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Modal analysis of graphene-based structures for large deformations, contact and material nonlinearities

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ABSTRACT

The nonlinear frequencies of pre-stressed graphene-based structures, such as flat graphene sheets and carbon nanotubes, are calculated. These structures are modeled with a nonlinear hyperelastic shell model. The model is calibrated with quantum mechanics data and is valid for high strains. Analytical solutions of the natural frequencies of various plates are obtained for the Canham bending model by assuming infinitesimal strains. These solutions are used for the verification of the numerical results. The performance of the model is illustrated by means of several examples. Modal analysis is performed for square plates under pure dilatation or uniaxial stretch, circular plates under pure dilatation or under the effects of an adhesive substrate, and carbon nanotubes under uniaxial compression or stretch. The adhesive substrate is modeled with van der Waals interaction (based on the Lennard-Jones potential) and a coarse grained contact model. It is shown that the analytical natural frequencies underestimate the real ones, and this should be considered in the design of devices based on graphene structures.

1. Introduction

The high mechanical strength [1], thermal conductivity [2,3] and electrical conductivity [4–6] of graphene have received much interest in recent years. The vibrational properties (i.e. frequencies and mode shapes) of graphene play an important role in analysis and design of graphene-based sensors and resonators. There are several studies on the development of new sensors using graphene-based structures [7,8]. For example, graphene can be used in oscillators and electro-mechanical resonators [9–11].

The effect of pre-stressing on the vibrational properties of graphene have been investigated by Gupta and Batra [12] and Mustapha [13], while foundation effects have been studied by Murmu and Pradhan [14], Lee and Chang [15], Lee et al. [16] and Mustapha [13]. Sadeghi and Naghdabadi [17] use an atomistic method at the temperature of 19.3 K to calculated the nonlinear frequencies of graphene sheets. The nonlinear vibration of sandwiches with graphene and piezoelectric layers have been modeled by Li et al. [18]. Favata and Podio-Guidugli [19] propose an orthotropic shell model for CNTs. Ansari et al. [20] use a nonlocal shell theory to include the size-effects in the calculation of the frequencies of single and double walled carbon nanotubes. Hussain et al. [21] obtain the natural frequencies of single walled carbon nanotubes by using Donnell thin shell theory. Li et al. [22] used a nonlinear finite element (FE) method to analyze large deformations and obtain the nonlinear frequencies of graphene membranes for nanomechanical applications. A linear material model works well for infinitesimal strains. But, the

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List of important symbols

$\mathbf{1}$	identity tensor in $\mathbb{R}^3$
$\boldsymbol{a}_\alpha$	co-variant tangent vectors of $\mathscr{S}$; $\alpha = 1,2$
$a_{\alpha\beta}$	co-variant components of the metric tensor of $\mathscr{S}$
$a^{\alpha\beta}$	contra-variant components of the metric tensor of $\mathscr{S}$
$\boldsymbol{a}^\alpha$	contra-variant tangent vectors of $\mathscr{S}$; $\alpha = 1,2$
$\mathscr{S}_0$	reference configuration of the manifold
$\mathscr{S}$	current configuration of the manifold
$b_{\alpha\beta}$	co-variant components curvature tensor of $\mathscr{S}$
$\boldsymbol{E}^{(0)}$	logarithmic surface strain
$\boldsymbol{E}^{(0)}_{\text{dev}}$	deviatoric part of the logarithmic strain
$\Gamma^\gamma_{\alpha\beta}$	Christoffel symbols of the second kind
H	mean curvature of $\mathscr{S}$
J	surface area change of $\mathscr{S}$
κ	Gaussian curvature of $\mathscr{S}$
κ_1, κ_2	principal curvatures of $\mathscr{S}$
k_{p}	penalty parameter
λ	square root of the stretch ratio, i.e. $\sqrt{\lambda_1/\lambda_2}$
λ_1, λ_2	principal surface stretches of $\mathscr{S}$
$\boldsymbol{n}$	surface normal of $\mathscr{S}$
ξ^α	parametric coordinates; $\alpha = 1,2$
$\boldsymbol{X}$	reference position of the manifold
$\boldsymbol{x}$	current position of the manifold

mechanical properties of graphene vary in large strains. Hence, nonlinear hyperelastic material models should be used to model the material behavior in large strains [23,24]. Thermal vibration of rectangular, circular and annual graphene sheets are studied by Kumar et al. [25], Wang and Hu [26], Mohammadi et al. [27] and Biswal and Rao [28]. The vibrational properties of multi-layer circular and rectangular graphene sheets are obtained by Kitipornchai et al. [29] and Allahyari and Fadaee [30]. Ke et al. [31] has modeled the size-effects on vibrational properties of rectangular plates. The vibrational properties of a graphene sheet can be calculated by molecular mechanics [32] and molecular dynamics [33]. Strozzi et al. [34] have calculated the natural frequencies and mode shapes of CNTs by analytical approaches and validated them by experimental, atomistic and FE results. Arghavan and Singh [35] have computed the natural frequencies, mode shapes and force vibration of CNTs.

All mentioned continuum models are limited by linear elastic material behavior. However, graphene shows nonlinear and anisotropic behavior under large deformations [23]. Kumar and Parks [23] develop a hyperelastic material model for graphene that is based on three strain invariants and several unknown material constants. Those constants need to be determined from appropriate tests. A suitable approach for this are ab-initio calculations. They are more accurate than molecular dynamics simulations, and they do not have difficulties with applying homogeneous strain states as is the case in experiments. In addition, atomistic potentials [36,37] underestimate elastic modulus [38]. A wide range for the elastic modulus for graphene have been reported by Cao [39] that under or overestimate experimental and ab-initio results [40,41]. It should be mentioned that Gupta and Batra [12] used the MM3 potential and obtained a very close results to experimental and ab-initio results, but further investigations should be considered for large deformations. The nonlinear material model of Ghaffari et al. [24] is used here to remedy these deficiencies and the consistency of the model with experimental and ab-initio results is verified analytically. Neglecting the bending stiffness can result in large frequency errors for low pre-tension and/or small sheets. However, the bending stiffness can be neglected for a large graphene sheet under significant pre-tension [24,42].

Isogeometric analysis (IGA) is a new computational technique that connects CAD and FE analysis [43]. Recently, an isogeometric FE formulation has been developed by Sauer et al. [44] for the analysis of liquid and solid membranes based on inherent curvilinear coordinates. It has been extended to anisotropic membranes by Roohbakhshan et al. [45] and rotation-free shells by Sauer and Duong [46] and Duong et al. [47]. This shell formulation has been applied to biomaterials and composites by Roohbakhshan and Sauer [48,49] and to graphene by Ghaffari et al. [24]. The latter work uses the anisotropic membrane model of Kumar and Parks [23] and extends it to a shell formulation by including the Canham model [50]. This new model can simulate the anisotropic behavior of graphene-based structures under large deformation and it has been used to simulate indentation and peeling of graphene sheets and torsion and bending of carbon nanotubes (CNT). Thermal fluctuation are not considered in the current study. But the proposed model does allow for an extension to those. Thermal fluctuations can result in structural softening, but they can be suppressed with small pre-strains above 1% [51,52]. Therefore Kumar et al. [53] and Ghaffari et al. [24] obtain similar material properties as the experimental results of Lee et al. [41] by using a hyperelastic constitutive law that disregards thermal fluctuations.