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Mechanical properties of defective hybrid graphene-boron nitride nanosheets: A molecular dynamics study

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ABSTRACT

In this paper, by using molecular dynamics simulation, the mechanical properties of butt-joined hybrid graphene-boron nitride (BN) sheets in the presence of various defects have been investigated. For this purpose, two types of defects including circular and square holes have been created in the examined specimens. The effects of increasing the hole diameter, hole length (circular and square), number of holes and also the effect of different locations of such defects in hybrid graphene-boron nitride sheets on their mechanical properties have been analyzed and discussed. The findings indicate that the presence of holes in the considered structures reduces their mechanical properties including the failure strength and strain and Young's modulus; but the effect of such defects on Young's modulus is much less than that on the other two mechanical parameters. Also, it has been demonstrated that the circular holes have a less severe effect on mechanical properties than the square holes. For example, by making circular holes of 10 Å diameter in a hybrid graphene-boron nitride sheet in the left graphene region (GFL), its failure strength is reduced 20% relative to that of a defect-free structure; while the Young's modulus diminishes by 10% under the same conditions. Different cases of these defects in the structure of hybrid graphene-boron nitride nanosheets and their effects on mechanical properties have been explored for the purpose of using them in nanotransistors and nanodiodes. As a key result, it was observed that the hybrid sheets behave as a more ductile material when the density of the defects increases.

1. Introduction

While the atomic structures of 2D materials such as graphene and boron nitride, with a 2% lattice mismatch in the interface in the newest syntheses of these materials, have attracted the attention of researchers, the combination of these two materials by means of sturdy interfaces or connections can lead to even more interesting functional properties [1]. Because of the band gap produced by integrate pure graphene and pure boron nitride, the electronic properties of hybrid super-layers resulting from these two materials can be tuned. Also, due to their structural similarity, when these two materials are combined, boron nitride is able to produce a band gap in graphene (which has a band gap of zero), which can be exploited in the nanoelectronics industry [1–3]. In recent years, many researchers have studied the presence of holes and defects within these two materials, whether in pure or hybrid forms. However, the semiconductor form of graphene, being free of any holes and cavities, has caused some limitations in the manufacturing of transistors. Some researchers have tried to create controlled pores in graphene and also other 2D materials structures [4–6]. In 2008, by producing small holes in thin graphene layers and thin sheets of carbon atoms and creating nanopores in graphene by means of electron radiation, Bayley investigated the application of such materials in medicine and in drug delivery within human body [7]. In 2012, by means of quantum computations, Brunetto et al. showed that porous graphene can automatically form 2D carbon allotropes called biphenylene carbon. Also, while porous graphene shows an inherently nonzero gap, carbon biphenylene presents well delocalized frontier orbitals, indicating a structure of high electrical activity [4]. In 2012, Ansari et al. employed molecular dynamics simulation to demonstrate the effect of pore defects on the mechanical properties of single-layer graphene. They maintained that structural defects slightly reduce the failure strain and strength, but their effect on Young's modulus is very negligible. They also showed the effects of force and load on single-layer graphene in both the armchair and zigzag directions and proved that the armchair direction is stronger in a defective graphene and that the holes and defects have much less of an effect in this direction [8]. Hydrogen separation by means of porous graphene membranes is another work carried out in recent years. In 2014, Tao et al. employed two computational methods of molecular dynamics and DFT to explore the performance of 2D porous graphene in hydrogen separation and

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refinement. Their findings indicated that, like other gas molecules found along with H_2 in industrial vapors (e.g. N_2, CO and CH_4), the H_2 molecules are extremely sensitive to the size of holes in graphene membranes. They also showed that the energy barrier of gas molecules that pass through a graphene membrane is generally increased by reducing the size of pores or increasing the kinetic diameter of molecules; which is due to the overlapping of different electrons between gas and membrane [9]. In 2015, porous graphene was used as a weed barrier for molecules. In this work, "holey graphene", produced by making numerous holes in graphene, was used as a mask against molecular adsorption [10]. Numerous reports have been presented in recent years regarding works on boron nitride (BN) nanoholes. In 2009, Meyer et al. investigated the preparation element selective damage mechanism in atomically thin boron nitride membranes. In this work, triangular holes appear in line with the crystallographic direction of each layer, and the defects are compared with those in graphene membranes. These researchers showed that, like graphene, thin boron nitride membranes can exist in a quasi-two-dimensional allotrope without requiring for a substrate [11]. In 2016, Abadi et al. used molecular dynamics simulation to explore the effects of crack propagation and existing notch on the mechanical properties of polycrystalline boron-nitride nanosheets. There, the effect of crack size on crack propagation velocity and direction was explored. Their findings indicate that a central crack reduces the tensile strength and failure strain of these nanosheets considerably, and that this reduction is independent of initial crack length. They also maintained that the samples' mechanical properties depend on crack position in these samples [12]. In another work, boron carbon nitride (BCN) nanosheets have been used as efficient metal-free catalysts for oxygen reduction reaction in both alkaline and acidic solutions. This report presents a novel approach for making metal-free oxygen reducing catalysts for industrial-scale fuel cells [13]. Also in 2016, Garnier et al. employed molecular dynamics simulation to study the surface tension of water on multilayer graphene and boron nitride nanosheets and to investigate the permeation of water through nanopores in BN and graphene membranes. They showed that surface tension is reduced by increasing the number of layers in multilayer graphene sheets. They attributed the negative surface tensions to the long-range wetting of water and also to the lower infiltration of water through two-layer membranes relative to single-layer membranes. They also demonstrated that the smaller surface tension of water on a single-layer boron nitride membrane with regards to graphene is due to the increased water permeation through the BN membrane. Their findings indicated that nanoporous BN membranes can be good candidates for water purification applications [14]. In a molecular dynamics study, Kommu and his colleague investigated the separation of water and ethanol by means of BN and graphene slit pores. They claimed that water contaminants can be removed by using nanoporous graphene and boron nitride. Their findings indicate that contaminant removal efficiency depends on pore width and the type of pore walls. Also, for all the considered pore widths, selectivity of ethanol is relatively higher for BN pores compared to the graphene pores. By reducing the pore width, the diffusion coefficients of water and ethanol molecules are reduced significantly for both graphene and boron nitride surfaces [15]. Shahbabaei and colleague used molecular dynamics simulation to investigate water transport mechanisms through nanoporous structures of graphene and boron nitride multilayers. Their results show that by increasing the water flow rate the inter-layer distance increases as well and also, due to a greater energy blocking and friction force, BN multilayers exhibit a weaker flow through them than graphene multilayers. In boron nitride multilayers, the friction force increases considerably with the increase in the number of layers; while in graphene, the friction force is independent of the distance between layers [16].

