Abstract

To have a proper guidance on the mechanical and thermal properties of nanomaterials, a lot of efforts have been put on their prediction through theoretical and numerical simulation. Currently, most of the numerical methods are based upon molecular dynamics simulation. Owing to the vast number of atoms involved in the simulation, it is usually very time consuming. To improve the computational process, recently a semi-analytical method called molecular-continuum model was proposed to estimate the stiffness, strength and fracture toughness of nanomaterials. This model was developed by combining the concept of molecular dynamics and continuum mechanics, in which the potential energy describing the interactions of atoms is not restricted to the harmonic potential function, and hence its deriving stress-strain relation is not restricted to be linear. The estimated properties can therefore be the ones defined based upon the initial linear region such as stiffness, or the ones occur at the later period of the materials such as strength and toughness. With the concept of this model, a MD-based nonlinear finite element method was also developed. By using the molecular-continuum model and nonlinear finite element method, several mechanical and thermal properties of nanomaterials such as Young’s modulus, Poisson’s ratio, shear modulus, ultimate strength, fracture toughness, coefficient of thermal expansion, and specific heat have been estimated. For the purpose of illustration and verification, some examples of graphene, carbon nanotubes and single crystal Cooper are presented in this study.

Keywords: molecular-continuum model, nonlinear finite element method, mechanical property, thermal property, nano-materials