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Curvature dependent surface energy for a free standing monolayer graphene: Some closed form solutions of the non-linear theory

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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. 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. We start by laying down the equations of a simplified model which can still capture bending effects. Initially, we ignore out of plane deformations. For this case, we solve analytically the equations ruling the auxiliary variables in terms of the shift vector; these equations are algebraic when the loading is specified. As a next step, still working on the simplified model, out-of-plane deformations are taken into account and the equations complicate dramatically. We describe how wrinkling/buckling can be introduced into the model and apply the Cauchy–Kowalevski theorem to get existence and uniqueness in terms of the shift vector for some characteristic cases. Finally, for the treatment of the most general problem, we classify the equations of momentum and give conditions for the Cauchy–Kowalevski theorem to apply.

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. For modeling graphene many different approaches at different scales can be found in the literature ranging from first principle calculations [14,16], atomistic calculations [36,37] and continuum mechanics [4,35,17]. Furthermore, mixed atomistic formulations with finite elements are being reported for graphene [3,2,33] based on the earlier notion of a quasi-continuum [31,30].

The mathematical theory of surface elasticity is established by Gurtin and Murdoch [13]. This pure membrane approach is incapable of taking into account out of plane deformations. Generalization of this framework to take into account bending effects is given by Steigmann and Ogden [29]. These authors propose a surface energy which depends, apart from a surface measure of the deformation, on the curvature tensor as well, in similar trends with previous works [7,18]. The curvature tensor is a measure of the out-of-plane deformations that the surface suffers and this way bending effects are introduced into the framework. Steigmann and Ogden, in the same work [29], also describe a rigorous way for defining the notion of material symmetry for curvature dependent surface energies in line with Noll's fundamental work [20]. Implications of such energies for nanostructures are studied by Chhapadia et al. [5].

In a recent work [27] we adopt the framework of Steigmann and Ogden [29] and utilize a surface energy function depending on three arguments for a free standing monolayer graphene. The first one is an in-surface strain measure describing changes happening on the surface. The second argument is the curvature tensor which describes the out of surface motions and introduces bending effects into the model. The third argument is the shift vector (SV) which connects the two simple lattices when graphene is seen as a monoatomic 2-lattice. The motivation for assuming the shift vector as an independent variable comes from the work of Pitteri and Zanzotto ([24] and references therein). These authors utilize an energy function depending on the shift vector when modeling a multilattice. We note that for graphene a similar assumption is made by E and Ming [8].

Using the above surface energy, calculation of the surface stress and the surface couple stress tensor at the continuum level is possible. This way the number of independent relations to be observed in experiments becomes available; these are 13 independent material parameters, in the simplest expression of the model. The surface stress tensor is responsible for in-plane motions while out-of-plane motions are due to the surface couple stress tensor. The elasticities of the material can then be calculated

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and one may also lay down the field equations characterizing the problem: the momentum, the moment of momentum equation as well as an equation for the evaluation of the shift vector.

Being aware of the molecular theories of elasticity, where the energy depends on the lattice vectors, we stress that this analysis [27] is confined to weak transformation neighborhoods [22]. This way the classical theory of invariants for continuum mechanics can be utilized, so we can obtain the invariants of the surface energy function. This is compatible with molecular theories when the Cauchy–Born rule is enforced, and also compatible with the global theory of Ericksen [10,12,9].

In this respect, we present the key findings of [27] which is the theoretical background for this work. When graphene is viewed as a monoatomic 2-lattice, its arithmetic symmetries can be deduced from the fundamental work of Fadda and Zanzotto [11]. To arrive at the classical symmetries, those employed by continuum mechanics, the analysis should be confined to weak transformation neighborhoods [24,22,23]. Also the Cauchy–Born rule [10] should be enforced. Under these assumptions, we work at the continuum level with an energy depending on three arguments: an in-surface strain measure, the curvature tensor and the shift vector. Since symmetries are now those employed by continuum mechanics, we are able to deduce the complete and irreducible representation of graphene's energy. This way calculation of the surface stress and the surface couple stress tensor becomes possible. These tensors participate to the field equations ruling the problem: the momentum, the moment of momentum equation and the shift vector. In Section 3 we derive the field equations in terms of the kinematic variables: the position vector of the points of the surface, the components of the curvature tensor and the components of the shift vector. These equations are designed for the geometrical and materially non-linear case.

