Mechanical properties of a G/h-BN heterobilayer nanosheets coupled by interlayer sp³ bonds and defects

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Abstract

The mechanical properties of graphene/hexagonal boron nitride (G/h-BN) heterobilayer nanosheets coupled by interlayer sp³ bonds and defects have been investigated by using the molecular dynamics (MD) simulation. For this purpose, interlayer sp³ bonds and two kinds of geometric imperfection (including rhombus and square nanopore) are formed in the G/h-BN heterobilayer nanosheets. The effects of adding the nanopore diameter, interlayer sp³ bonds fraction, and the influence of different position of geometric imperfection in heterobilayer nanostructure on mechanical properties have been investigated. The result shows that when sp³ bonds and nanopore coexist, the mechanical properties of defective graphene layer are higher than that of defective hexagonal boron nitride (h-BN) layer. Meanwhile, the negative effect of rhomboid nanohole on mechanical properties of heterostructure is weaker than that of square nanohole. It is observed that that interlayer sp³ bonds have greatest influence on the fracture strain of G/h-BN heterobilayer nanostructure, followed by fracture stress, and finally Young’s modulus. Another important point is that interlayer sp³ bonds can be regarded as a special defect, and its value seems to outweigh the intrinsic defects.

Abbreviations

- graphene/hexagonal boron nitride (G/h-BN)
- Van Der Waals Interaction (vdW)
- graphene (G)
- hexagonal boron nitride (h-BN)
- thermal conductivity (TC)
- large-scale atomic/molecular mass parallel simulator (LAMMPS)
- carbon (C)
- boron (B)
- nitride (N)
- Lennard Jones (LJ)
- molecular dynamics (MD)
- constant pressure and temperature (NPT)
- Multi-walled carbon nanotubes (MWCNTs)
- 1/2Lₓ region of upper layer graphene (CG)
- 1/4Lₓ region of upper layer graphene (LG)
- 1/2Lₓ region of lower layer boron nitride (CBN)
- 1/4Lₓ region of lower layer boron nitride (LBN)
1. Introduction

Graphene is made up of carbon atoms of covalent bonding, and because of its unique properties. It triggers prosperity in different fields [1, 2]. This superior performance and promising applications make it available in a wide range of areas, such as structural reinforced composites [3–5] and Nano electromechanical systems [6, 7]. However, Graphene has a band gap of 0, which may limit its use in some applications. Because of Van Der Waals Interaction (vdW), double-layer and multilayer graphene has different characteristics from single-layer graphene. For example, Yancong Qiao et al reported that multilayer graphene epidermis electronic skin has a very high sensitivity. Multi-layer graphene can be directly applied to the skin, in a more comfortable and stable way to detect breathing and heart rate [8]. Again, Youguo Yan et al reported that compared with the two-dimensional channel of single-layer graphene, the three-dimensional channel of multilayer graphene has stronger ion selectivity. At the same time, the chiral channel also realizes the selective transshipment of the enantiomers [9]. In another work, Chen Xudong et al found that twisted double-layer graphene has electrical and optical properties, which is different from single-layer graphene.

More importantly, the angle of rotation between layers can be adjusted according to its nature [10]. From a structural point of view, graphene is similar to h-BN, and their lattice difference is only 2% [11, 12]. As a result, the hybrid structures made up of them can achieve better performance, and these hybrid structures exhibit superior performance [13–15]. In recent years, a good idea for stacking single layers, including graphene and boron nitride, has led to vdW heterogeneous structures [16, 17]. In order to achieve excellent performance, the hybrid structures are combined with the physical and chemical properties of each phase [18–21].

