

Atomistic simulation study of mechanical properties of periodic graphene nanobuds



A. Fereidoon^a, M. khorasani^b, M. Darvish Ganji^{c,*}, F. Memarian^{a,*}

^a Department of Mechanical Engineering, Semnan University, Semnan, Iran

^b Department of Mechanical Engineering, Semnan Branch, Islamic Azad University, Semnan, Iran

^c Young Researchers and Elite club, Central Tehran Branch, Islamic Azad University, Tehran, Iran

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ABSTRACT

Among the graphene-based hybrid nanostructures, graphene nanobuds (GNBs); a hybrid of graphene/fullerene architecture, are one of the most interesting nanostructured materials. In this study we have investigated the mechanical properties of graphene nanobud through molecular dynamic simulations. The effects of temperature, size of graphene sheet and also neck's length on the mechanical properties of this novel material were investigated, for the first time. The calculated Young's modulus ranges from 440 to 760 GPa and the failure stress changes from 100 to 200 GPa. The results show that the Young's modulus changes a little with temperature increment while, with increasing the neck's length the Young's modulus decreases. We found that with both temperature and neck's length increment, the failure stress decreases. Furthermore, when the size of graphene sheet was increased all the respected mechanical properties were increased too. These findings will augment the current understanding of the mechanical performance of GNBs, which will conduct the design of GNBs and shed lights on its various applications.

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1. Introduction

Graphene is an allotrope of carbon in the form of a two-dimensional, atomic-scale, hexagonal lattice which consists of covalently bonded carbon atoms. Its intrinsic strength, predicted to exceed that of any other material. Many studies have shown that graphene Young's modulus is around 1 TPa and its fracture strength is above 100 GPa [1–9]. Also graphene is the basic structural element of other allotropes, including graphite, charcoal, carbon nanotubes and fullerenes. Fullerene C₆₀, which is discovered in 1985 [10], is a molecule composed entirely of 60 sp²-hybridized carbon atoms which forms a hollow sphere with twenty hexagonal and twelve pentagonal rings [11]. Because of its exceptional structure, fullerene has the ability of attaching to different atoms or small molecules for modification or getting better properties [12]. Although fullerene has remarkable properties such as super conductivity, ferromagnetism, mechanical strength and thermal stability, because of its weak accessibility these properties are still unknown [13]. Two types of C–C bonds occurs in fullerene: one

type between hexagonal and pentagonal rings and the other between two hexagonal rings (Fig. 1(a)) [14]. The discoveries of these carbon nanostructures have played critical roles in the advancement of modern nanoscience and nanotechnology [15], due to their supernatural electrical [16], mechanical [5] and thermal [17] properties. Over the past decade, many efforts have been done to synthesize hybrid of carbon nanostructures with novel properties. The first hybrid nanostructure which is experimentally fabricated was carbon nanopeapod [18], in which carbon nanotube encapsulating fullerenes. Carbon nanobud (CNB) is another hybrid nanostructure which was constructed successfully in 2007. In this structure one or two C₆₀ molecules covalently attached to the sidewall of single-walled carbon nanotubes (SWCNTs) [19]. It is expected that chemical interactions between C₆₀ and SWCNT modified CNBs properties. In addition presence of C₆₀ molecules weakening the tendency of adhesion among SWCNTs and prevent slipping of SWCNTs in composite materials. So it is predicted that CNBs with mentioned operation can increase mechanical properties of composite materials [11].

Another hybrid nanostructure which is predicted theoretically, is obtained from fullerene and graphene sheet. The combination of these two novel structures, will develop a 3D carbon-based network, which is named graphene nanobuds (GNBs) [20]. GNBs can reinforce composite materials similar to CNBs and it is forecasted

* Corresponding authors. Tel./fax: +98 1132320342 (M.D. Ganji). Tel./fax: +98 23 33383331 (F. Memarian).

E-mail addresses: ganji_md@yahoo.com (M.D. Ganji), f-memarian@semnan.ac.ir (F. Memarian).

