CONTINUUM MECHANICS AND CARBON NANOTUBES

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Summary The understanding of the mechanics of atomistic systems greatly benefits from continuum mechanics. One appealing approach aims at deductively constructing continuum theories starting from models of the interatomic interactions. This viewpoint has become extremely popular with the quasicontinuum method. The application of these ideas to carbon nanotubes presents a peculiarity with respect to usual crystalline materials: their structure relies on a two-dimensional curved lattice. This renders the cornerstone of crystal elasticity, the Cauchy-Born rule, insufficient to describe the effect of curvature. We discuss the application of a theory which corrects this deficiency to the mechanics of carbon nanotubes. We review recent large scale simulations based on this theory, which have unveiled the complex nonlinear elastic response of thick multiwalled carbon nanotubes. We also discuss simplifications of the continuum theory, useful for fast engineering computations, and its application to the prediction of nanotube failure, refining other recent analysis.

INTRODUCTION

Continuum mechanics rationalizes the mechanics of materials in terms of irreducible sets of parameters (e.g. elastic moduli, Peierls stress), is amenable to analytical calculations, and affords very efficient simulations (e.g. finite elements). The most classic approach for continuum modelling of atomistic systems adopts a standard continuum theory (e.g. linear elasticity), and adjusts the material parameters to the data available. This phenomenological approach is simple and useful, particularly when the mechanics are well understood *a priori*, and the phenomena are simple enough to be encoded in the model. Another approach aims at deductively constructing continuum theories starting from models of the interatomic interactions as realistic as possible, with a minimal set of assumptions [1]. We are interested in this systematic approach.

The analysis of mechanics of carbon nanotubes by continuum models has attracted the attention of many researchers in the recent years. Let us cite the seminal work of Yakobson and co-workers [2], as the first to fully acknowledge the shell-like behavior of these nanostructures, and the relationship of their mechanics with the buckling of elastic shells. While most of the available works rely on the above mentioned phenomenological approach, some authors have tackled the problem within the framework of finite crystal elasticity. This approach is very attractive for carbon nanotubes given their nearly defect-free crystalline structure, and the very large deformations that they sustain reversibly. In [3], we pointed out the fundamental limitations of the Cauchy-Born rule for curved lattices of reduced dimensionality, and a generalized kinematical rule inspired in the geometric structure of the kinematics of two dimensional continua was proposed. This method consistently derives a hyperelastic surface model from the atomistic interactions. One feature of this model is that the continuum object under consideration is two-dimensional, i.e. a surface without thickness. In our view, this model overcomes the futile issue, so often discussed in the literature, about the appropriate thickness in a thin shell theory for this two-dimensional lattice.

SUMMARY OF THE THEORY AND VALIDATION

The essential idea behind the present theory, as in classical finite crystal elasticity, is to use the Cauchy-Born rule (here the generalized CB rule) to express the geometric quantities characterizing the deformation of the lattice in terms of the deformation of the continuum. For bulk materials, the bond lengths and angles are expressed in terms of a Lagrangian strain measure such as the right Cauchy-Green tensor. In the case of curved two-dimensional continua, such as that required for carbon nanotubes, the geometry of the deformed lattice is explicitly expressed in terms of the stretch (first fundamental form) and the curvature (second fundamental form) of the surface. The discretization of this continuum theory by finite elements yields a coarse-grained simulation method, which very accurately captures the nonlinear mechanics of carbon nanotubes, and can afford huge computational savings as illustrated in the next section.

Figure 1 shows simulations for a twisted (10,10) nanotube. Three representative snapshots of the deformation process are shown. The evolution of the strain energy is presented for both the atomistic and the continuum/finite element calculations. The snapshots demonstrate that, even for these intricate deformed morphologies, the continuum mechanics theory is surprisingly accurate, and the finite element model remarkably fits the atomic positions. When it comes to the energetics, the agreement is also excellent. A comprehensive set of comparisons between atomistic and continuum simulations can be found in [4].

MECHANICS OF THICK MULTI-WALLED CARBON NANOTUBES

The computational method that results from combining the present theory with finite elements allows for simulations of multimillion atom systems to be easily performed at a fraction of the cost. Figure 2(a) shows simulations reproducing the rippling deformations observed in recent experiments. These simulations reveal the three dimensional structure of the rippling deformations, reminiscent of the Yoshimura pattern (b). Furthermore, the analysis of the energetics of these deformations manifests a well-defined genuinely nonlinear response. See [5] for further details.

