Engineering Fracture Mechanics 136 (2015) 158–171

Contents lists available at ScienceDirect

Engineering Fracture Mechanics

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

Stress distribution in carbon nanotubes with bending fracture

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ARTICLE INFO

Article history:
Received 6 September 2014
Received in revised form 18 January 2015
Accepted 26 January 2015
Available online 11 February 2015

Keywords:
Carbon nanotubes
Analytical modeling
Finite element method
Bending

ABSTRACT

The previous experimental evidence indicated that bending fracture of a carbon nanotube (CNT) is triggered from the outermost layer of the graphene sheets, and then the crack grows toward the inner sheets. The unique feature is that the CNT is fractured in a form of cone-shaped pullout, meaning that the crack grows along an inclined direction into the inner layers. Based on the experimental observation, a model of bending fracture is proposed. The stress distribution in fractured CNTs under bending is analyzed by both the shear-lag model and the Finite Element Analysis (FEA). The effects of the layer number and the aspect ratio on the load transfer efficiency are examined. This study also examines the crack growth angle by using FEA.

1. Introduction

Carbon nanotubes are known for their potential in various applications owning to its exceptional properties. It was reported that the Young's modulus can be as high as 1 TPa and the failure strain up to 5% [1–3]. Conventional reinforcing fibers, such as carbon fibers, are typically brittle and cannot survive a large extension or bending without breakage. In comparison, CNTs are composed of graphene sheets which are exceptionally resilient, and thus the elastic range of CNTs is remarkably large [4,5]. While CNTs are resilient along the axial direction, they are susceptible to inter-layer stresses inside the CNT.

For a CNT to be stressed, the load must be applied on surface and then transferred into inner layers through the interlayer shear stress. The mechanism of load transfer between the graphite layers associated with non-fractured as well as fractured has been an important research topic studied both theoretically and experimentally [6–12]. Once a CNT is loaded, it could undergo fracture that renders the material unusable. To exploit its potential in many applications, the knowledge of CNT deformation and fracture is essential [13,14]. Nikiforov utilized the molecular dynamics to study the bending behavior of CNTs [15]. They predicted and characterized a Fourier-type rippling mode that dominates the incipient nonlinear elastic response of MWCNTs with closed cores. Wang used the molecular mechanics simulations to study the local buckling of a SWNT under bending [16]. The critical deformation at the force location was observed and the indentations or kinks at the onset of the local buckling were described. Belytschko observed a measured drop of the effective bending stiffness of MWNTs with larger diameters [17]. In addition, ripples were also predicted for MWNTs subjected to torsion. Falvo studied the resilience of MWNTs by applying a repeated bending motion. They observed reversible, periodic buckling of nanotubes [18]. Xu Guo investigated the bending stiffness of SWCNTs and some related issues by the combined use of the molecular-mechanics model and the deformation mapping technique [19]. An analytical expression for the bending stiffness of SWCNTs based on the molecular mechanics model under infinitesimal deformation was presented. It shows that the bending stiffness

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http://dx.doi.org/10.1016/j.engfracmech.2015.01.023
0013-7944/

Nomenclature

t	the distance between two layers
$R_{o.1}$, $R_{i.1}$, $R_{i.2}$, $R_{i.3} \ldots R_{i.7}$	the outer and inner radii of each graphite layer
D_1, D_2, D_3, D_4	diameters
RK-4	Runge–Kutta algorithm
$R_{o.1}$, $R_{i.7}$	the outer and inner radius of outermost and innermost layer
$R_{i.1}$, $R_{i.2} \ldots R_{i.7}$	inner radii of layer 1, 2, 3 and 4
dy	infinitesimal element
G_{is}	interlayer shear modulus
A_1	cross sectional area of the layer
$R_{i.m}$, A_m	inner radius, and cross sectional area
s	the gap size
j	interface index
vdW	van der Waals
w_h	crack opening
e_h	exposed length
$\tau_{a.i.m-1}$, $\tau_{a.i.m}$	two curved interfacial shearing tractions
σ_{01}	normal stress
σ_m^s	saturated normal stress in the layer m
$\sigma_{cen.m}$, $\sigma_{0.m}$	stresses at the central cross section
$\sigma_{cen.m}^{non}$	internal stress at the central cross section
ε_j, ε_{j+1}	the axial strains of shell j and shell $j+1$
$\tau_{a.i.1}$, $\tau_{a.i.2}$, $\tau_{a.i.3}$	interfacial shear stresses acting on the interface 1, 2, and 3

of SWCNTs is approximately proportional to the cube of the tube radius. Still, the progress in the analysis of the bending behavior has been slow, especially for MWCNTs.

Along with the efforts on studying stress transfer in MWCNTs, the cracking mechanisms of MWCNTs are also investigated experimentally. Yu first conducted tensile tests and observed pullout of the inner CNT [20], and this was termed as sword-in-sheath. Recently, Kuo adopted a special approach to incur bending fracture in CNTs [21,22]. They observed two major modes of bending fracture, including the cone-shaped and the shear-cut. Because the fracture modes in CNTs are unusual and unprecedented in micron-scale filaments, such as carbon fibers, it is necessary that these modes be well characterized analytically.

In this work, new formulations based on the experimental observations have been developed to study the deformation and stresses in a CNT under bending. The previous microscopic observations showed that many CNTs were partially fractured. Some outer graphene layers of a CNT were fractured, while the inner layers remain intact. This indicated that the crack starts from the outermost layer and follows a stepwise, stop-and-go manner to the inner layers. The crack grows when the stress and the stored strain energy are sufficiently high. Once the energy is dissipated, it stops and can proceed only more energy is supplied from external loads. This stop-and-go manner allows us to analyze the detailed stress distribution within the layers for any stage of crack growth. This information is important as it dominates the nucleation and development of a crack. Both non-fractured and partially fractured CNTs are examined, referring to the cases of crack initiation and propagation, respectively. The shear-lag model and the finite element method are employed to study the stress distribution in partially fractured CNTs. Without loss of generality, the influence of layer number is analyzed up to ten. The finite element method is used to calculate the crack growth angle.

2. Experimental observation

According to the previous experimental observation, CNTs showed unique fracture modes when bent to fracture [21]. Similar to the sword-and-sheath type of tensile fracture, the bending fracture is separated into two regions: the outer-tube and the inner-tube. The outer-tube is failed in tensile rupture, similar to the sheath. The inner-tube is fractured and pulled out. Unlike the sword, the pullout has an inclined side surface. The inclined crack propagation was due to the stepwise fracture in the graphene layers, as a result of the combination of bending-induced tensile rupture and interlayer separation. When the stepwise crack growth is symmetric with respect to the CNT centerline, a cone shape is formed as shown in Fig. 1.

3. Model transformation

Despite the gap in the layered structure, there exist some mechanisms for load transfer between graphene layers [23,24]. If the structure of a CNT is commensurate (with parallel chiral vectors), the efficiency of load transfer through shear is optimum as explained by Zalamea et al. [9] and Kolmogorov and Crespi [25]. To study of the load transfer among the layers, the