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Application of gradient elasticity to armchair carbon nanotubes: Size effects and constitutive parameters assessment

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ABSTRACT

The central focus of the paper is set on modelling of bending of armchair carbon nanotubes by means of the gradient elasticity theory. Influence of small-size effects on the Young's modulus is investigated. An attempt to determine small size (or nonlocal) parameter employed in the Bernoulli-Euler and Timoshenko gradient formulations is presented. To obtain such a goal, the paper provides an extensive set of molecular structural mechanics simulations of armchair nanotubes with different loading and kinematic boundary conditions. Dependence of the Young's modulus on small size effects is clearly noticed. Based on these results, small scale parameters for the gradient model are identified and limits of the method are pointed out. Results of the study indicate that the widely used theory should be modified to obtain a physically justified and reliable nanobeam model based on Bernoulli-Euler or Timoshenko kinematic assumptions.

1. Introduction

With increasing development of nanotechology, the need for precise mechanical measurement at the nanometer level is becoming increasingly important. Most frequently measured physical variables are the force, the mass and the displacement. Design of nanosensors used in aforesaid measurements considers carbon nanotubes (CNTs) as a very promising candidate due to theirs extraordinary mechanical properties. On the other side of scale - the macro level - sensors frequently operate exploiting very basic mechanical principles like the beam deflection and elongation or by exploiting resonance principles. Therefore, it is natural to expect that the same principles could be applied at the nanoscale level as well. However, applications of the macroscale mechanical laws at nanoscale is far from justified. In particular, various small size effects become important thus implying the need for the non-classical mechanical models (Eringen, 1983, 2002; Mindlin, 1964). The essential assumption of this class of models is that the stress state does not depend only on the local strain/stress state at the point being considered, but rather the neighbourhood stress state has also certain influence. However, as recently discussed in (Romano and Barretta, 2016; Romano et al., 2017), the nonlocal elastic model proposed by Eringen cannot be used in order to study size-effects in nanostructures. Gradient elasticity theory is adopted in the present paper in order to get a satisfactory mathematical modelling of scale-effects in nanobeams, see e.g. (Barretta et al., 2015a; Marotti de Sciarra and Barretta, 2014). Valuable contributions on this fascinating topic can be found in (Lam et al., 2003; Giannakopoulos and Stamoulis, 2007; Lazopoulos and Lazopoulos, 2010; Papargyri-Beskou et al., 2003). Scale-dependent structural behaviour is described by a characteristic length, named small-size material parameter c.

A good starting point for the overview of the start-of-art in the field is the review paper (Arash and Wang, 2012). Among other issues, it notes that the nonlocal parameter can depend on boundary conditions, chirality, mode shapes, number of walls and the nature of motions. Also, the Bernoulli-Euler and Timoshenko beam models, along with the elastic shell model based on the classical or first-order shear deformation theories are quite satisfactory tools for CNT static or dynamic mechanical analysis. In another research (Wang and Hu, 2005), the Timoshenko beam formulation gives better results for flexular wave propagation in

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single-walled carbon nanotubes than the Bernoulli-Euler beam formulation.

Returning to the specific values for the small size parameter, the issue was analysed in vibrational behaviour by means of molecular dynamics (MD) in the case of Timoshenko beam (Zhang et al., 2009). Reactive empirical bond-order (REBO) potential was used while the CNTs investigated were of armchair (5,5) type. Thus, no dependence on the diameter was investigated. However, different CNT lengths were used with the aspect ratio in the range 4.67−35.34 nm. Regarding kinematic boundary conditions, simulations were performed for the cantilever beam and the doubly clamped beam. Results indicate that both local and nonlocal Timoshemko models can give good results, with the condition that the Young's' modulus E is properly chosen. Differences in the first natural frequency when the Timoshenko beam (either local or nonocal model) is compared to the MD results are up to 10% for the smaller CNT thickness, while higher thickness (0.34 nm) gives somewhat larger discrepancy (up to 15%).

Another vibrational analysis, provided by the nonlocal shell model, was performed in (Arash and Ansari, 2010). As the benchmark, MD results described in (Zhang et al., 2009) were used. Yet again, dependence on the thickness/Young's modulus, boundary conditions and geometry was found to influence the small size effects. Different boundary conditions lead toward different values of the nonlocal parameter ($c = 1.7$ nm for the doubly clamped beam and $c = 2.0$ nm for the cantilever beam in the case of thickness 0.34 nm; somewhat lower values are reported for thickness 0.066 nm). Therefore, unlike (Zhang et al., 2009), different values are reported for c depending on used boundary conditions. Adding complexity to the issue of thickness selection, the authors conclude that thickness of 0.34 nm is more suitable in the case of initial compressive strain, while the thickness of 0.066 nm is to be preferred if the initial strains are tensile.

