Multiscale numerical simulations for elastic properties and the flexural response of graphene sheets at finite temperature

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Abstract

Abstract: Among the different nanomaterials synthesized in recent decades, carbon-based nanomaterials such as carbon nanotubes, nanocones, etc., have garnered the attention of the scientific community due to their exceptional mechanical, electrical, properties and biomedical compatibility. Considering graphene as a basic building block to these nanomaterials and their wide range of potential applications in sensing, actuation, biosensors, biomedicines and other electronic devices, it is imperative to investigate their elastic properties thoroughly and study mechanical behaviour under different loading conditions. To the best of the authors' knowledge, few experimental studies were conducted for the elastic and mechanical characterization of carbon nanostructures. For instance, Treacy et. al. (1996) reported Young's modulus of CNTs with a value ranging from 1.06 to 3.7 TPa using a transmission electron microscope. Due to the experimental difficulties involved in the direct measurement at the nanoscale level and in the physical characterisation of these nanomaterials, the theoretical modelling techniques are found to be quite efficient and appropriate alternatives. The different theoretical techniques include quantum mechanics calculations, molecular statics/molecular dynamics (MS/MD) simulations, continuum models and multiscale modelling methods. The atomistic simulations based on quantum mechanics using first-principles calculations, density functional theory (DFT) and ab initio study are considered the most accurate methods among the different theoretical techniques. However, their applications are suitable for systems with a few hundred atoms only due to the requirement of high computational time and power. Contrary to this, atomistic simulations based on MS/MD study can handle systems which may require significant computational resources. It is crucial to note that the accuracy of simulations based on MS/MD study primarily depends upon the proper parameterization of interatomic potentials governing the atomic interactions. The popular interatomic potentials for carbon-based nanomaterials are (i) Tersoff potential (Tersoff, 1989), MM3 potential (Allinger et al., 1989), first and second-generation reactive bond order potential (REBO- I & II) (Brenner, 1990; Brenner 2002), and Tersoff-Brenner potential with revised parameters (Singh, 2021). The results observed using these interatomic potentials are found to be underestimated and overestimated when compared to available DFT calculations. For instance, the Brenner potential underestimates the tensile stiffness (_˜236 nN/nm) and where parameters proposed by Singh (2021) overestimate the bending stiffness (_˜0.42 nNnm) of graphene sheet in comparison to values of _˜350 nN/nm and _˜0.256 nNnm, respectively using DFT based models (Shao et al., 2012; Zhang et al., 2011). Keeping in view the same, the present work involves the investigation of elastic properties of the graphene sheet using recalibrated empirical parameters

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and its mechanical response under transversely distributed load at different finite temperatures. An atomistic continuum-coupled multiscale approach is used to integrate the atomic level deformations (bond lengths, bond angles) to a continuum scale through quadratic-type Cauchy-Born (Zhang et al., 2002). The cohesive interactions between the carbon atoms are modelled through Tersoff-Brenner interatomic potentials by accounting for the effects of dihedral energy terms in the constitutive model (Singh, 2018). The derived stress/moments resultants and tangent constitutive matrix are embedded in the Gauss-quadrature numerical integration of elemental level governing equations of finite element formulation. Both material and Green-Lagrange geometric nonlinearities are considered in the present study. The results of the recalibrated interatomic potentials are tested for different numerical problems such as investigating the elastic properties and bending response of graphene sheets at finite temperatures under different boundary conditions. The results are compared with available DFT-based models and with those obtained using other interatomic potentials (Brenner, 1990; Singh, 2021). It is observed that the proposed set of empirical parameters predicts better results compared to other interatomic potentials for carbon-based nanomaterials and close to DFT studies reported in the literature. *Keywords*: Multiscale modelling, Elastic properties, Bending response, Finite element method, Graphene, Finite temperature.