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A new efficient hyperelastic finite element model for graphene and its application to carbon nanotubes and nanocones

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ABSTRACT

A new hyperelastic material model is proposed for graphene-based structures, such as graphene, carbon nanotubes (CNTs) and carbon nanocones (CNC). The proposed model is based on a set of invariants obtained from the right surface Cauchy-Green strain tensor and a structural tensor. The model is fully nonlinear and can simulate buckling and postbuckling behavior. It is calibrated from existing quantum data. It is implemented within a rotation-free isogeometric shell formulation. The speedup of the model is 1.5 relative to the finite element model of Ghaffari et al. [1], which is based on the logarithmic strain formulation of Kumar and Parks [2]. The material behavior is verified by testing uniaxial tension and pure shear. The performance of the material model is illustrated by several numerical examples. The examples include bending, twisting, and wall contact of CNTs and CNCs. The wall contact is modeled with a coarse grained contact model based on the Lennard-Jones potential. The buckling and post-buckling behavior is captured in the examples. The results are compared with reference results from the literature and there is good agreement.

1. Introduction

Graphene and graphene-based structures such as carbon nanotubes (CNT) and carbon nanocones (CNC) [3–8] have unique mechanical [9–11], thermal [12–15] and electrical [16–19] properties. They can be used in sensors [20], energy storage devices [21], healthcare [22] and as a coating against corrosion [23]. They are used to improve mechanical, thermal and electrical properties of composites [24–28]. CNTs and CNCs can be obtained by rolling of a graphene sheet [29,30]. Robust and efficient analysis methods should be developed in order to reduce the time and cost of design and production.

There are several different approaches in the literature for modeling graphene. One is based on the Cauchy-Born rule applied to intermolecular potentials. Arroyo and Belytschko [31] propose an exponential Cauchy-Born rule to simulate the mechanical behavior of CNTs. Guo et al. [32] and Wang et al. [33] use a higher order Cauchy-Born rule to model CNTs. Yan et al. [34] use a higher order gradient continuum theory[1] and the Tersoff-Brenner potential to obtain the properties of single-walled CNCs. A second approach is based on the quasi-continuum method [35]. Yan et al. [36] apply the quasi-continuum to simulate buckling and post-buckling of CNCs. A temperature-related quasi-continuum model is proposed by Wang et al. [37] to model the behavior of CNCs under axial compression. A third approach is based on classical continuum material models. Those are popular for graphene in the context of isotropic linear material models. Firouz-Abadi et al. [38] obtain the natural frequencies of nanocones by using a nonlocal continuum theory and linear elasticity assumptions. Their work is extended to the stability analysis under external pressure and axial loads by Firouz-Abadi et al. [39] and the stability analysis of CNCs conveying fluid by Gandomani et al. [40]. Lee and Lee [29] use the finite element (FE) method to obtain the natural frequencies of CNTs and CNCs. The interaction of carbon atoms is modeled as continuum frame elements. Graphene has an anisotropic behavior under large strains. There are several continuum material models for anisotropic behavior of graphene. Sfyris et al. [41] and Sfyris et al. [42] use Taylor expansion and a set of invariants to propose strain energy functionals for graphene based on its lattice structure. Delfani et al. [43] and Delfani and Shodja [44,45] use a similar Taylor expansion for the strain energy and apply symmetry operators to the elasticity tensors in order to reduce the number of independent variables. Nonlinear membrane material models are proposed by Xu et al. [46] and Kumar and Parks [2]. They use ab-initio results to calibrate their models. The model of Kumar and Parks [2] is

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[1] This method is similar to the Cauchy-Born rule.

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based on the logarithmic strain and the symmetry group of the graphene lattice [47–49]. This symmetry group reduces the number of parameters in the model of Xu et al. [46] by a half. The membrane model of Kumar and Parks [2] is extended by Ghaffari et al. [1] to a FE shell model by adding a bending energy term. Such FE models tend to be much more efficient than all-atom models: Ghaffari et al. [1] study the indentation of a square sheet with length 550 nm and found that the FE model requires 122,412 nodes, while the corresponding atomistic system has about 12 million atoms, i.e. about 100 times more. Ghaffari and Sauer [50] conduct a modal analysis of graphene sheets and CNTs under various nonlinearities. A finite thickness for graphene is considered in the most of the mentioned works. Thus, an integration through the thickness needs be conducted to obtain the bending stiffness. The finite thickness assumption can be avoided by writing the strain energy density per unit area of the surface as in Ghaffari et al. [1], Kumar and Parks [2], Xu et al. [46] and Ghaffari and Sauer [50].