The need for describing graphene using non-linear elasticity is based on graphene's very high strength. Efficient computational methods, such as ab initio and/or molecular mechanics, report that graphene can deform elastically at tension up to more than 20 per cent of strain (see e.g. [16]). Compression can also reach such high levels, even though buckling occurs at lower strains; this buckling is elastic so graphene can accommodate even higher compressive strains in an elastic manner (see e.g. [40]). The present approach is designed as the theoretical backbone, at the continuum level, of this non-linear behavior graphene shows.

Earlier attempts to use non-linear elasticity for graphene can be found to the work of Lee et al. [15] who 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 et al. [4]. These authors view graphene as an isotropic body and they utilize an energy cubic in strains (second order elasticity in words of Murnaghan [19] and Rivlin [26]). 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 of bending effects. It also models graphene as an isotropic body; dependence on the zigzag 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 et al. [34]. 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.

At Section 4, a model for the problem is presented, where five (5) out of the thirteen (13) material parameters of the model are set to zero, with the purpose of simplifying the mathematical analysis while capturing bending effects. Initially, by focusing on in-plane motions for simple mechanical loadings, we disregard dependence on the curvature tensor. As an outcome of that, the equation of moment of momentum need not be taken into account. By also assuming that the shape of the body, at the reference state, is a rectangular plate, we examine axial, biaxial tension/compression and simple shear loadings. The strategy consists of assuming the form of the solution for the position vector $\mathbf{x}$ of the surface and seeking for suitable forms of the SV that guarantees fulfillment of the field equations. The outcome consists of expressions for the SV, which is denoted by $\mathbf{p}$ that, in general, depend on the material parameters and the loading constant as well. What allows us to give these closed form solutions is the fact that the equations ruling the auxiliary variables are algebraic and solvable in terms of $\mathbf{p}$.

When out-of-plane motions are taken into account, the field equations of the simplified model become much more complicated. In our model wrinkling/buckling is a product of in-plane mechanical tension/compression. The equations ruling the auxiliary variables are algebraic as previously, but now they are not solvable in a closed form. We describe how wrinkling/buckling can be introduced into the present framework following standard assumptions on the topic [32,25] and write down the field equations describing the problem at hand. More specifically, we treat the case when wrinkling/buckling is a product of tension/compression on the in plane. We note that the different behavior of graphene at tension and compression is not taken into account here, since that would require extension of the model to include this hardening behavior which is beyond the scope of this work. We classify the momentum equation viewed as a system of quasilinear equations for the shift vector and also give conditions for the Cauchy–Kowalevski theorem to apply. This theorem guarantees existence and uniqueness of solutions for the SV; these conditions are expressions in terms of the material parameters and the SV. The presence of the shift vector in such equations results from the fact that momentum equation is a quasilinear system in terms of $\mathbf{p}$. These are the contents of Section 5.

In its most general form, the problem of free standing monolayer graphene sheet under mechanical loading is extremely difficult to tackle analytically; nevertheless, at Section 6 we present and classify the momentum equations and we also give necessary conditions for the Cauchy–Kowalevski theorem to apply. Finally, in Section 7 we conclude with a summary of the results and some remarks highlighting future directions. The appendix section giver a short reminder of issues like classification, existence and uniqueness of solutions for quasilinear systems [21].

2. Curvature dependent surface energy for graphene

Following the classification of 2-lattices by Fadda and Zanzotto [11], we treat a monolayer graphene as a hexagonal monoatomic 2-lattice with unit cell of the form of Fig. 1.

The lattice and shift vectors are depicted in Fig. 2 and defined as

$$\mathbf{e}_1=(\sqrt{3}l,0),\quad \mathbf{e}_2=\left(\tfrac{\sqrt{3}}{2}l,\tfrac{3}{2}l\right),\quad \mathbf{p}=\left(\tfrac{\sqrt{3}}{2}l,\tfrac{1}{2}l\right), \tag{1}$$

l being the lattice size, namely the interatomic distance at ease which is approximately 1, 42 Å. The two simple hexagonal lattices are

$$L_1(l)=\{\mathbf{x}\in\mathcal{R}^2:\mathbf{x}=n^1\mathbf{e}_1+n^2\mathbf{e}_2,(n^1,n^2)\in\mathcal{Z}^2\},$$
$$L_2(l)=\mathbf{p}+L_1(l). \tag{2}$$