In recent years, the idea of using G/h-BN heterobilayer with interlayer sp³ bonds and for a hot trend has been set off in new fields. For example, by using MD simulation, interlayer sp³ bonds are created in graphene with different layers. Guo et al investigated that the influence of sp³ bonds on the thermal conductivity (TC) of graphene with different layers. They found that interlayer sp³ bonds can greatly reduce thermal conductivity to 80%, and tensile strain can reduce thermal conductivity further by up to 50% [22]. Furthermore, Y Y Zhang et al studied the effect of interlayer sp³ bonds on the mechanical properties of bilayer structure by using molecular dynamics simulation. The result indicated that sp³ bonds will decrease the mechanical properties of bilayer structure [23]. In 2018, by creating sp³ bonds in G/h-BN heterobilayer, T. Iwata et al revealed that a few sp³ bonds drastically decreases TC of system, while TC of G/h-BN heterobilayer gradually increases when fraction sp³ bonds exceeds 0.25 [24]. Also, Rajabpour et al proposed that sp³ bonds may be considered a defect for graphene [25].

In recent years, the trend of heat, interlayer interaction and Electron properties of G/h-BN heterogeneous bodies has been reported [24]. However, its mechanical properties are rarely reported. Therefore, an important issue to be studied is how interlayer sp³ bonds affect the mechanical properties of G/h-BN heterobilayer nanostructure and how much they affect. Most importantly, how much stress a hybrid system bear compared with the pristine? Moreover, what would happen to the mechanical properties of graphene if it had both interlayer sp³ bonds and defects?

In this paper, interlayer sp³ bonds and defects are formed in the G/h-BN heterobilayer nanostructure. Its mechanical properties have been analyzed. In addition, the effects of different conditions on mechanical properties were studied by molecular dynamics method, including the diameter (length), position and different kinds of nanopore (square and rhombus nanopore), and the number of interlayer sp³ bonds.

2. Computational model and method

The MD simulation Software (large-scale atomic/molecular mass parallel simulator, LAMMPS) [26] in this paper has been completed.

In the current study, Tersoff potential is better to play and calculate the short-range interaction between carbon (C), boron (B) and nitride (N) atoms [27, 28]. Therefore, in our simulation, the in-plane interaction between carbons has been characterized by Tersoff Potential, which has been studied by Rajasekaran G [29]. In addition, the in-plane interaction between boron and nitride is characterized by the Tersoff potential [30]. Like with previous work [24], the short interactions between C and B atoms should also be characterized for their interlayer sp³ bonds by Tersoff Potential, which was investigated by Kinaci et al [31]. Another point is that the long-range interaction between carbon, boron and nitride should be characterized by the potential of Lennard Jones (LJ) [32].

The simulated values between carbon, boron and nitrogen in this article are shown in table 1. In this section, we assume that the Tersoff and LJ potential energy are related to the named Atomic group parameters. For
example, suppose the boron atoms are present in the h-BN layer, and these boron atoms do not have interlayer bonds, so the first set of atoms (group-1) is boron atoms. In addition, if boron belongs to the h-BN region, it also contains the B-C interlayer bond, and then the boron atoms are called the second set (group-2). In addition, it should be assumed that carbon atoms exist in the graphene layer, and these carbon atoms do not have interlayer bonds, so the carbon atoms are called the third set (group-3). Eventually, there are nitrogen atoms in the boron nitride layer, and these nitrogen atoms do not have interlayer bonds, and then the nitrogen atoms are called the group-5. In the current work, Table 2 shows the potential for parameters related to named atomic groups, which are used to calculate the interactions between named atomic groups.

First of all, the numerical model of G/h-BN heterobilayers with interlayer sp³ bonds are formed for six types of sp³ bonds content 0%, 1%, 2%, 3%, 5% and 10%. In the present simulation, all G/h-BN heterobilayers are with length 129.12 Å, with width 29.82 Å. The lattice constants of graphene and h-BN are displayed to 2.46 Å and 2.51 Å, respectively. Although this lattice constant setting results in a lattice mismatch of about 2% h-BN. According to the former works, for example, results of Zou [33], Zhang [34] and T. Iwata [35], exhibit that the effect of a lattice mismatch of about 2% on properties of G/h-BN nanostructures can be ignored. We assume that the interlayer distance is 0.3389 nm. The assumptions of the simulation are consistent with previous work [24]. In this simulation work, a G/h-BN heterostructure containing B–C interlayer sp³ bonds of content 3% as an example. Figure 1 shows local side view of a G/h-BN heterostructure containing B–C interlayer sp³ bonds of content 3%.

