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Study of mechanical behavior of BNNT-reinforced aluminum composites using molecular dynamics simulations

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ABSTRACT

Fabrication of metallic matrix boron nitride nanotubes (BNNT) composites have remained challenging due to their high reactivity of metals at elevated processing temperatures. Recently, however, the successful fabrication of BNNT-metal composites has been reported using a plasma technique. Since carbon nanotubes (CNT), which are a structural analogy of BNNTs, easily react with aluminum to form aluminum carbides at the interface, serving as mechanically weak points, BNNTs can be a good alternative for the reinforcing component of metal-matrix composites (MMC). In this study, we conducted several molecular dynamics (MD) simulations to investigate the mechanical behaviors of BNNT-Al composites under tensile loading. The simulations provided quantitative information on the mechanical properties of the BNNT composite, revealing the effect of various BNNT diameters and volume fractions. The contributions of the BNNT and Al component to the total improvement of mechanical properties were quantified through a component analysis. The analysis revealed that the effect of the volume fraction of BNNTs is more significant than that of the size. In addition, the quantified relation between the volume fraction of BNNTs and the enhancement in elasticity can be effectively used for the engineering design of BNNT-Al MMCs.

1. Introduction

In the 1990s, two renown discoveries were made in nano-scale materials: carbon nanotubes (CNTs) in 1991 [1] and boron nitride nanotubes (BNNTs) in 1994 [2]. Due to the strong mechanical properties of CNTs, CNT-reinforced composites have received considerable attention for engineering applications with polymeric matrices [3–6] and metallic matrices [7–11]. BNNTs have attracted significant attention due to their structural similarity to CNTs, of which their lattice parameters, bond angles, and bond lengths are almost identical [12]. However, compared with CNTs, the features of BNNTs differ, including larger neutron absorption [13], superior piezoelectricity [14], superior oxidation stability [15], superior mechanical flexibility [16], and greater strength [17]. Using these characteristics, BNNT composites are considered as a promising functional material for use in mechanical reinforcements, electrical insulators, and mechanical sensors.

Most studies on BNNT composites have focused on polymer-based composites due to their manufacturability. The elasticity of polystyrene (PS) showed a 21% increase by adding only 1 wt% BNNT [18], and 10 wt% BNNT-poly(methyl methacrylate) (PMMA) composites showed a 3-fold increase in thermal conductivity [19]. It has been reported that the mechanical strength of polymer-BNNT composites can be enhanced by the chemical functionalization of BNNTs due to the strong interfacial interactions between the BNNTs and matrices [20]. Saran-polymer based BNNT composites have been demonstrated as a successful anti-degradation material against the exposure of oxygen, moisture, and radiation for organic photovoltaic devices while maintaining the high transparency in the visible region [21]. The addition of BNNTs to biodegradable polylactide-polycaprolactone copolymers (PLC) has shown a significant enhancement of mechanical properties [22]. The BNNT-PCL composite can be used for orthopedic scaffolds, suggesting their high potential for bioengineering applications.

Recently, several studies on metal-BNNT composites have been reported. Inspired by a chemical vapor deposition (CVD) approach for iron-CNT composites [23,24], iron-BNNT composites were fabricated by the CVD method [25]. The composites showed 24% higher specific yield strength and 50% higher hardness than those of pure iron due to the bridging of BNNTs across the iron particles. Recently, aluminum-BNNT composites were prepared by spark plasma sintering (SPS) and high pressure torsion (HPT) methods, showing 2 times increase in hardness and 1.5 times increase in tensile strength [26].

Compared with the experimental works, limited theoretical studies have been reported. Atomistic simulations can effectively predict the mechanical properties of nanoscale structures [27–35]. In terms of

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BNNTs, Tang et al. studied the strengthening effect at the interface between two BNNTs by molecular dynamics (MD) simulations [36]. An MD study showed that the interfacial binding strength of BNNT/polymer interfaces is stronger than that of CNT/polymer interfaces, suggesting BNNTs are more efficient nanofillers for reinforcement of nanocomposites than CNTs [37].

In this study, we conducted a series of MD simulations to investigate the mechanical behaviors of BNNT-Al composites under unidirectional tensile loading. Studies on the effect of the volume fractions and sizes of BNNT reinforcements have focused on the contribution of the enhancement in mechanical properties. In addition, MD simulations have captured detailed fracture mechanisms, including plastic deformations and crack evolution inside the composite at the atomic scale. The remainder of this paper is organized as follows. In Section 2, the MD model, interatomic potentials, and simulation conditions are described. In Section 3, the MD simulation results are provided for the effect of volume fractions and sizes of BNNTs. Finally, in Section 4, our findings are summarized.

2. MD methodology and model

The MD simulation model is shown in Fig. 1. Periodic boundary conditions (PBCs) are applied in the x, y, and z directions in order to represent the volume of the inside of the MMC. Tensile loads are applied in the z direction. We prepared four models according to the size of BNNTs as shown in Fig. 2. The aluminum matrix is created in a rectangular shape with dimensions of 60.75 Å × 60.75 Å × 83.02 Å. In the middle of the matrix, a cubic hole with a side length of 20.26 Å is generated for insertion of BNNTs. The armchair nanotubes of (4,4) BNNT, (6,6)BNNT, (8,8)BNNT, and (10,10)BNNT are placed in the hole. It was observed that the mechanical behavior of the aluminum matrix depends on the size of the hole, since the hole acts as a defect. In order to avoid the effect of the defects, the largest hole that can include all BNNTs was chosen, and the same size hole was maintained for all the simulations. To examine the effect of volume fractions, the outer boundary length of the aluminum matrix was changed. The number of atoms for each model is 18,184 (B: 277, N: 277, Al: 17,640), 19,296 (B: 408, N: 408, Al: 17,640), 19,568 (B: 544, N: 544, Al: 17,640), and 19,840 (B: 680, N: 680, Al: 17,640).

