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Curvature dependent surface energy for free standing monolayer graphene: Geometrical and material linearization with closed form solutions

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ABSTRACT

Continuum modeling of a free-standing graphene monolayer, viewed as a two dimensional 2-lattice, requires specifications of the components of the shift vector that act as an auxiliary variable. The field equations are then the equations ruling the shift vector, together with momentum and moment of momentum equations. To introduce material linearity energy is assumed to have a quadratic dependence on the strain tensor, the curvature tensor, the shift vector, as well as to combinations of them. Hexagonal symmetry then reduces the overall number of independent material constants to nine. We present an analysis of simple loading histories such as axial, biaxial tension/compression and simple shear for a range of problems of increasing difficulty for the geometrically and materially linear case. We start with the problem of in-plane motions only. By prescribing the displacement, the components of the shift vector are evaluated. This way the field equations are satisfied trivially. Out-of-plane motions are treated as well; we assume in-plane tension/compression that leads to buckling/wrinkling and solve for the components of the shift vector as well as the function present in buckling's modeling. The assumptions of linearity adopted here simplifies the analysis and facilitates analytical results.

1. Introduction

Graphene is a two dimensional sheet that constitutes the building unit of all graphitic forms of matter, such as graphite, carbon nanotubes and carbon fibers. Lee, Wei, Kysar, and Hove (2008) use a nanoindentation experiment in an atomic force microscope to measure the elastic properties and intrinsic strength of graphene. Using second order elasticity they evaluate Young's modulus, the second order elastic constant as well as graphene's breaking strength. Their analysis models graphene as an isotropic body in one dimension, due to symmetry in the loading.

Generalization of their approach to two dimensions is done by Cadelano, Palla, Giordano, and Colombo (2009). These authors view graphene as an isotropic body and they utilize an energy cubic in strains (second order elasticity in words of Rivlin (1963) and Murnaghan (1951)). Utilizing tight-binding atomistic simulations they calculate Young's modulus, Poisson ratio as well as higher order constants for graphene. While interesting and novel their approach is, it lacks the treatment

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of bending effects. It also models graphene as an isotropic body; dependence on the zig-zag and the armchair direction is not incorporated to the constitutive law through dependence on a structural tensor. Fifth order models for graphene are presented by Wei, Fragneand, Marianetti, and Kysar (2009). These authors utilize an energy that depends on strains of the fifth order. Using density functional theory for simple loading histories they evaluate higher order constants for graphene. Their approach does not include bending effects neither anisotropy; graphene is modeled as an isotropic body.

To introduce anisotropy for a free-standing monolayer graphene as well as for incorporating bending effects we recently proposed a finite elasticity model for graphene (Sfyris & Galiotis, in press). Viewing graphene as a two dimensional 2-lattice, we obtain its arithmetic symmetries (Fadda & Zanzotto, 2000; Pitteri & Zanzotto, 2003). Confined to weak transformation neighborhoods (Ericksen, 1979; Pitteri, 1984, 1985) and invoking the Cauchy–Born rule (Ericksen, 2008), we arrive to the classical symmetries continuum mechanics uses. We lay down the complete and irreducible representation (Zheng, 1994; Zheng, 1997) for an energy depending on the Cauchy–Green deformation tensor, the curvature tensor as well as the shift vector. Cauchy–Green's surface tensor is a measure of in-plane motions, the curvature tensor measures out-of-plane motions, while dependence on the shift vector stems from viewing graphene as a 2-lattice. Dependence of the energy on the curvature tensor is motivated by the fundamental works of Murdoch and Cohen (1979) and Steigmann and Ogden (1999). We note that E and Ming (2007) report dependence on the energy on the shift vector for graphene as well. The need for introducing the shift vector as an independent variable in continuum modeling of graphene is also apparent in the approach of Zhou and Huang (2008). Additionally, the corrugation vector that is introduced in the homogenization scheme of Davini (2014) is very close in spirit to the shift vector of our approach.