Next, nanopore was created in G/h-BN heterostructure with B–C interlayer sp³ bonds. Two kinds of geometric imperfection (rhombus and square nanopore) at four different positions in the heterostructure were established. Figure 2 shows panorama of G/h-BN heterostructure coupled by interlayer sp³ bonds and rhombus nanohole. Figure 3 exhibits panorama of G/h-BN heterostructure coupled by interlayer sp³ bonds and square nanohole.

Last but not least, we studied the mechanical properties of G/h-BN heterobilayer nanosheets coupled by interlayer sp³ bonds and defects. In this section, the X, Y and Z directions are all periodic conditions, the time step is 0.5 fs. Before uniaxial tensile strain is applied along the X direction, the energy minimization method is used to simulate the strain in equilibrium state. In the whole computational simulation, we adopted the Nosé-Hoover arithmetic of 50 ps under constant temperature and pressure (NPT). The strain rate of the tested model is 0.001 ps⁻¹ during the tensile load. All mechanical simulations are performed at 300 K.

3. Results and discussion

3.1. Validation

To verify the simulation, tables 3 and 4 show the results of previous work compared with the three mechanical values (fracture stress, strain and Young’s modulus) of graphene and boron nitride in this study.

As shown in tables 3 and 4, the comparison shows that the calculation method and the selection of potential function are very reasonable, and the results obtained are also very consistent with previous work. For example, Young’s modulus of boron nitride and graphene were found to be 925 GPa and 923 GPa, respectively. These values in the study have approached to the corresponding experimental value of 1000 GPa and previous simulation value of 889 GPa. Again, fracture stress and strain in the study has also approached to the previous work.

3.2. Mechanical properties of a G/h-BN heterobilayer nanosheets coupled by interlayer sp³ bonds and defects

The interwall bonds are created for graphite and pristine Multi-walled carbon nanotubes (MWCNTs) by using femtosecond laser excitation and electron irradiation in previous reports [33, 34]. The research results show that mechanical properties of MWCNTs with interwall sp³ bonds are higher than that of pristine. It can be attributed the fact that the formation of interwall sp³ bonds plays an important role in increasing mechanical properties of MWCNTs. Moreover, YY Zhang et al studied that the effect of interlayer sp³ bonding on mechanical properties of double layer of graphene sheet. Their finding show that in the presence of sp³ bonding,
**Table 2.** Usage of the Tersoff and LJ potentials for a G/

| Named atomic groups | 1–3 | 1–4 | 1–5 | 2–3 | 2–4 | 2–5 | 3–3 | 3–4 | 3–5 | 4–5 |
|---------------------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| Applied potential   | LJ B-C | LJ B-C | Tersoff B-N | LJ B-C | Tersoff B-C | Tersoff B-N | Tersoff C-C | Tersoff C-C | LJ C-N | LJ C-N |

The group numbers of atoms from 1 to 5 are defined in the text.
Figure 1. Local side view of a G/h-BN heterostructure containing B–C interlayer sp³ bonds of content 3%.

Figure 2. Panorama of G/h-BN heterostructure coupled by interlayer sp³ bonds and rhombus nanohole (Rhombus nanohole in four different of region) (Lx is the length of the heterostructure).

Figure 3. Panorama of G/h-BN heterostructure coupled by interlayer sp³ bonds and square nanohole (Square nanohole in four different of region) (Lx is the length of the heterostructure).
the shear modulus and load transfer rate of bilayer can be improved [23]. However, due to the limitations of preparation methods and equipment conditions, the synthesis of heterogeneous double-layer nanomaterials, various geometrical shapes, dimensions and types of defects may occur anywhere in the nanostructure. So, if defects and interlayer sp³ bonds appear in the heterobilayer hybrid nanostructures in the same time, what impact it have on the mechanical properties of the hybrid nanostructures? What types of defects, in the heterobilayer hybrid nanostructures couple with interlayer sp³ bonds, and can perform the mechanical properties that we expect to see? More importantly, where does the defect appear in heterobilayer hybrid nanostructures containing interlayer sp³ bonds, can the system have better mechanical properties?

