Materials and Design 32 (2011) 2949–2955

Contents lists available at ScienceDirect

Materials and Design

journal homepage: www.elsevier.com/locate/matdes

New approach to model the buckling and stable length of multi walled carbon nanotube probes near graphite sheets

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ARTICLE INFO

Article history:
Received 6 April 2010
Accepted 2 August 2010
Available online 6 August 2010

Keywords:
A. Nanomaterials
I. Buckling
H. Selection of components

ABSTRACT

Modeling the buckling of multi walled carbon nanotube (MWCNT) probes/actuators in the vicinity of thin and thick graphite has been carried out for the first time via two analytical approximation methods as well as a numerical one. A hybrid nano-scale continuum model based on Lennard–Jones potential is applied to simulate the intermolecular force-induced deflection of MWCNT. The critical values of MWCNT tip deflection and MWCNT-graphite attraction at the onset of the instability are computed. In addition, minimum nanotube-graphite initial gap and stable length of freestanding CNT are determined as basic parameters for engineering applications and nano-devices design. The stable length of MWCNT is determined as a function of its geometrical and material characteristics, initial gap and number of graphene layers.

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1. Introduction

Multi walled carbon nanotubes (MWCNTs) have attracted considerable attention among other nanomaterials. These novel materials can usually be visualized as nano-scale concentric cylinders rolled up by graphene sheets. MWCNTs are produced by different techniques, such as chemical vapor deposition, laser ablation, and arc discharge. It has been reported that the stiffness, flexibility and strength of carbon nanotubes are much higher than the conventional materials [1]. Furthermore, nanotubes can provide various ranges of conductive properties depending on their atomic and geometrical structure [2]. The extraordinary properties of MWCNTs have motivated worldwide engineers to explore their applications in different fields. With recent growth in nanotechnology, MWCNTs are increasingly used in developing atomic force microscope (AFM) probes [2–4] and nano-electromechanical system (NEMS) switches [5–7]. Consider a typical cantilever MWCNT probe/switch suspended near graphite surface with a small gap in between. As the gap decreases from micro to nano-scale, the van der Waals interaction deflects MWCNT to the surface. When the separation is small enough, nanotube buckles onto graphite. The prediction of the molecular force-induced instability of MWCNTs near the surface is a critical subject in design AFM probes and NEMS switches. With decrease in distance between the AFM probe and sample surfaces, the probe jumps into contact with the surfaces and renders its imaging performance [8–10]. Similarly, a NEMS switch might adhere to its substrate even without an applied voltage as a result of molecular force, if the minimum gap between the switch and substrate is not considered [11–13].

In order to study nanomaterials, several approaches are employed. Molecular dynamics (MD) and molecular mechanics (MM) simulations could be used to study the mechanical behavior of carbon-based nanomaterials [14–17]. However these methods are very time-consuming and might not be easily used in complex structures. An alternative reliable trend to simulate the instability behavior of MWCNT interacting with extremely large number of graphite atoms, is to apply nano-scale continuum models. A hybrid continuum model can be used to calculate the van der Waals energy, in lieu of the discrete Lennard-Jones potential, similarly [16–18]. Although continuum models are more time-saving than MM and MD, their approach often leads to nonlinear equations that might not be worked out by analytical methods, accurately [16,19].

In this paper, we utilize a hybrid continuum model to investigate the molecular force-induced deflection and buckling of the cantilever freestanding MWCNT probes/actuators suspended over graphite. Two new analytical approximation methods, Adomian decomposition [20–22] and Green's function [23–25] are introduced to simulate the instability of MWCNT and the obtained results are compared with numerical data. In addition we compute the permissible length of MWCNT that does not stick to graphite

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0261-3069/$ - see front matter © 2011 Published by Elsevier Ltd.
doi:10.1016/j.matdes.2010.08.002