In Sfyris and Galiotis (in press) anisotropy is introduced through a sixth-order structural tensor which describes the zig-zag and armchair directions of graphene. This model predicts 13 independent material moduli, in contrast to the seemingly endless Taylor expansion models in terms of the strains adopted at third and fifth order elasticity (Cadelano et al., 2009; Wei et al., 2009). It is worth mentioning that bending effects are considered in the work of Wei, Wang, Wu, Yang, and Dunn (2013). These authors utilize an energy depending on one in-plane measure and two out-of-plane: bending rigidity and Gaussian bending stiffness. These two quantities are work conjugate to the mean and the Gaussian curvature, respectively. Using density functional calculations for single wall carbon nanotubes, they evaluate bending rigidity and Gaussian bending stiffness for a monolayer graphene. Their calculations are based on assuming infinitely long constant radius carbon nanotubes, so they can relate energy per atom of the carbon nanotube to the energy per atom of the graphene sheet.

Another interesting study incorporating bending effects is that of Lu and Huang (2009). Using von-Karman kinematical assumptions together with a measure of curvature they provide stress–strain curves using the virial theorem and molecular calculations. In-plane constants are calculated together with bending stiffness which is work-conjugate to curvature. Mixed atomistic-continuum methods are reported by Arroyo and Belytschko (2002, 2004) based on the earlier notion of the quasicontinuum (Tadmor, Ortiz, & Phillips, 1996; Tadmor, Smith, Bernstein, & Kaxiras, 1999). Arroyo and Belytschko provide a finite continuum theory derived from interatomic potential; the material moduli are expressed in an explicit form in terms of the interatomic potential. They also provide a generalization of the Cauchy–Born rule appropriate for modeling surfaces.

The present work is the linearized counterpart of our previous contributions (Sfyris & Galiotis, in press; Sfyris, Sfyris, & Galiotis, in press). Linearization is understood at two levels: material linearity as well as geometrical linearity. Geometrical linearity means confinement to small deformations; mathematically this means that higher order terms of the displacement gradient are negligible. Material linearity means that energy is a quadratic function of the strain tensor, the curvature tensor, the shift vector, as well as to combinations of them. Anisotropy is introduced by requiring the tensors of material constants to be independent under rotations by 60°: graphene's symmetry. This reduces the independent moduli to 9.

We then examine what this framework gives for simple loading histories. Initially, we treat the case of in-plane deformations only. We thus disregard out-of-plane effects setting the curvature tensor equal to zero. In this case we need not take into account the equations of moment of momentum. Assuming the form of the displacement components that correspond to axial tension/compression, we solve for the components of the shift vector. It turns out that shift's vector components are homogeneous; they depend on the loading parameter as well as on the material constants. Same homogeneity of the shift vector components holds true for the case of biaxial tension/compression and for the simple shear case. Analogous procedure is done in the nonlinear counterpart of the present theory (Sfyris & Galiotis, in press; Sfyris et al., in press). Results there (Sfyris et al., in press) are obtained using the same procedure, nevertheless they are much more complicated than the results of this study. This is due to the linearity assumptions that simplify the analysis here severely. This is apparent especially in the equations describing the shift vector. In the linearized problem they are algebraic equations of the first order, while for the nonlinear case they are algebraic equations of the fifth order. This order reduction simplifies the analysis and facilitates analytical results.

This difference in the algebraic nature of the equations ruling the shift vector permit closed form solutions for the buckling/wrinkling case as well, in contrast to the nonlinear case. By making a suitable assumption for the buckling mode (Puntel, Deseri, & Fried, 2011), we solve for the components of the shift vector. These expressions are substituted to one of the momentum equation. From this equation we obtain the form the function present in the buckling mode has. Then, this final expression is substituted to all the other field equations thereby rendering constraints that the material parameters, the loading constant and the constants of integration should satisfy so that all field equations are satisfied.

The paper is structured as follows. Section 2 reminds the modeling of graphene as a 2-lattice, as well as the passage to the continuum theory. The field equations as well as the constitutive laws that introduce material linearity are given there. Section 3 deals with evaluating the number of independent constants for the constitutive law. Following standard