A series of interlayer sp³ bonds and controlled defects are created in G/h-BN heterobilayer nanostructures in order to tune its mechanical properties. It also provides a significant insight for adjusting other properties of G/h-BN heterobilayer nanostructures.

### 3.3. The effect of rhombus defects and interlayer sp³ bonds coupling

In this section, different sizes of rhombus defects have been formed in four types of regions of G/h-BN heterobilayer nanostructures with six kinds of interlayer sp³ bonds: one nanopore in $\frac{1}{4}L_x$ region of upper layer graphene (CG), one nanopore in $\frac{1}{4}L_x$ region of upper layer graphene (LG), a nanopore in $\frac{1}{4}L_x$ region of lower layer boron nitride (CBN) and a nanopore in $\frac{1}{4}L_x$ region of lower layer boron nitride (LBN), as shown in figure 2. Finally, for each region, mechanical properties of a G/h-BN heterobilayer nanosheets coupled by different fraction of interlayer sp³ bonds (0%, 1%, 2%, 3%, 5% and 10%) and different diagonal length of rhombus defects in length direction (0, 10 and 20 Å) have been investigated. The stress-strain curves for defect-free G/h-BN heterobilayer nanostructures with different interlayer sp³ bonds fraction are observed in figure 4. Variations of three mechanical values for different cases of rhombus hole are shown in figure 5. It is noted in figure 5 that CG-10 Å represents diagonal length 10 Å of rhombus nanopore in CG region, and other symbols are the same as before.

In general, the fracture stress and strain of heterogeneous structures do follow a similar trend. For example, with the increase of the size of the nanohole and the number of nanoholes, the fracture stress and strain of heterogeneous structures decrease, and these two mechanical values usually show a decreasing trend of similarity. However, in the upper graphene layer of G/h-BN heterobilayer nanosheets, fracture strain decreases by 25% when the fraction of interlayer sp³ bonds is 5%, its fracture stress diminishes only by 14.57%, relative to that of pristine model. In addition, Young’s modulus is not in line with the overall trend, and its Young’s modulus is down 10.7% according to the previous example. It is also observed that, under the same conditions, the mechanical value of the defective lower h-BN layer is similar to that of the upper graphene layer. These trends are different from the general situation, as shown in figure 4. As a result, an important point can be obtained that when interlayer sp³ bonds exists, they have the greatest influence on the fracture strain of G/h-BN heterobilayer nanostructure, followed by fracture stress, and finally Young’s modulus. Another important point is that the

| Table 3. Comparing the mechanical properties of pure graphene achieved by the present study and by previous experimental and computational works. |
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| **Direction** | **Various types** | **Assessment Method (Potential)** | **Failure strain** | **Failure strength (GPa)** | **Young’s modulus (GPa)** | **References** |
| AC | Single-layer | MD (Tersoff) | 0.208 | 127 | 925 | Present study |
| AC | Single-layer | MD (Tersoff) | 0.24 | 125 | 889 | Zhao et al [36] |
| AC | Single-layer | MD (Airebo) | 0.17 | 105 | 890 | Pei et al [37] |
| — | Two-layer | MD (Airebo) | 0.184 | 86.53 | 907 | Zhang et al [23] |
| — | — | Experimental | 0.13 | 90 | 1000 | Zhao et al [38] |

| Table 4. Comparing the mechanical properties of boron nitride achieved by the present study and by previous experimental and computational works. |
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| **Direction** | **Various types** | **Assessment Method (Potential)** | **Failure strain** | **Failure strength (GPa)** | **Young’s modulus (GPa)** | **References** |
| AC | Single-layer | MD (Tersoff) | 0.210 | 128 | 923 | Present study |
| AC | Single-layer | MD (Tersoff) | 0.332 | 133.2 | 881.1 | Han et al [39] |
| AC | Single-layer | MD (Airebo) | 0.280 | 120.4 | 716.3 | Zhao et al [36] |
| AC | Single-layer | MD (Tersoff) | 0.3 | 150 | 800 | Bohayra et al [40] |
| — | — | Experimental | — | — | 881 | Bosak et al [41] |
mechanical properties of a defective G/h-BN heterobilayer nanosheets decrease with increase of sp³ bond fraction. In addition, the interlayer sp³ bonds can be seen as a special defect in heterobilayer nanostructure.

