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Mechanical Properties of Carbon Nanotubes Using Molecular Dynamics Simulations with the Inlayer van der Waals Interactions

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Summary

The evaluation of the fundamental mechanical properties of single/multi-walled carbon nanotubes(S/MWCNTs) is of great importance for their industrial applications. The present work is thus devoted to the determination of various mechanical properties of S/MWCNTs using molecular dynamics (MD) simulations. The study first focuses on the exploration of the effect of the weak inlayer van der Waals (vdW) atomistic interactions on the mechanical properties of S/MWCNTs. Secondly, in addition to the zig-zag and armchair types of CNTs, the hybrid type of MWCNTs that comprise a zig-zag outer tube and an inner armchair tube is also analyzed. Thirdly, the investigation is extended to deal with the influence of the axial orientation mismatch between the inner and outer layers of MWCNTs on the associated mechanical properties. Lastly, the behaviors of the interlayer shear force/strength of MWCNTs are discussed in detail. In the MD simulations, the force field between two carbon atoms is modeled with the Tersoff-Brenner (TB) potential while the inlayer/interlayer vdW atomistic interactions are simulated with the Lennard-Jones (L-J) potential. The effectiveness of the MD simulations is demonstrated by comparing the computed results with the theoretical/experimental data available in literature. Some interesting and essential results are presented. With different dimensions and geometries of CNTs, the inlayer vdW atomistic interactions can have up to about 9% increase of the elastic moduli, 27% decrease of the Poissona?Ts ratios, 12% growth of the shear moduli, and 13% enhancement of the interlayer shear strength. The mechanical properties of the hybrid MWCNTs are found to be midway between the zig-zag and armchair MWCNTs. It is also detected that the axial orientation mismatch between the inner and outer layers of a double-walled CNT has a trivial impact on the mechanical properties of CNTs. To separate the inner layer of a double-walled CNT from its outer layer, it requires a minimum external force of 0.889nN for the zig-zag.