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Dynamic instability of graphene sheets subjected to in-plane compressive loads involving nonlinearities at finite temperature using a multiscale model

Akash Raikwar[1], Sandeep Singh[2]

[1] Department of Mechanical Engineering, Indian Institute of Technology Indore, Indore, 453552, Madhya Pradesh, India, India. akashraikwar92@gmail.com
[2] Department of Mechanical Engineering, Indian Institute of Technology Indore, Indore, 453552, Madhya Pradesh, India, India. mechmehal@gmail.com

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Extended Abstract

Abstract

Among various nanomaterials synthesized over the last three decades, graphene has attracted the scientific community due to its distinctive properties and biomedical compatibility. Graphene is used in various fields, including nanosensors, nanoresonators, medical treatment/diagnosis equipment, and nanocomposites, which may be subjected to combined static and periodic axial loads. These nanomaterials under such loading conditions may lose stability and become dynamically unstable. Therefore, it is crucial to study the instability characteristics of graphene under these loading conditions to ensure the safe and sustainable design of nanodevices. Theoretical techniques such as atomistic simulations and continuum modeling are commonly used methods for the mechanical characterization of these nanomaterials. Atomistic simulations based on density functional theory, ab initio studies, and molecular statics/dynamics simulations are the most accurate and best suited for systems with a small number of atoms. Continuum modelling methods can handle large structures, in which the discrete nature of lattice is neglected, and material nonlinearities due to bond interactions cannot be incorporated until hyperelastic models are developed. Multiscale modelling methods based on Cauchy-Born coupling are another alternative for larger systems, capable

of preserving the accuracy of results (close to DFT calculations) by accounting for nonlinear atomic interactions and maintaining computational efficiency. Using these methods, several studies on bending, static buckling, and free vibration analyses of graphene have been reported. In dynamic analysis, the instability behaviour of viscoelastic graphene sheets was investigated using nonlocal strain-gradient theory [1, 2]. To the best of the authors' knowledge, no work has been reported on the dynamic instability of graphene sheets accounting for material and geometric nonlinearities at finite temperature using a multiscale model. Owing to this, the present work deals with the instability analysis of graphene sheets subjected to periodic in-plane compressive load, including material and geometric nonlinearities, using a multiscale model. In present atomistic-continuum-coupled framework, interatomic interactions are modelled using the Tersoff-Brenner potential [3, 4], which includes dihedral energy term at finite temperature. The strain energy density function and constitutive relations are derived by coupling atomic-level deformations to continuum scale using a temperature-based quadratic-type Cauchy-Born rule [5, 6]. The governing equation of motion is formulated using Hamilton's energy principle, and spatial approximation of graphene at the continuum scale is obtained through finite element method, incorporating geometric nonlinearities in von Karman and Green-Lagrange sense, as well as material nonlinearity due to nonlinear interatomic interactions. The dynamic instability behaviour of graphene sheets is described through ordinary differential equations (Mathieu-Hill type equation), and the boundaries of the instability zones are determined using Bolotin's method [7]. The results of the present finite element model are found in close agreement with those reported in existing literature [8]. The dynamic instability zones of graphene sheets obtained using the recalibrated set of empirical parameters are also compared with those obtained with earlier sets [4, 9]. The effect of geometric properties, dihedral energy term, empirical parameters, boundary conditions, and material and geometric nonlinearities on the dynamic instability zones of GSs will be presented in the full-length manuscript.

Keywords:

Dynamic instability Multiscale model Nonlinearity Graphene Finite temperature