Figure 5 shows variations of Fracture stress, strain and Young’s modulus for G/h-BN heterobilayer nanostructures with different interlayer sp³ bonds fraction and different size of rhombus nanopore. Figures 6–9 shows fracture process and stress distribution of a G/h-BN heterobilayer nanosheets coupled by interlayer sp³ bonds and rhombus defects. In general, mechanical properties can vary greatly as the location of the defect changes. For example, Kasra Einalipour Eshkalak et al reported that when the nanohole appears in an area, the ideal value of Young’s modulus is obtained, while the ideal fracture stress and strain value are obtained in other regions [35]. We observed from figure 5 that the mechanical properties of a G/h-BN heterostructure coupled by interlayer sp³ bonds and defects do not follow the general trends. It can be found that ideal values of mechanical properties in heterobilayer nanostructure are obtained when the nanopore is located at graphene region (LG), and this lead to the conclusion that mechanical properties of graphene region (LG) are higher than that of LBN or CBN region. In addition, it is found from figures 6–9 that in the presence of sp³ and nanopore, the mechanical properties of defective graphene layer are higher than that of defective h-BN. We can be ascribed to the fact that when the nanopore was created in G/h-BN heterostructure with interlayer sp³ bonds, graphene layer shows greater stability and toughness than h-BN layer. Ultimately, it can be also found that the introduction of sp³ bonds increases the initial strain of the heterostructure, intensifies the cracking process and leads to the decline of mechanical properties.

An important conclusion can be drawn that if nanoholes or defects are formed in the G/h-BN heterogeneous structures, they should be controlled in the graphene area rather than in the h-BN area in order to achieve better mechanical properties.

The Von mises stresses in figures 6–9 is calculated by the following formula:

\[ \sigma_{\text{Von mises}} = \sqrt{\frac{(\sigma_1 - \sigma_2)^2 + (\sigma_1 - \sigma_3)^2 + (\sigma_2 - \sigma_3)^2}{2}} \]

3.4. The effect of square defects and interlayer sp³ bonds coupling

The rhombus nanopore in the previous section was replaced by square nanopore, in same conditions. Square nanopore was created in G/h-BN heterobilayer nanosheets coupled by sp³ bonds, and we studied that the effect of square defects and sp³ bonds coupling on mechanical properties of G/h-BN heterobilayer nanosheets. The stress-strain curves for G/h-BN heterobilayer nanosheets coupled by different amount of interlayer sp³ bonds and square defects have been depicted in figure 10. It can be observed from figure 10 that the mechanical properties generally decrease with the increase in the size of square nanopore. This tendency is consistent with previous experimental studies. The mechanical properties of graphene or graphene/boron nitride heterostructures are affected by various defects, and the mechanical properties of graphene/boron nitride heterostructures decrease with the increase of defects [42–45]. In addition, similar to rhombus nanopore, the ideal mechanical value of G/h-BN heterobilayer with interlayer sp³ bonds are achieved when the square nanopore are at graphene layer. These trends in this section are similar as results of the previous section.

![Figure 4](image-url)
However, this section is also different from the results of previous section. The adverse effect of square nanopore on mechanical properties of G/h-BN heterobilayer with interlayer sp$^3$ bonds is higher than that of rhombus nanopore.

