Composites Science and Technology 110 (2015) 159–165

Contents lists available at ScienceDirect

Composites Science and Technology

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

Tensile failure mechanisms of individual junctions assembled by two carbon nanotubes

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ARTICLE INFO

Article history:
Received 19 September 2014
Received in revised form 2 January 2015
Accepted 7 February 2015
Available online 13 February 2015

Keywords:
A. Carbon nanotubes
B. Interface
B. Debonding
C. Stress transfer
D. Atomic force microscopy (AFM)

ABSTRACT

The tensile mechanical behaviors of junctions between carbon nanotubes (CNTs) were experimentally and theoretically studied. For sidewall-contact junctions, we found that tensile failure stress can be enhanced by radial deformation of CNTs. Meanwhile, a re-formation mechanism of junctions expected to contribute to interfacial toughness was found, for which a theoretical prediction was presented. For end-contact junction, it is found that the maximum pulling force is dependent on the diameters and wall numbers of CNTs. Most importantly, the interaction strength between two open-ends of CNTs was first experimentally estimated to be 21 MPa. This study would be helpful not only in understanding the failure behaviors, but also in quantifying the mechanical properties of the CNT-based fibers, films and blocks.

1. Introduction

In recent years, carbon nanotubes (CNTs) have been utilized to fabricate a series of high performance of yarn-like fibers [1–9], films and blocks [10–13] (Fig. 1a–c) due to their extraordinary properties such as high strength and stiffness, high aspect ratio and low density [14–18]. The joining mechanisms to build these multifunctional materials are junctions between two CNTs formed by self-assembly. The junction types may be classified as sidewall-contact junction and end-contact junction, as shown in Fig. 1d and e. Mechanical characteristics of sidewall-contact and end-contact junctions are fundamentals to study mechanical performance of these CNT-based hierarchical materials as the two junctions are their basic structures.

So far, limited experimental and theoretical works have been performed to study mechanical properties of the two junctions. Suekane et al. [19] used an *in-situ* transmission electron microscope with a nano-manipulation system to investigate static friction force of the sidewall-contact junction with two individual CNTs. They found that the surface roughness of CNTs affected interfacial shear force significantly and the van der Waals (vdW) interaction between CNTs is subordinate. Wei et al. [20] studied CNT interactions with sidewall-contact junction by using the *in-situ* scanning electron microscope (SEM) testing system combining with a theoretical model, where relationships between the maximum shear force and overlap length of CNTs were derived. They reveal that the maximum shear force linearly increases with an increase of junction length in a short range and tends to be saturated when the junction is larger than a characteristic length. Li et al. [21] investigated the interfacial shear strength between two CNTs by using molecular dynamic (MD) simulation and found that the shear strength was 0.05–0.35 GPa. They indicated that variations of interfacial shear strength are strongly dependent on chiralities of CNTs. It is seen that roughness, chirality, characteristic length and the vdW bond can affect CNT interactions of the sidewall-contact junction and thus they are very complicated.

Nagataki et al. [22] investigated effects of covalent bond linking on interaction force between two capped CNTs. They found that the interaction force is not only related to the number of covalent bond, but also controlled by wresting the formed covalent bond. To our best knowledge, there is no experiment on the end-contact junction between two open-end CNTs based on vdW interaction in open publications. In this paper, we will conduct an *in-situ* tensile testing and MD simulation to study tensile mechanical behaviors of the two junctions between two CNTs.

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http://dx.doi.org/10.1016/j.compscitech.2015.02.003
0266-3538/

2. Experimental and simulation method

2.1. Materials preparation

In this study, we employed a hierarchical structure, where the CNTs were uniformly grown on the surfaces of carbon fibers (CFs) prepared by chemical vapor infiltration (Fig. 2a) to obtain the CNT junctions and achieve *in-situ* pulling of junctions. The length of grafted CNTs ranges from 0.5 to 20 μm, and the diameter of CNTs is 50–120 nm. The diameter of CFs is about 7 μm. The detailed preparation process can be referred to the literatures [23,24].

2.2. In-situ tensile testing

One CF with CNTs was drawn out from the bundles of CFs, and cut into several segments with a length of ~3 mm in the optical microscope. Then, these CF segments were fixed on a metal holder used in SEM. Here, we employed a force measurement system (FMS) (Kleindiek Nanotechnik) to achieve the measurement of force, which is composed of a nano-manipulator (the minimum moving resolution can reach 0.25 nm), atomic force microscope (AFM) tip (the maximum tolerate value of force is ~80 μN) and a sensitive force sensor (measurement resolution of force is ~1 nN) (Kleindiek Nanotechnik). The samples and the AFM tip were putted into the chamber so that we can perform the nano-manipulation. As shown in Fig. 2b, the AFM tip was slowly close to a selected CNT, and then the free end of CNT was bonded onto the AFM tip using compatible SEM-glue. It is noted that this glue remains uncured under low and can rapidly polymerize upon exposure to strong electron beam, ensuring that there is enough time to search selected samples and form strong bonding between AFM tip and CNTs. The selected CNT was pulled away along the direction perpendicular to the CF surface until the CNT was fractured, by which partial or whole CNT can be remained on the AFM tip. Then, the CNT on AFM tip was gradually close to another CNT which was chose to be perpendicular to the CF surface, and due to vdW interaction sidewall-contact and end-contact junctions can be formed (Fig. 2c and d). Lastly, the CNT on AFM tip was moved with a constant speed along the direction perpendicular to the CF surface, until the junction was broken.

