Computational Materials Science 144 (2018) 193–209

Contents lists available at ScienceDirect

Computational Materials Science

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

Mechanical behavior of a novel carbon-based nanostructured aluminum material

Ahmet Semih Erturk, Yunus Onur Yildiz, Mesut Kirca *

Department of Mechanical Engineering, Istanbul Technical University, 34437 Istanbul, Turkey

ARTICLE INFO

Article history:
Received 15 September 2017
Received in revised form 16 November 2017
Accepted 14 December 2017

Keywords:
Amorphization
Carbon based aluminum
Deformation characteristics
Mechanical behavior
Molecular dynamics
Nanocomposite

ABSTRACT

In this paper, a novel carbon-based composite material, which is a hybrid structure consisting of aluminum, fullerene and graphene units, is presented. The proposed structure is basically built by a covalently bonded fullerene-graphene sandwich structure merged into an aluminum block. In order to examine the mechanical characteristics and underlying deformation mechanisms of the structure, tensile and compressive experiments of the specimens with different types of fullerenes (i.e. C_{60}, C_{80}, C_{180}, C_{240} and C_{320}) are conducted at several loading rates (i.e. 0.5, 0.3, 0.1, 0.05 and 0.005 ps^{-1}) by performing classical molecular dynamics simulations. According to the results, it is found that for both tensile and compressive loadings the hybrid structure becomes much more sensitive to the loading rate as the size of the fullerenes increases. Furthermore, the examination of the compressive behavior shows that increase in loading rate and decrease in fullerene size improves the compressive strength of the hybrid structure. Interestingly, it is also observed that the specimens are amorphized at higher loading rates for both tensile and compressive tests, which provide the enhancement of the strength. In addition to these, a comparison between the proposed nanostructure with C_{60} fullerenes and pristine aluminum indicates an improved tensile load bearing capability at high loading rates.

1. Introduction

Since their discovery, carbon based nanomaterials such as carbon nanotube (CNT), graphene and fullerene attracted the attention of countless researchers due to their astonishingly extraordinary mechanical [1,2], electrical [3,4] and thermal properties [5,6]. Due to their significant properties, carbon nanomaterials have a superior potential to improve the applications in electronics, thermal systems and mechanical reinforcements. Enhancement of ionic polymer actuators reinforced by adding fullerene particles [7] and improvement of solar cells by using CNTs [8] are just a few examples of the exploitation of this potential.

In addition to utilizations in the pristine form of these carbon nanomaterials, researchers are also highly interested in the hybrid structure composed of their combination with each other and other nanostructural materials. Many of these studies are related to composites of polymers reinforced with carbon nanomaterials. For example, Kim et al. [9] investigated the electrical conductivity of chemically treated carbon nanotube-epoxy composites by presenting some comparisons. For the same material combination with different types of carbon materials (i.e. carbon powders and different commercial CNTs), Castellino et al. [10] examined electrical characteristics by employing simulations based on Finite Element Method (FEM). Instead of CNTs, An & Jeong [11] used different amounts of graphene (0–10 wt%) additives to prepare series of epoxy based composite films and examined their electric heating performance. As a result, they report that the electrical resistance of the composite material varies significantly from $\sim 10^{13}$ to $\sim 10^{3}$ Ω by increasing the graphene content. Furthermore, molecular dynamics (MD) simulations are performed by Jeyranpour et al. [12] to determine effects of the fullerene addition to epoxy resin on thermo-mechanical properties of the structure. Their results show that adding fullerenes decreases the thermal expansion coefficient while improving the mechanical properties such as Young's modulus and shear modulus as well as Poisson's ratio.

In addition to the many other studies about electrical properties of carbon-polymer composites [13,14], mechanical characteristics of these nanostructured composites are also intensively investigated. For instance, Kulkarni et al. [15] recovered the weakness of fiber reinforced polymer composites by replacing fibers with CNTs as a reinforcement, which increases the strength of the structure as a result of increased interaction surface. Additionally, they determined the elastic properties such as Young's modulus, shear

* Corresponding author at: Department of Mechanical Engineering, Istanbul Technical University, Inonu Cad. No: 65, 34437, Gumussuyu, Istanbul, Turkey.
E-mail address: kircam@itu.edu.tr (M. Kirca).

https://doi.org/10.1016/j.commatsci.2017.12.033
0927-0256/

modulus and Poisson's ratio of the composite structure with enhanced properties by both numerically and experimentally. In another study, Kun et al. [16] compared mechanical properties of graphene-silicon nitride composite structures by changing the amount (i.e. 1 and 3 wt%) and type of carbon nanomaterials (i.e. multilayer graphene, graphite nanoplatelets and graphene platelets). Furthermore, the effect of CNTs lengths in the composite structure with elastomer matrixes is examined by Li et al. [17]. They presented higher strength values at low strains, which is a desired characteristic for elastomers with a minor reduction of thermal and electrical conductivity.

