Materials Science & Engineering A 614 (2014) 273–283

Contents lists available at ScienceDirect

Materials Science & Engineering A

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

Computational structural modeling and mechanical behavior of carbon nanotube reinforced aluminum matrix composites

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ARTICLE INFO

Article history:
Received 30 March 2014
Received in revised form
15 July 2014
Accepted 16 July 2014
Available online 23 July 2014

Keywords:
CNT–metal composite
Structural modeling
Layered structure
Interfacial behavior
Mechanical behavior

ABSTRACT

Due to their remarkable mechanical properties, carbon nanotube (CNT) reinforced aluminum (Al) matrix composites have attracted a wide range of research interests. This work attempts to experimentally and numerically investigate the relationship between the micro-structures and mechanical behavior of CNT/Al composites. Three-dimensional (3D) computational structural modeling of CNT/Al composites is performed, in which the size, morphology, orientation, location and volume fraction of CNTs are reproduced to be similar to those of the actual micro-structures of CNT/Al composites. The strengthening of the mechanical properties of the constituent materials of CNT/Al composites and reasonable load and boundary conditions are studied based on the models of CNT/Al composites developed. The tensile mechanical behavior of CNT/Al composites is numerically evaluated and experimentally verified. Results show that the enhanced mechanical properties of CNT/Al composites can be attributed to three factors: CNT reinforcements, matrix grain refinement and layered architectures. Through the microscopic structural modeling methods presented herein, the effects of model size, interfacial behavior, volume fraction of CNTs and layered structures on the mechanical behaviors of CNT/Al composites can be reproduced to understand the strengthening and deformation mechanisms of CNT/Al composites.

1. Introduction

Carbon nanotubes (CNTs) possess a unique combination of high stiffness, strength and tenacity [1,2], as well as superior thermal and electrical properties [3] for structural and functional material applications. It is generally believed that CNTs can be used as reinforcements to produce novel composites [4,5]. CNT reinforced polymer and metal matrix composites have been widely developed based on various types of matrix material [6,7]. However, in contrast to the intensive research on CNT/polymer composites, relatively few studies have been conducted on CNT/metal composites, particularly CNT/Al composites. Although the excellent performance of CNT/Al composites has been reported in several experimental investigations and CNT/Al composites are promising for the development of ultra-strong, lightweight materials [8–10], few numerical studies on this material have yet to be conducted, hindering a deep understanding of the phenomena relevant to the composite [11,12].

Herein, we establish a series of 3D microscopic structural models for CNT/Al composites, in which the size, morphology, orientation, location and volume fraction of CNTs can be reproduced. For a single CNT, a detailed model is created based on statistical information gathered from numerous CNTs, such as the CNT diameter, length and orientation. The mechanical properties and interfacial behaviors of the constituent materials in CNT/Al composites are introduced to conduct uniaxial tensile tests, whereas fine meshes and proper load and boundary conditions are imposed to balance the computational accuracy and cost. With respect to the physical structures and processing factors of CNT/Al composites, the effects of model size, interfacial behavior, volume fraction of CNTs, and layered structure on the mechanical behavior of CNT/Al composites are simulated. The simulation results are in accordance with experimental data, indicating a remarkable reinforcing effect originating from the CNT structures. Overall, the 3D microscopic structural modeling method developed in this study is demonstrated to be an effective route to understand the strengthening and deformation mechanisms of CNT/Al composites.

2. Experimental procedures

To prepare CNT/Al composites, commercial CNTs functionalized with carboxyl groups (–COOH) were purchased, and ball-milled Al