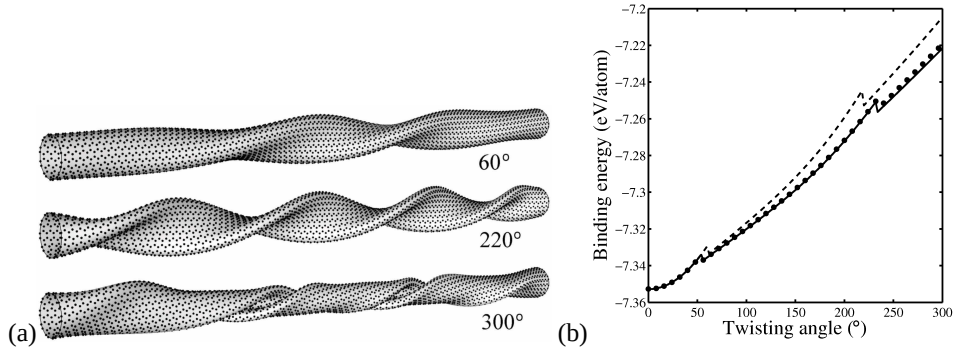

Figure 1. (a) Twisted 25.11 nm long (10,10) nanotube: super-imposed deformed configurations at three twisting angles for atomistic calculation (black spheres) and continuum finite element calculation (gray surface). (b) Comparison of the strain energy as a function of the twisting angle for atomistic calculation (—), and continuum/FE calculation (•), and strain energy evolution for the simplified model (- - -).

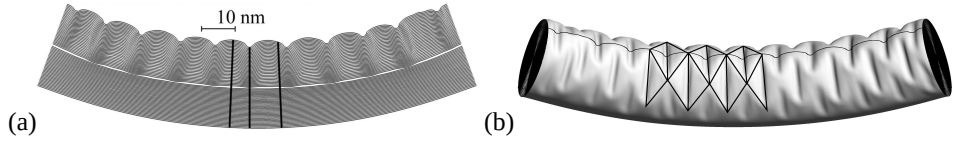

Figure 2. (a) Simulated rippling deformations in a 34-walled carbon nanotube, and (b) three dimensional structure of the deformation.

SIMPLIFIED MODEL

Although the continuum models described above affords very accurate and efficient computations, it is relatively complex and its computational cost is higher than that of standard engineering material models; it is strongly non-linear, its evaluation requires the inner displacement relaxation, and the membrane and bending contributions are tightly coupled. On the other hand, the simulations suggest that the nonlinearity of the mechanical response is mostly geometrical, rather than stemming from the material model. In this section we show that following rational arguments, it is possible to deduct the simplest nonlinear model, capable of reproducing the essential mechanics, and consistent with an irreducible set of elastic parameters.

It is well known that the infinitesimal in-plane elastic response of graphene is isotropic. In [6] we showed that the bending response is also isotropic. By analogy with the Kirchhoff-Saint Venant model of finite elasticity, the simplest isotropic model for a two-dimensional continuum splits the energy into membrane and bending energy, and is of the form

$$W_{\rm approx} = W_{\rm m} + W_{\rm b} = \frac{1}{2}[2\mu \mathbf{E} : \mathbf{E} + \lambda(\mathrm{tr}\ \mathbf{E})^2] + \frac{1}{2}[a(2H)^2 + bK]$$

where μ and λ are the 2D Lamé coefficients [6], $\mathbf{E}$ is the Green strain tensor, the mean curvature H and the Gaussian curvature K are the invariants of the curvature tensor, and a and b are bending elastic moduli. Since $\int_\Omega K\ dX$ is a topological invariant of the surface, the term involving K can be disregarded from the strain energy density. In [6] we provided explicit expressions for the bending modulus a in terms of the inter-atomic potential, as well as for the Lamé coefficients. Fig 1(b) (dashed line) shows that indeed this simple model captures the essential geometric nonlinearities of the problem, and provides quite good energetics. It also shows that for very large deformations, when presumably the material nonlinearities become more important, this model does not perform as well as the complete model discussed above. Although not shown, the agreement in the deformed configurations is also good for the simplified model.

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