To observe effects of carbon nanomaterials added into metals, Wang et al. [18] conducted tensile loading experiments on graphene-aluminum composite and determined its tensile strength as 249 MPa, which presents a 62% improvement over pure aluminum. In a different study, Shin et al. [19] employed few-layer graphenes and multi-layer CNTs as reinforcement units in an aluminum matrix to investigate the strengthening behavior of graphene-aluminum composite structure. Similarly, Shin & Bae [20] examined the microstructure and mechanical properties of the nanocomposite composed of aluminum alloy 2024 and few-layer graphene. Besides, fullerene-aluminum composites are studied to explore their strengthening and hardening mechanisms in [21] while their fracture toughness, which is shown to be improved to a value of 16.5 MPa $m^{1/2}$, and electrical conductivity are presented as a result of characterization and mechanical testing in [22]. Considering the CNT reinforced composites, He et al. [23] demonstrated effects of the CNT length on properties of CNT-aluminum composites produced by chemical vapor deposition method. Because of the fact that the performance of the hybrid structure is not only dependent on the CNT length but also on the diameter and density of CNTs in the composite structure, they supported their findings by numerical modelling and simulations to achieve a detailed characterization of the hybrid composite. Other than carbon-aluminum composites, Klaver et al. [24] implemented MD simulations to provide a detailed information about the coating formation and interaction of graphene on copper. Additionally, a graphene-MnO_2 composite is used as electrodes in a capacitor, which resulted in a high-performance energy storage called supercapacitor [25] and graphene is used as a coating on cobalt to improve wear and corrosion resistance of cobalt [26].

Day by day, more advanced and complicated composite structures are becoming available by fusing carbon nanomaterials with each other. In this regard, performing molecular dynamics simulations is an essential way of understanding their characteristics in detail. For instance, Wu et al. [27] investigated the deformation mechanisms of CNT-fullerene composite by using MD simulations. By the help of the same simulation method, Fang et al. [28] explored the mechanical behavior of CNT-graphene composite by presenting effects of temperature and diameter of CNTs. Furthermore, Kirca [29] designed a novel sandwich structure generated from fullerenes sandwiched between monolayer graphene sheets. The behavior of the structure is examined in detail with the aspects of mechanical energy absorption and compressive behavior by numerical experiments. The same structure is inspected by Ozturk et al. [30] in terms of its hydrogen storage, which resulted in remarkable potential of storage.

Among the numerical studies performed on the polymer-carbon nanocomposites, Zhang et al. [31] investigated the mechanical properties of graphene-CNT-polyethylene hybrid nanocomposite by focusing on the load transfer capability. Besides of polyethylene, Patole et al. [32] used same carbon combination with polystyrene to investigate the improved mechanical and thermal properties of the structure. Other than a few studies about electrical properties of these complicated polymer based nanocomposite materials [33,34], as a practical study, Chen et al. [35] enhanced the performance of capacitors by using CNT-graphene-Ni composite, which improved specific capacitance and cycling stability.

In addition to the aforementioned studies, which are concentrated on the synthesis or characterization of advanced composite structures of carbon nanomaterials, the studies about advanced nanostructures of carbon-metal nanocomposites are very limited. Motivated by this fact, a novel carbon-metal hybrid nanostructure, which can be called AFG (i.e. aluminum-fullerene-graphene) is presented in this study. This novel composite structure is formed by randomly distributed fullerenes between two graphene sheets, which are placed between two layers of aluminum. For the purpose of identifying the effect of fullerene size on the mechanical performance, different fullerene types (i.e. C_{60}, C_{80}, C_{180}, C_{240} and C_{320}) are employed for the construction of atomistic models. To understand the mechanical behavior and deformation characteristics, MD simulations are performed under compressive and tensile loading. Moreover, different loading rates are applied to observe the strain rate effect on the mechanical characteristics of this novel structure. Finally, the AFG specimen with C_{60} fullerenes is compared with pristine aluminum block to demonstrate the mechanical enhancement maintained by the proposed nanostructured material.

2. Atomistic modelling and simulation details

Proposed material architecture is illustrated in Fig. 1. According to this a sandwich-structured composite unit is created by placing graphene sheets as the sandwich skin and fullerenes as the sandwich core, which are covalently bonded to graphene sheets, between two aluminum sheets. As a pre-processing step, atomistic models of this AFG structure are generated to be utilized in MD simulations.

In the modelling process, randomly distributed fullerenes [36] are placed between two 10×10 nm monolayer graphene sheets, which are obtained by using VMD software [37], under two different distance constraints. The first constraint prevents the intersection of the fullerenes with each other while the second constraint maintains the periodic boundary conditions along the planar directions (i.e. X and Y directions) by limiting the distance between fullerenes and the edge of the model. Furthermore, two aluminum sheets with a thickness of 2 nm are placed on both upper and lower free surfaces of graphene sheets by allowing a distance of 0.224 nm, which is considered as the bond length between aluminum and carbon atoms as referenced in [38].

For MD simulations, an open source code, namely LAMMPS (i.e. Large-scale Atomic/Molecular Massively Parallel Simulator), which is developed by Sandia National Laboratories [39], is employed. To represent atomic interactions between carbon atoms (i.e. fullerene and graphene), Adaptive Intermolecular Reactive Empirical Bond Order (AIREBO) potential is employed while Embedded Atom Method (EAM) with an appropriate potential file is used for force calculations between metal atoms (i.e. aluminum). Moreover, Morse potential is utilized with the parameters referenced in [40] for hybrid interactions between carbon and metal atoms.

The covalent bonding between fullerenes and graphene sheets are created by using heat welding method [41], which is, in general, an annealing process applied at high temperatures to the junction regions between fullerenes and graphene sheets. In Fig. 2, created bonds and junction regions for one fullerene are shown. In order to accelerate the heat welding process, junction regions are pre-conditioned by removing the atoms encapsulated by a spherical volume, which is centered at a point where the fullerene and the graphene sheet intersects. The diameter of this spherical volume is adjusted to different values for the different fullerene types.