A further support for the notion that the nonlocal parameter is not a single value is provided in (Narendar and Gopalakrishnan, 2011) in which the nonlocal parameter turns out to be a linear function of the CNT diameter. The result is obtained for the case of the torsional mode of wave propagation by means of analytical molecular structural mechanics. Similarly to this, MD investigation (Duan et al., 2007) finds that the nonlocal parameter cannot be a single value in the case of vibrations of a Timoshenko beam, thus again contradicting (Zhang et al., 2009). In particular, for a cantilever CNT beam, the authors report values of $c = 1.35$ nm and $c = 2.64$ nm for aspect ratios 10.16 and 15.24, respectively, while $c = 0.308$ nm for a doubly clamped beam. It is emphasized that all these results do not include influence of loading, i.e. the static boundary conditions.

Therefore, based on the above literature review, the following issues in the determination of the small size parameter can be identified as disputable:

- *CNT thickness.* There is no unanimous understanding about the thickness value among the researchers, see (Huang et al., 2006) for a thorough discussion. The thickness reported in the literature ranges ten-fold: from 0.066 nm to 0.69 nm. There are also reports indicating the thickness being dependent on the diameter (Wang et al., 2005). Naturally, the value of the Young's modulus is directly affected by this choice.
- *Small-size parameter functional dependence.* There are some results indicating that the small-size parameter is a constant. Most of literature points out that the small size parameter is the function of diameter, length, boundary conditions (both kinematic and static), chirality and initial strain.
- *Statics vs vibrations.* Performed modal analyses by molecular structural mechanics (MSM) or MD do not account for the static boundary conditions (apart from the initial axial strain in (Arash and Ansari, 2010)). Static analyses can easily account for the static boundary conditions.
- *Choice of the potential.* There are different possibilities for the choice of the potentials available in the literature and it was shown that this somewhat affects the nonlocal behaviour as well.
- *Gradient theory.* Most authors rely on the validity of the gradient nonlocal theory. However, simulations of tensile tests of the CNT indicate dependence of Young's modulus on the diameter; in the presence of the homogeneous stress field a gradient theory cannot explain such effects. Although these effects are small, they are unwanted nevertheless.
- *Bernoulli-Euler vs Timoshenko formulation.* Most studies of the CNT vibrations finds Timoshenko formulation better suited. On the other hand, the Bernoulli-Euler formulation does not need so many parameters that are not easy to determine.

Consequently, this paper hopes to contribute to the determination of the small size parameter representing nonlocality of normal stresses by performing a series of linear static MSM simulations, aiming to provide estimates of the Young's modulus depending on the armchair CNT diameter and the length. Although axial loading will be considered as well, the special emphasis will be given to bending of armchair CNT with various static and kinematic boundary conditions. Having provided such a comprehensive set of simulations with the Young's modulus variation as the result, small size parameters for the Bernoulli-Euler and Timoshenko beam gradient models are determined, even tough some unexpected results are obtained. Shortcomings of the application of the gradient model to the Bernoulli-Euler and the Timoshenko formulation are pointed out. Such a thorough analysis of the nonlocal bending behaviour of armchair CNTs is not available in the literature, to the best of the authors' knowledge.

The paper is structured as follows. Second section provides short summary of the molecular structural mechanics procedure. The subsequent section carefully documents performed numerical simulations. The third section deals with each loading case, applies the nonlocal gradient Bernoulli-Euler and the Timoshenko beam model and thoroughly reports the results. At the end, the Conclusion section summarize main findings.

2. Interatomic potential and molecular structural mechanics

Molecular structural mechanics is a numerical method aiming to substitute molecular dynamics in some simpler problems. It was originally developed by Li and Chou in 2003 (Li and Chou, 2003a). The central idea is to model interatomic bonds by standard spatial beam finite elements with 6 degrees of freedom per node, while nodes are positioned at atom positions. Therefore, an atomic structure is treated as a spatial frame, Fig. 1. The simplicity of the procedure and the possibility to apply it in any kind of finite element software was a main reason for the today's popularity of the method.

To accurately represent physical behaviour of interatomic bonds, the proper interatomic potential U must be selected. The general form is:

$$U = \sum_{i=1}^{N} \sum_{j=i+1}^{N} U_2(\mathbf{r}_i, \mathbf{r}_j) + \\ + \sum_{i=1}^{N} \sum_{j=i+1}^{N} \sum_{k=j+1}^{N} U_3(\mathbf{r}_i, \mathbf{r}_j, \mathbf{r}_k) + \sum_{i=1}^{N} \sum_{j=i+1}^{N} \sum_{k=j+1}^{N} \sum_{l=k+1}^{N} U_4(\mathbf{r}_i, \mathbf{r}_j, \mathbf{r}_j, \mathbf{r}_l), \tag{1}$$