Using molecular dynamics simulation, extensive research works have been conducted to analyze the mechanical properties of defect-free graphene and boron nitride. In 2016, Sadeghzadeh employed molecular dynamics simulation to investigate the mechanical properties of pure defect-free graphene and obtained the Young's modulus, failure strength and failure strain of this material as 833 GPa, 139 GPa and 0.275, respectively [17]. Also, by altering the simulation conditions, Mortazavi et al. have determined the Young's modulus of pure graphene as 960 GPa. In exploring the mechanical properties of pure boron nitride through molecular dynamics simulation, Mortazavi et al. have obtained the Young's modulus, failure strength and failure strain of BN single-layer as 825 GPa, 165 GPa and 0.28, respectively [18].

The extensiveness of the conducted works point to the importance of studying the mechanical characteristics of thin graphene and boron nitride layers, whether as pure and separate materials or as hybrids. There are some studies on the properties of grain boundaries in hybrid graphene – BN sheets. The mechanical properties of grain boundaries in planar heterostructures of graphene and h-BN were studied using the molecular dynamics method in combination with the density functional theory and classical disclination theory [19]. The hybrid interface between graphene and h-BN grains was optimally matched by a non-bisector grain boundary composed of pentagon–heptagon defects arranged in a periodic manner [20]. Recently, the authors studied the effect of the interface structure on the mechanical properties of a hybrid graphene/boron nitride [21].

In recent years, the idea of using nanoporous graphene and boron nitride materials under various conditions and for a variety of applications has engaged the minds of many researchers. Hence, it is important to understand what effects the nanopores in defective graphene and boron nitride will have on their mechanical properties and what mechanical loads and pressures can be withstood by defective hybrids made of these two materials. Most importantly, how will a defect in the most important part of a hybrid graphene-boron nitride sheet (i.e. the interface (connection point) of two single-layers) affect the mechanical properties we expect to see? As is shown in Fig. 1, because of the defects that may arise at the interface of graphene and boron nitride layers during the synthesis process or even during the use of these hybrids, the bonding between atoms is weaker at these boundaries, and these defects could lead to functional drawbacks.

In the present work, the presence of circular and square holes and defects in the structure of graphene-boron nitride hybrid plates and the mechanical properties of such defective material have been investigated. Also, the effects of the size, location and number of holes on mechanical properties have been studied by means of molecular dynamics simulation.

2. Theory and modeling

The molecular dynamic simulation in this paper has been performed by using the large-scale atomic/molecular mass parallel simulator (LAMMPS) [22]. The interactions between carbon, nitrogen and boron atoms have been described by means of Tersoff Potential, which has been reported by Kinaci et al. [23]. In this potential, the relationship between the energy and the displacement of atoms relative to one another is expressed by the following equation:

$$U_{ij} = f_c(r_{ij})[f_R(r_{ij}) + b_{ij} f_A(r_{ij})] \tag{1}$$

Function $f_R(r_{ij})$ expresses the repulsion potential of two particles, i.e. nucleus-nucleus interaction, and $f_A(r_{ij})$ represents the attraction potential resulting from valence electrons. b_{ij} denotes a bond strength term that depends on the local atomic medium around a specific bond and is a decreasing function of atoms rearrangement number. b_{ij} contains all the potential multi-particle effects. The existing functions in these potentials are expressed by the following equations [24]:

$$f_R(r_{ij}) = -A_{ij} e^{-\lambda_{ij} r_{ij}}, \quad f_A(r_{ij}) = -B_{ij} e^{-\mu_{ij} r_{ij}}$$