The material model of Ghaffari et al. [1] and the proposed new material model in the current paper are implemented in the rotation-free isogeometric finite shell element formulation of Sauer et al. [51], Sauer and Duong [52] and Duong et al. [53]. This formulation is based on displacement degree of freedoms (DOFs) and avoids rotation DOFs through the use of Kirchhoff-Love kinematics and NURBS discretization [54]. The avoidance of rotational DOFs increases efficiency and simplifies the formulation [55]. A material model based on continuum mechanics is necessary for the development of a shell formulation. The model of Ghaffari et al. [1] is quite complicated and computationally expensive. It is based on a logarithmic strain formulations, which requires using chain rule and summation over fourth and sixth order tensors (see Sec. 2 for more details). This high computational cost is avoided in the new proposed material model.

In summary, the novelties of the current work are:

- It can be used both in curvilinear and Cartesian shell formulations.
- It is simpler to implement and thus 1.5 faster[2] than the model of Ghaffari et al. [1].
- It is fully nonlinear and can capture buckling and post-buckling behavior.
- It is suitable to simulate and study carbon nanocones under large deformations.
- It is applied to simulate contact of CNTs and CNCs with a Lennard-Jones wall.
- The latter example demonstrates that CNCs are ideal candidates for AFM tips.

The remainder of this paper is organized as follows: In Sec. 2 the finite element formulation is summarized and the development of a new material model is motivated. In Sec. 3, a new hyperelastic shell material model for graphene-based structures is proposed. In Sec. 4, the model is verified and compared with the model of Ghaffari et al. [1] considering various test cases. Sec. 5 presents several numerical examples involving buckling and contact of CNTs and CNCs. The behavior is compared with molecular dynamics and quasi-continuum results from the literature. The paper is concluded in Sec. 6.

2. Finite element formulation for Kirchhoff-Love shells

It this section, the discretized weak form is summarized and the development of a new material model is motivated. The Cauchy stress tensor of Kirchhoff-Love shell theory can be written as[3] [52]

$$\boldsymbol{\sigma}_{\mathrm{KL}} = N^{\alpha\beta}\,\boldsymbol{a}_\alpha \otimes \boldsymbol{a}_\beta + S^\alpha\,\boldsymbol{a}_\alpha \otimes \boldsymbol{n}\,, \tag{1}$$

where

$$N^{\alpha\beta} = \sigma^{\alpha\beta} + b^\beta_\gamma\, M^{\gamma\alpha} \tag{2}$$

and

$$S^\alpha = -M^{\beta\alpha}_{;\beta} \tag{3}$$

are the components of the membrane stress and out-of-plane shear. Here, ";" denotes the co-variant derivative, and $\boldsymbol{a}_\alpha$ and $\boldsymbol{n}$ are the tangent and normal vectors of the shell surface in the current configuration, see Appendix A. For hyperelastic materials, $\sigma^{\alpha\beta}$ and $M^{\alpha\beta}$ are given by

$$\sigma^{\alpha\beta} = \tau^{\alpha\beta}/J\,, \quad \tau^{\alpha\beta} = \frac{\partial W}{\partial a_{\alpha\beta}}\,, \tag{4}$$

$$M^{\alpha\beta} = M_0^{\alpha\beta}/J\,, \quad M_0^{\alpha\beta} = \frac{\partial W}{\partial b_{\alpha\beta}}\,, \tag{5}$$

where W is the strain energy density per unit area of the initial configuration, and $a_{\alpha\beta}$ and $b_{\alpha\beta}$ are the covariant components of the metric and curvature tensor [52]. b^β_α in Eq. (2) are the mixed components of the curvature tensor (see Appendix A). The discretized weak form for Kirchhoff-Love shells can be written as [53].

$$\sum_{e=1}^{n_{\mathrm{el}}} (G^e_{\mathrm{int}} + G^e_{\mathrm{c}} - G^e_{\mathrm{ext}}) = 0\,, \forall\ \delta\mathbf{x}_e \in \mathcal{V}\,, \tag{6}$$

where $\delta\mathbf{x}_e$ is the variation of the element nodes, n_{el} is the number of elements and $\mathcal{V}$ is the space of admissible variations. G^e_{c} and G^e_{ext} are related to contact and external forces [1]. G^e_{int} is the internal virtual work of element Ω^e_0 defined as

$$G^e_{\mathrm{int}} \coloneqq \delta\mathbf{x}_e^{\mathrm{T}}\,(\mathbf{f}^e_{\mathrm{int}\tau} + \mathbf{f}^e_{\mathrm{int}M})\,, \tag{7}$$

