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An elastica model that predicts radial corrugations in a double- walled carbon nanotube

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ABSTRACT

In this paper we study a variation on the classical problem of a ring subject to a uniform radial load. An initially circular elastic ring, modeled as an elastica, is concentric with a second circular ring, which is rigid and is either outside or inside the elastic ring. On each point of the elastic ring, the rigid ring exerts a *nonuniform* radial load that depends on the distance between the point and the rigid ring. The two rings can be viewed as a continuum description of the cross-section of a double-walled carbon nanotube. The force between the elastic ring and the rigid ring is a continuum approximation to the van der Waals interaction between atoms on the two walls of the double-walled tube. We use this model to study the buckling of the elastic ring as the radius of the rigid ring is varied. Our model predicts radial corrugations, a type of deformation studied recently in (Shima and Sato, 2008, 2009; Shima et al., 2010).

1. Introduction

A classical problem in mechanics is the buckling of a circular elastic ring subject to a uniform radial load (Dickey and Roseman, 1993; Sills and Budiansky, 1978; Simitses and Hodges, 2006; Singer and Babcock, 1970; Stoker, 1968). In this paper we consider an interesting variation on this classical problem. An initially circular elastic ring is concentric with a second circular ring, which is rigid and is either outside or inside the elastic ring. See the upper middle and lower middle parts of Fig. 1. The elastic ring is modeled using the classical elastica assumptions (Antman, 2005). On each point of the elastic ring, the rigid ring exerts a *nonuniform* radial load that depends on the distance between the point and the rigid ring. As we discuss further below, this load models a van der Waals interaction between the rings. The most salient features of this interaction are the following: a point on the elastic ring that is near the rigid ring is pushed strongly away from the rigid ring, a point that is relatively far from the rigid ring is pulled weakly toward the rigid ring, and a point that is very far from the rigid ring essentially feels no force from the rigid ring. Hence, for example, when the rigid ring is outside the elastic ring and the radii of the two rings are sufficiently close, all points on the elastic ring are pushed radially inward, putting the elastic ring under circumferential compression. We study the buckling of the elastic ring as the radius of the rigid ring is varied.

Our treatment of this problem is in general motivated by an interest in understanding the mechanics of carbon nanotubes. A single-walled carbon nanotube is a one-atom thick lattice of carbon atoms wrapped into a cylinder, which typically has circular cross-sections (Dresselhaus et al., 1996) A multi-walled carbon nanotube (MWNT) is a collection of single-walled nanotubes nested about a common axis (Dresselhaus et al., 1996). A typical inner radius for a MWNT can be is small as 1 nm, while a typical outer radius is on the order of 10 nm, and the separation between adjacent walls is around 0.34 nm (Dresselhaus et al., 1996; Terrones, 2003). At this length scale, atoms on a wall of a MWNT interact with other nearby atoms on adjacent walls by weak (non-bonded) interatomic forces called van der Waals forces. These interactions, though weak, are critical for understanding the mechanical response of MWNT and, in particular, for explaining the radial deformations of cross-sections of a MWNT (He et al., 2010; Popescu et al., Mar 2008; Ru, 2000; Wang et al., 2003).

A continuum model recently developed by Shima and Sato (2008, 2009) predicts that a MWNT, when subject to hydrostatic pressure, may undergo a radial deformation that the authors call a *radial corrugation*. The key feature of this class of deformations is

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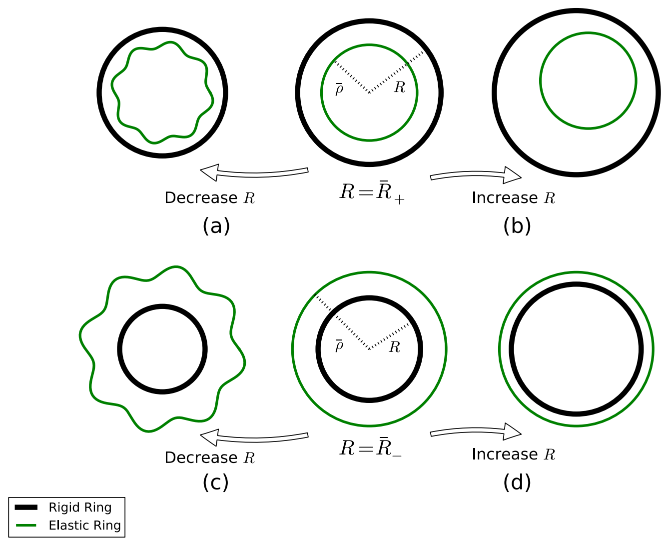

Fig. 1. The top and bottom middle figures show the initially circular elastic ring with the circular rigid ring either outside or inside. From each of these initial geometries, we can either decrease or increase R.

that the walls of the tube exhibit wavy structures along the circumferential direction. Radially corrugated MWNT have yet to be observed experimentally. However in (Shima et al., 2010), Shima et al. formulate a problem in which the inner walls of a MWNT are subjected to pressure by the radial shrinkage of the outer walls of the tube. This pressure occurs because, as the radii of the outer walls shrink, the van der Waals interaction between the outer walls and the inner walls becomes repulsive. Shima et al. conjecture that this shrinkage could be achieved experimentally by the electon-beam irradiation of the outer walls of the tube (Krasheninnikov and Banhart, 2007; Sun et al., 2006). In (Shima et al., 2010), this problem is studied by treating the collection of radially shrunken outer walls of the MWNT as a continuum elastic medium in which the inner walls are imbedded. The authors use their model to predict cross-sectional shapes, critical pressures, and corrugation amplitudes associated with radial corrugations (Shima et al., 2010). We note that radial corrugations have also been observed in atomistic simulations (Huang et al., 2011).

