

Estimation and Validation of Elastic Modulus of Carbon Nanotubes Using Nano-Scale Tensile and Vibrational Analysis

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Summary

In this paper, the atomistic-continuum mechanics method (ACM) is applied for carbon nanotube modeling. The atomistic-continuum mechanics is based on the transformation of chemical bonds between atoms in molecular mechanics into appropriate elements in finite element method and continuum mechanics. Spring elements are treated as chemical bonds between carbon atoms in carbon nanotube, whose force-displacement function is determined by the Reactive Empirical Bond Order (REBO) potential model. As a result, not only Young's modulus could be obtained but also modal analysis could be achieved with affordable computational time by personal computers. The validity of the results is demonstrated through comparisons to numerical and experimental results provided by other papers. In addition, based on classic structural dynamics, the feasibility of the ACM method has been verified by comparing the results of Young's modulus analysis and modal analysis.