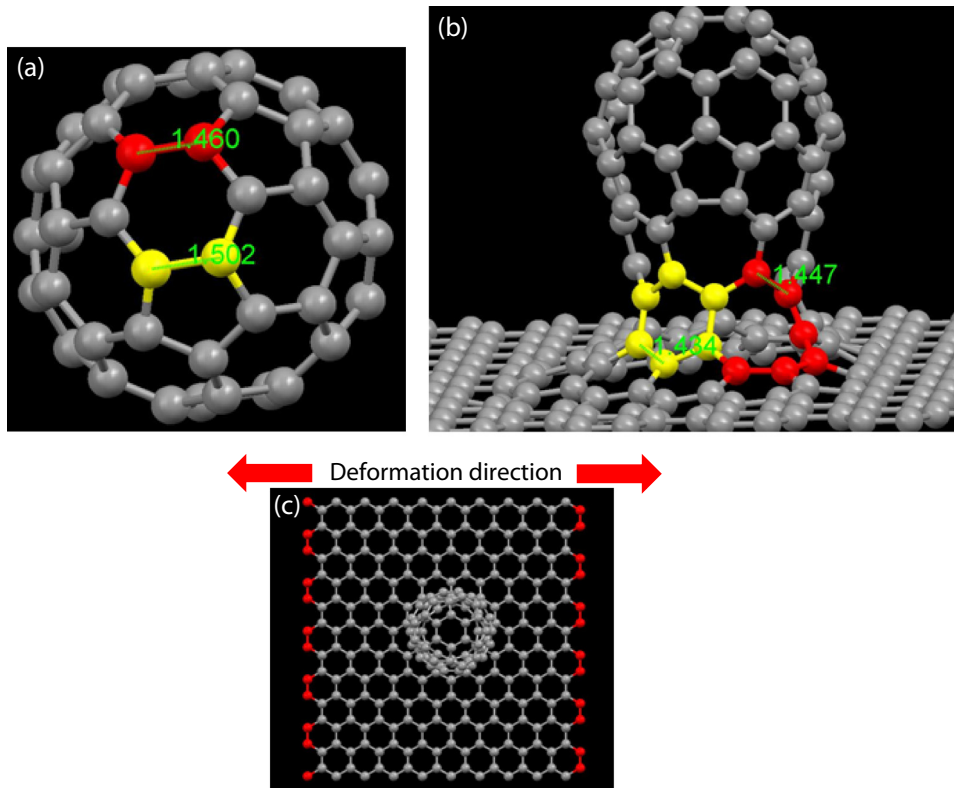


Fig. 1. (a) Two types of C–C bonds occurs in fullerene, (b) octagonal and hexagonal rings at junction region, and (c) GNB under tension load along armchair direction.

that mechanical properties improve significantly in the presence of this unique nanostructure. Different properties of GNBs were investigated in recent years. Wang et al. [21] studied the magnetic properties of GNBs using spin-polarized density functional theory. Furthermore by using GCMC simulations the mechanism of argon adsorption onto GNBs were investigated [22]. Also structural and electronic properties of two prototype periodic GNBs by means of the *first-principles* calculations was considered by Wu et al. [20].

In GNBs, fullerenes are attached to a graphene monolayer. These junctions can formed differently: in first type C_{60} molecules are covalently bonded to a graphene monolayer [20] whereas in second type fragmented C_{60} are fused onto a defective graphene monolayer [20]. In both cases, the C_{60} molecules form a periodic lattice on the graphene monolayer. In this study we use the second type with different length of neck attached to defective graphene sheet. Effects of these junctions in electronic structures and thermal transport [23,24] have been studied, but how the mechanical properties can be affected by junctions is a novel field of interest that is investigated in this study. GNBs can reinforce composite materials similar to CNBs and it is forecasted that mechanical properties improve significantly in the presence of this unique nanostructure.

Temperature is an important factor for producing new hybrid nanostructure and usually these structures are fabricated in high temperature [25]. Also carbon-based materials are useful in many electronic devices working in high temperature such as CPUs [26], transistors [27], diodes [28] and capacitors [29]. Furthermore from reported studies we believe that the elastic properties of single layer graphene sheet, such as Young's moduli is temperature-dependent [30]. So elastic properties of the combination of graphene sheet and fullerene is predicted to be temperature dependent. Therefore understanding the behavior of GNBs in different temperatures is necessary for fabricating high quality

graphene based devices. Because of above mentioned reasons, in this work a series of GNBs are investigated in eight temperatures in order to consider effect of temperature on mechanical properties of GNBs entirely. Furthermore, additional attention is paid to the role of junctions, necks length and sheet size in the 3D network to gain further conception insight into the different mechanical properties. The revealed understanding of junction's role at molecular-level can help control the performance of these structures [31].

2. Atomistic modeling of graphene nanobud

The powerful Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) code and Visual Molecular Dynamics (VMD) visualizer were performed for studying mechanical properties of GNBs. VMD software was used for animating and coloring molecules which supports more than 60 molecular file formats including LAMMPS output files [32]. The adaptive intermolecular reactive empirical bond order (AIREBO) potential was employed as a force field in LAMMPS package [33]. The AIREBO potential which was originated from Tersoff–Brenner potential allows the intermolecular and torsional interactions [34–36] in addition to the simulation of bond breaking and formation. So this potential can easily shows failure process in nanostructured systems. The AIREBO potential can be represented by a sum over pairwise interactions, including covalent bonding REBO interactions (E_{ij}^{REBO}), LJ terms (E_{ij}^{LJ}), and torsion interactions (E_{kijl}^{TORS}) [30].

The full expressions of energy items are given in Eq. (1) [37].

$$E = \frac{1}{2} \sum_i \sum_{j \neq i} \left[E_{ij}^{REBO} + E_{ij}^{LJ} + \sum_{k \neq i, j, l \neq i, j, k} E_{kijl}^{TORS} \right] \quad (1)$$

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