with

$$\begin{aligned} \mathbf{f}^e_{\mathrm{int}\tau} &= \int_{\Omega^e_0} \tau^{\alpha\beta}\,\mathbf{N}^{\mathrm{T}}_{,\alpha}\,\boldsymbol{a}_\beta\ \mathrm{d}A\,, \\ \mathbf{f}^e_{\mathrm{int}M} &= \int_{\Omega^e_0} M_0^{\alpha\beta}\,\widetilde{\mathbf{N}}^{\mathrm{T}}_{;\alpha\beta}\,\boldsymbol{n}\ \mathrm{d}A\,, \end{aligned} \tag{8}$$

where $\mathbf{N}$, $\mathbf{N}_{,\alpha}$ and $\widetilde{\mathbf{N}}_{;\alpha\beta}$ are the shape function arrays of the element that are defined as

$$\begin{aligned} \mathbf{N} &:= [N_1\,\mathbf{1}, N_2\,\mathbf{1}, \dots, N_{n_e}\,\mathbf{1}]\,, \\ \mathbf{N}_{,\alpha} &:= [N_{1,\alpha}\,\mathbf{1}, N_{2,\alpha}\,\mathbf{1}, \dots, N_{n_e,\alpha}\,\mathbf{1}]\,, \\ \widetilde{\mathbf{N}}_{;\alpha\beta} &:= \mathbf{N}_{,\alpha\beta} - \Gamma^\gamma_{\alpha\beta}\,\mathbf{N}_{,\gamma}\,, \\ \mathbf{N}_{,\alpha\beta} &:= [N_{1,\alpha\beta}\,\mathbf{1}, N_{2,\alpha\beta}\,\mathbf{1}, \dots, N_{n_e,\alpha\beta}\,\mathbf{1}]\,. \end{aligned} \tag{9}$$

Here, "$\bullet, \alpha$" denotes the parametric derivative $\partial\bullet/\partial\xi^\alpha$, and $\mathbf{1}$ and N_i are the three dimensional identity tensor and the NURBS shape functions [54]. $\tau^{\alpha\beta}$ and $M_0^{\alpha\beta}$ need to be specified for the finite element implementation through Eqs. (4) and (5). $\tau^{\alpha\beta}$ corresponds to the components of the in-plane Kirchhoff stress tensor $\boldsymbol{\tau} = J\boldsymbol{\sigma}$. They are equal to the components $S^{\alpha\beta}$ of the in-plane second Piola-Kirchhoff (2.PK) stress $\boldsymbol{S} = S^{\alpha\beta}\,\boldsymbol{A}_\alpha \otimes \boldsymbol{A}_\beta$ since

$$\tau^{\alpha\beta} = \boldsymbol{a}^\alpha \cdot \boldsymbol{\tau}\boldsymbol{a}^\beta = \boldsymbol{A}^\alpha \cdot \boldsymbol{S}\boldsymbol{A}^\beta = S^{\alpha\beta}\,, \tag{10}$$

due to $\boldsymbol{\tau} = \boldsymbol{F}\,\boldsymbol{S}\,\boldsymbol{F}^{\mathrm{T}}$ and $\boldsymbol{a}^\alpha = \boldsymbol{F}^{-\mathrm{T}}\boldsymbol{A}^\alpha$. Here $\boldsymbol{F} = \boldsymbol{a}_\alpha \otimes \boldsymbol{A}^\alpha$ is the surface deformation gradient. $\boldsymbol{A}_\alpha$ ($\boldsymbol{a}_\alpha$) and $\boldsymbol{A}^\alpha$ ($\boldsymbol{a}^\alpha$) are the tangent and dual vectors in the reference (current) configuration (see Appendix A). Following Eq. (4), the 2.PK stress $\boldsymbol{S}$ can also be written as

$$\boldsymbol{S} = 2\frac{\partial W}{\partial \boldsymbol{C}}\,, \tag{11}$$

where $\boldsymbol{C} = \boldsymbol{F}^{\mathrm{T}}\,\boldsymbol{F}$ is the right surface Cauchy-Green deformation tensor. $\boldsymbol{S}$ can be computed by using Eq. (11). However, if the model is developed

[2] In computing the stiffness matrix.

[3] Subscript KL is added here to distinguish the total Cauchy stress $\boldsymbol{\sigma}_{\mathrm{KL}}$ from its membrane contribution $\boldsymbol{\sigma} \coloneqq \sigma^{\alpha\beta}\boldsymbol{a}_\alpha \otimes \boldsymbol{a}_\beta$.