One way to specifically motivate the problem represented by Fig. 1(a)—in which the outer ring is rigid and its radius is decreased—is to view it as an alternative model for the problem suggested by Shima et al. in (2010). In this case the inner, elastic ring describes the inner wall of a double-walled nanotube, which is subject to a van der Waals force as the outer wall shrinks. Although we are modeling a double-walled tube, to keep the problem tractable we do not allow the outer ring to deform. This simplifies the description of the interaction between the rings. Specifically, the van der Waals force that the rigid ring exerts on a point on the deformable ring is a function of just the radial distance between that point and the rigid ring. Keeping the outer ring rigid limits the applicability of our results. One could expect, however, that any buckling would be initiated by deformaton of the inner wall, because when the two rings are relatively close, the van der Waals interaction puts the outer wall under circumferential tension but the inner wall under circumferential compression. The case in which both rings can deform will be treated in a future study.

As a second motivation for the problem described by Fig. 1(a), we note that this problem models the response of a single-walled nanotube imbedded in a relatively stiff elastic medium. In this case, the van der Waals force exerted by the outer rigid ring represents the interaction between the medium and the wall of the nanotube. By varying the radius of the outer rigid ring, we vary the strength of the interaction between the medium and the nanotube. Numerous continuum models of a nanotube embedded in an elastic medium have been studied. See, for example, (Han and Lu, 2003; Ru, 2001; Sun and Liu, 2008), among many possibilities. We note that in our model, unlike the model in (Shima et al., 2010), we do not include a contribution to the energy from the deformation of the medium because we do not allow the outer wall to deform.

The problems depicted in Fig. 1(c), (d)—in which the inner ring is rigid—are motivated by noting that the interaction between the rings in this case could model the force on a nanotube exerted by a relatively rigid inclusion introduced into the nanotube. An interesting example of this type of system is provided by different techniques for introducing metals into carbon nanotubes. Metal-filled nanotubes have significantly different conducting, electronic, and mechanical properties (Wang et al., 2008). We note also that single-walled nanotubes have also been successfully filled with clusters of metal atoms and C_{60} molecules (Buckeyballs) (Monthioux, 2002).

We show that our model predicts solutions analogous to the radial corrugations observed in (Shima and Sato, 2008, 2009; Shima et al., 2010). First, we establish the existence of a branch of solutions in which the elastic ring is circular and concentric with the rigid ring. These solutions exist for any positive radius R of the rigid ring and any positive radius $\bar{\rho} \neq R$ of the elastic ring. For a given $\bar{\rho}$, there are two values of R—denoted $\bar{R}_-$ and $\bar{R}_+$, with $\bar{R}_- < \bar{\rho} < \bar{R}_+$—such that if $R = \bar{R}_\pm$, then the rigid ring exerts no force on the elastic ring. See Fig. 2. Treating R as a bifurcation parameter, we can recover a version of the problem studied in (Shima et al., 2010) by starting initially with $R = \bar{R}_+$ and seeking bifurcations as we decrease R. See Fig. 1(a). We also treat 3 other closely related problems: starting initially with $R = \bar{R}_+$ and increasing R (Fig. 1b), and starting initially with $R = \bar{R}_-$ and either decreasing or increasing R (Fig. 1c and d). (We shall refer to the problem depicted in Fig. 1(a), (b) as the *outer-ring problem* and to the problem depicted in Fig. 1(c), (d) as the *inner-ring problem.*) For both the outer-ring problem in which we decrease R and the inner-ring in which we decrease R, we show that the elastic ring buckles into a solution corresponding to what Shima et al. call a radial corrugation. We use our model to predict the buckling radii and the mode number of the buckled solutions. For the inner-ring problem in which we increase R, we show that buckling does not occur. Lastly, for the outer-ring problem in which we increase R, we show that the two-ring system loses stability by a translation of the elastic ring. We make some comparisons between these results and the classical problem of the buckling of a circular ring subject to a uniform radial load.

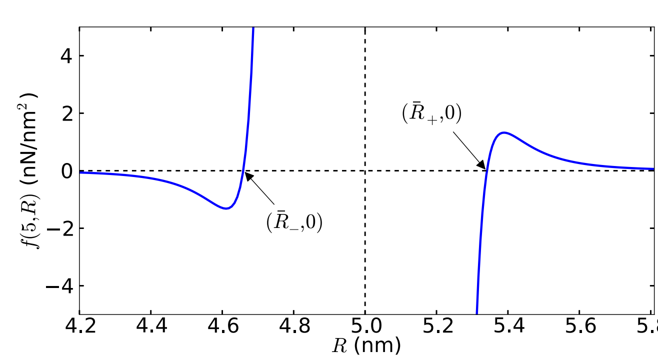

Fig. 2. $f(\rho,R)$ as a function of R for $\rho = 5$ nm. The van der Waals force that a rigid ring of radius R exerts on a point on the elastic ring with polar coordinates (ρ,γ) is $f(\rho,R)\xi_1(\gamma)$, where $\rho\xi_1(\gamma)$ is the position vector for the point (ρ,γ).