Moreover, it is observed that the interlayer sp$^3$ bonds seem to have great influence on the fracture strain of G/h-BN heterobilayer nanostructure, but less on the fracture stress and Young’s modulus on G/h-BN heterostructures. For example, fracture strain of free-defect G/h-BN nanostructure decreases by 10% when the fraction of interlayer sp$^3$ bonds is 2%, its fracture stress diminishes only by 6%, relative to that of pristine model. However, fracture strain of G/h-BN nanostructure with 10 Å square nanopore and no sp$^3$ bonds in CG region decreases by 15%, its fracture stress diminishes by 24.67%, relative to that of pristine model. The effect of intrinsic defects (including square and rhombus nanopore in this paper) on mechanical properties of G/h-BN heterobilayer nanostructure is higher than that of interlayer sp$^3$ bonds when the content of intrinsic
defects is the similar as that of interlayer sp³ bonds. A key conclusion can be obtained that interlayer sp³ bonds can be regarded as a special defect, and its value seems to outweigh the intrinsic defects.

Figures 11–14 shows fracture process and stress distribution of a G/h-BN heterostructure and square nanopore. It can be found that the negative effect of rhombus nanopore on mechanical properties of G/h-BN heterostructure is weaker than that of square nanopore. It can be drawn an important conclusion that mechanical properties of G/h-BN heterostructure with square nanopore is weaker than that of G/h-BN heterostructure with rhombus nanopore. Also, it can be attributed the fact that rhombus nanopore can withstand higher pressure and load than square nanopore in G/h-BN with interlayer sp³ bonds. Another important reason is that this article maintains three criteria for creating nanoholes: Diamond and square nanoholes consist of the same single number of individual empty defects, which are the same atomic
center coordinates, and the length of the nanoholes is similar. However, asymmetric square nanoholes may also lead to accelerated failure of the six-element ring in stress concentration and heterogeneous structures.

4. Conclusion

In this paper, interlayer sp³ bonds and defects are formed in the G/h-BN heterobilayer nanostructure. Its mechanical properties have been analyzed. Besides, by using molecular dynamics method, the influences of different cases on mechanical properties were investigated, including the diameter (length), position and
different kinds of nanopore (square and rhombus nanopore), and the number of interlayer sp\(^3\) bonds. Draw the following conclusions:

In the presence of sp\(^3\) bonds and nanopore, the mechanical properties of defective graphene layer are higher than that of defective h-BN. In other words, when the nanopore was created in G/h-BN heterostructure with interlayer sp\(^3\) bonds, graphene layer shows greater stability and toughness than h-BN layer. An important conclusion can be drawn that if nanoholes or defects are formed in the G/h-BN nanostructure, they should be controlled in the graphene area rather than in the h-BN area in order to achieve better mechanical properties. If the nanohole can be controlled in the LG area, the heterogeneous double-layer nanomaterials can withstand higher pressure. At the same time, we observed that the negative effect of rhomboid nanopores on the properties of heterogeneous structural mechanics was weaker than that of square nanopores.

The effect of intrinsic defects (including square and rhombus nanopore in this paper) on mechanical properties of G/h-BN heterobilayer nanostructure is higher than that of interlayer sp\(^3\) bonds when the content

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**Figure 10.** Variations of Fracture stress, strain and Young’s modulus for G/h-BN heterobilayer nanostructures with different interlayer sp\(^3\) bonds fraction and different size of square nanopore. (a)–(c) Effect of square nanopore in graphene region of G/h-BN heterostructures, (d)–(f) Effect of square nanopore in h-BN region of G/h-BN heterostructures.
of intrinsic defects is the same as that of interlayer sp$^3$ bonds. Moreover, it is observed that the interlayer sp$^3$ bonds seem to have great influence on the fracture strain of G/h-BN heterobilayer nanostructure, but less on the fracture stress and Young's modulus on G/h-BN heterobilayer nanostructure. Ultimately, it can be also found that the introduction of sp$^3$ bonds increases the initial strain of the heterostructure, intensifies the cracking process and leads to the decline of mechanical properties.

Based on study in this paper a key conclusion can be obtained that interlayer sp$^3$ bonds can be regarded as a special defect, and its value seems to outweigh the intrinsic defects. It can also prove the importance of interlayer sp$^3$ bonds, which can be used to regulate the mechanical, thermal and other properties of heterogeneous structures, and can also be combined with a variety of defects (empty space, stone walls, heterogeneous defects, etc).
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