for CNT/PE composites with volume fractions greater than 10%. Moreover, the molecular dynamics results are employed in verifying the accuracy of analytical continuum mechanics models based on Euler beam theory, classical shell theory and first-order shell theory combined with
Winkler foundation model. The results show that the molecular dynamics results closely follow the values of buckling stress and increment of buckling stress obtained from the first-order shell theory combined with Winkler foundation model. It is expected that these findings will be helpful in designing nanocomposites and nanomechanical devices.