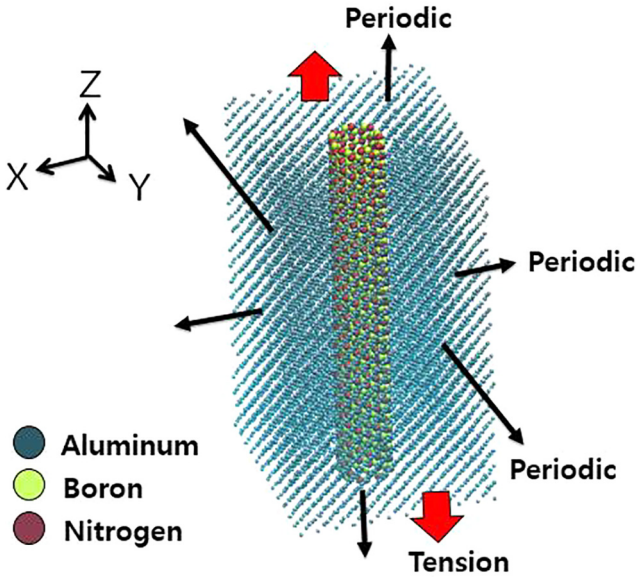

Fig. 1. Atomic model for MD simulations, representing the inside of a BNNT-Al composite material under tensile loading. The cyan, yellow, and purple atoms denote aluminum, boron, and nitrogen, respectively. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

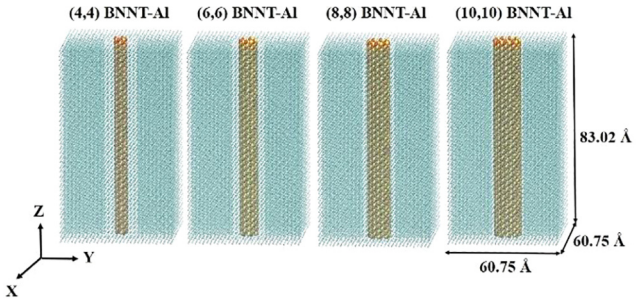

Fig. 2. Four cases with the different sizes of BNNTs inside the same size of the aluminum matrix.

Table 1
LJ potential parameters for the atomic interactions.

Atoms	Al-Al	B-B	N-N	Al-B	Al-N
ε (eV)	0.4157	0.004116	0.006281	0.04136	0.05109
σ (Å)	2.62	3.453	3.365	3.0365	2.9925
Reference	[28]	[46,47]	[46,47]	–	–

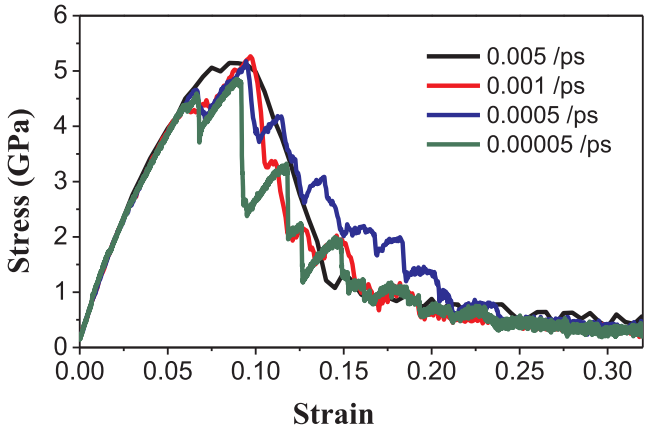

Fig. 3. Stress-strain responses at various strain rates applied to the pure aluminum material.

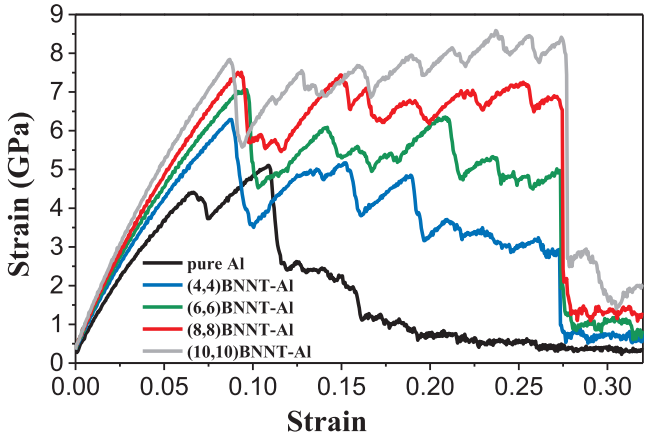

Fig. 4. Stress-strain curves of the BNNT-Al composites with different BNNTs and pure aluminum.

The B-N, B-B, and N-N interactions within the BNNTs have been described by the Tersoff potential [38]. The Tersoff potential is a three-body potential functional, which explicitly includes an angular contribution of the force. This potential has been widely used in various materials for silicon, carbon, and germanium. The potential field is