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http://dx.doi.org/10.1016/j.msea.2014.07.048
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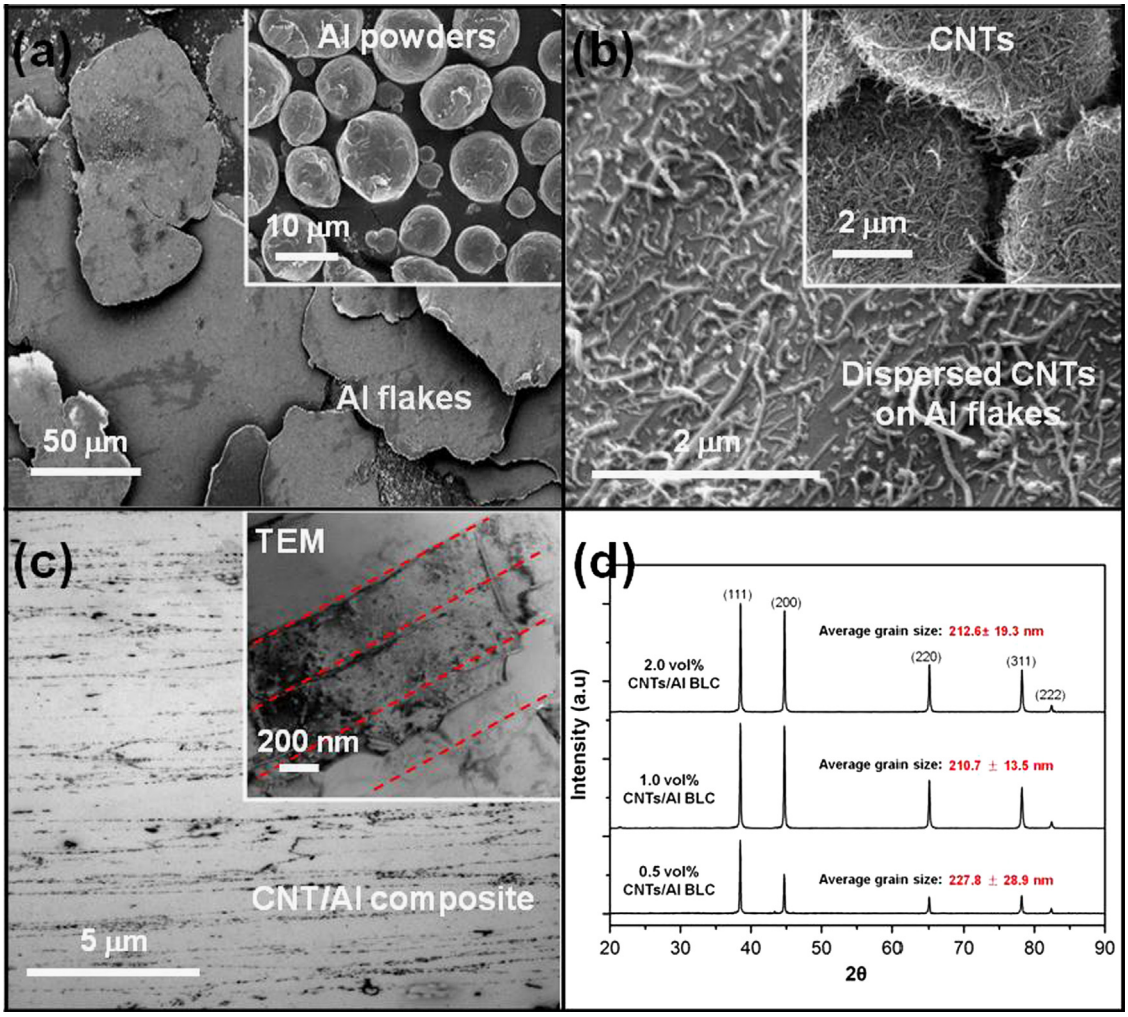

Fig. 1. Preparation and experimental tests of CNT/Al composites: (a) ball-milled Al flakes, (b) dispersed CNTs on Al flakes, (c) 1.0 vol% CNT/Al BLC and (d) Al matrix grain size.

flakes (~500 nm in average thickness) were produced from spherical powders (10 μm in diameter and 99.5% pure) [13], as shown in Fig. 1(a). The surfaces of Al flakes were then modified using polyvinyl alcohol (PVA) and uniformly mixed with the CNTs dispersed in a suspension, as shown in Fig. 1(b). The mixture of Al flakes and CNTs was then pre-heated in a flowing Ar atmosphere at 500 °C for 2 h to remove the PVA, compressed under a pressure of 500 MPa, sintered at 550 °C for 2 h, and cooled in a furnace to room temperature. Finally, the mixture was gradually heated to 440 °C and extruded to an extrusion ratio of 20:1 at a speed of 0.5 mm/min in a vacuum furnace. Therefore, CNT/Al composites denoted "biomimetic laminated composites" (BLCs) with a final compactness of over 99.5% were produced. Based on microscopic observations of the CNT/Al composites, the average thicknesses of the Al flakes were reduced to 400 nm; further details have been reported in a previous study [14]. After the preparation of the CNT/Al composites, uniaxial tensile specimens of the composites with varying volume fractions of CNTs were prepared and machined. The tests were conducted at a strain rate of $5 \times 10^{-4}\,s^{-1}$ at room temperature on a universal testing machine (AUTO-GRAPH AG-I, Shimadzu Co. Ltd., Japan). Fig. 1(c) presents the micro-structure of a 1.0 vol% CNT/Al BLC imaged on an optical microscope and a transmission electron microscope (TEM JEM-2100, JEOL, Japan), whereas Fig. 1(d) presents the grain size of the Al matrix in CNT/Al BLCs with CNT volume fractions of 0.5 vol%, 1.0 vol% and 2.0 vol%, respectively.

3. Numerical modeling

3.1. Computational structural modeling

3.1.1. Single CNT

As shown in Fig. 2(a), CNTs are an allotrope of carbon that exhibit a cylindrical structure. For microscopic structural modeling, a single CNT can be treated as two coaxial cylinders with different radii [11], as shown in Fig. 2(b), where symbols R_o, R_i and l are the outer radius, the inner radius and the length of the CNT, respectively. Moreover, the flexural morphology of CNTs is considered as well by using a random factor. To evaluate the size distribution of CNTs, such as their diameter and length, a large number of CNTs were analyzed to achieve statistical results. Fig. 2(c) and (d) presents the length and diameter distributions of numerous CNTs, respectively. These results were measured from SEM and TEM images of randomly dispersed CNTs on Al flakes.

Because the material between the outer and inner walls of single CNTs is simply graphite, a mathematical relation between the outer radius R_o and inner radius R_i can be established as follows:

$$R_i = (1 - \rho_{CNT}/\rho_G)^{1/2} R_o \tag{1}$$

where p_{CNT} and p_G are the densities of CNTs and graphite, respectively. In this work, the density of CNTs and graphite was 1.60 g/cm^3 and 2.25 g/cm^3, respectively [15]. Based on the statistical results, the