Chapter 43
On the Modeling of Carbon Nanotubes as Drug Delivery Nanocapsules

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ABSTRACT

The structure of carbon nanotubes is recognized to be suitable for medical applications such as encapsulating drugs or genes with the aim of targeted deliveries. In this regard, knowing about the suction force exerted on a nonoscale object which is supposed to be sucked into a carbon nanotube, and whether the object is accepted by the carbon nanotube are important issues to be studied. In this chapter, considering the nanoscale object as a carbon nanotube, a new semi-analytical method is developed to determine the van der Waals interaction between two concentric single-walled carbon nanotubes.

1. INTRODUCTION

Since the appearance of the landmark paper by Iijima (1991), carbon nanotubes (CNTs) have evoked a great deal of interest due to their superior physical and chemical properties over other materials known. In terms of mechanical properties, CNTs have proved to be amongst the lightest, stiffest and strongest materials yet measured with high elastic modulus of greater than 1 TPa comparable to that of diamond and strengths many times higher than the strongest steel at a fraction of the weight. CNTs are expected to withstand large strains of up to 10% (Nardelli & Bernholc, 1999).They are also quite flexible and can return to their original shape after bending and buckling (Falvo et al., 1997).

Among the various attractive application of CNTs, Gigahertz oscillators have been the focus of considerable research due to the difficulties encountered for micromechanical oscillators to achieve frequencies in Gigahertz range (Cox et al., 2007; Liu et al., 2005; Rivera et al., 2003; Zheng et al., 2002; Zheng & Jiang, 2002). There

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are different theoretical approaches to study these nanoscale oscillators. Atomistic methods such as molecular dynamics (MD) simulation have been widely applied by research workers. Using microcanonical molecular dynamics, Wong et al. (2006) studied effects of single defects on the performance of a nanoscale oscillator composed of coaxial double-walled carbon nanotubes (DWCNTs). Su et al. (2006) investigated a single-walled carbon nanotube (SWCNT) with one buckyball inside with an operating frequency in the tens-of-gigahertz range via MD simulation. Based upon an atomistic model, Legoas et al. (2003) showed that multi-walled carbon nanotubes (MWCNTs) as Gigahertz oscillators are dynamically stable when the radii difference values between inner and outer tubes are of:3.4Å.

Even though the MD simulations have generated plentiful results for understanding the performance of nanoscale oscillators, they are often computationally expensive and very time consuming. Another way for analyzing nanostructures is based upon the continuum mechanics. Continuum models are one of the most applied theoretical approaches for the investigation of Gigahertz oscillators due to their computational efficiency and the capability to generate accurate results which are comparable to those of atomistic models. Herein, some of the studies based on continuum models are cited.

Using continuum approximation, Baowan et al. (2008) investigated the suction energy and offset configuration for DWCNTs. Cox et al. (2008) developed a continuum model to study the acceptance conditions and suction energies of spherical and spheroidal fullerenes entering carbon nanotubes. Based upon continuum mechanics, the oscillatory behavior of DWCNTs was analyzed by Baowan & Hill (2007). An expression for the van der Waals interaction energy between two parallel torus-shaped colloidal particles was derived by Ohshima & Hyono (2009). They indicated that for small particle separations the torus–torus interaction energy is well approximated by the interaction energy between two parallel cylinders, each being produced by cutting a torus and unrolling it. On the basis of hybrid discrete–continuum formulation, Hilder & Hill (2008) used an acceptance condition and the suction energy to determine the suction behavior of a particular drug molecule entering a nanotube. Based on the continuum Lennard–Jones model, Sun et al. (2005) presented the potential energies of van der Waals (vdW) interactions between two parallel, infinitely long and perfect single-walled nanotubes with identical and different sizes. The oscillation of a fullerene that is moving within the center of a bundle of nanotubes was studied by Thamwattana & Hill (2009) using the Lennard–Jones potential and the continuum approach. Ansari & Motevalli (2009) investigated the effects of geometrical parameters on force distribution and mechanics of carbon nanotubes. They also presented a correction factor capable of converting the results of DWCNTs to the correlated multi-walled. The recent work by Alisafaei & Ansari (2011) on the mechanics of concentric carbon nanotubes was also based upon the continuum approximation. A universal potential curve was also presented for an inner tube entering various semi-infinite outer ones in their work.

In this study, the discrete distribution of atoms on the two surfaces is replaced by a constant atom density on the surfaces of each of them. In general case, to estimate the interaction between two nanostructures using continuum approximation, surface integrals must be performed over both smeared surfaces, which leads to a quadruple integral. This quadruple integral is analytically reduced to a single integral expression for the concentric tubes. The resultant integrals can be numerically computed which is very quick in comparison with other methods. Also, it is shown that the nature of potential energy and interaction force at the entering point can be fully explained by the terms introduced in the above mentioned expression.