2.3. MD simulation

We utilize the molecular simulation package LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator) (http://lammps.sandia.gov/) to establish the molecular models of sidewall-contact and end-contact junction between two CNTs. The adaptive intermolecular reactive bond order (AIREBO) potential as implemented in the LAMMPS was used to describe the interactions among carbon atoms, which has been approved to be capable to accurately account for the mechanical behaviors of CNTs [25,26]. In this study, the cut-off distance was set at 2.0 Å. The initial molecular models were equilibrated using an NVT ensemble with a time step of 0.001 ps for 30 ps, where Berendsen thermostat was used to control the temperature (300 K). To carry out the tension of CNTs, a constant strain rate of 0.0001 ps^{-1} was applied in loading directions until the two CNTs were completely separated each other. The tensile stress was obtained by averaging over the stresses of all atoms in the simulation system, and the detailed computing principle can be referred in related literatures [25].

3. Results and discussion

To conduct pulling testing for the two types of CNT junctions, we devised a simple and efficient process to prepare samples used in the experiment as shown in Fig. 2a, where multi-walled CNTs were grown on the CF surfaces based on a "base-growth" mode (see detailed prepared process in experimental section). The outermost diameter d_{out} and innermost diameter d_{inn} of the used CNTs are 90 and 54 nm, respectively. The detailed preparation process was given in experimental section. In the experiment, the CNTs grown on the CFs were used for the *in-situ* tensile testing. To apply a pulling force on an individual CNT jointed to another one, the FMS equipped in SEM was used to record the pulling process data so that curves of pulling force F versus time s could be obtained. The testing procedure was given in experimental section.

To implement the pulling test for the sidewall-contact junction under tensile load, F was carefully applied with calibration to ensure that loading direction is parallel to the axial direction of CNTs. The pulling displacement δ is defined as an increment of full length L of the pulled CNT along loading direction as in Fig. 3a. A typical F–δ curve and several selected snapshots were shown in Fig. 3a and b (see Video S1 for whole pulling process), respectively. Initially, the F increases at a lower rate (~1 nN/nm) with δ due to the straightening of CNT with the initial curvature (stage I). When δ increases to ~200 nm, F starts to increase with the stretching of CNT at a higher rate (~10 nN/nm) until it reaches the maximum value of 1405 nN (point ②, stage II), at which the junction breaks abruptly and the two CNT ends move in opposite directions at high

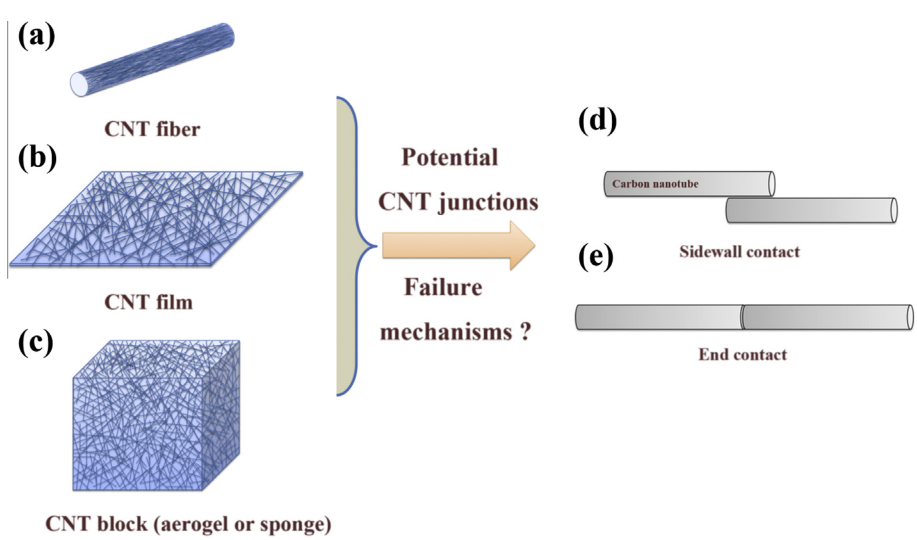

Fig. 1. (a–c) CNT-based fiber, film and blocks, (d) sidewall-contact junction and (e) end-contact junction.