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Mechanical properties of graphene grain boundary and hexagonal boron nitride lateral heterostructure with controlled domain size

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ABSTRACT

In this paper, the mechanical properties of in-plane heterostructure with alternating stripes of graphene grain boundary (GB) and hexagonal boron nitride (*h*-BN) are investigated using classical Molecular Dynamics method. The graphene GB contains an array of pentagon-heptagon (5–7) defects, and has good interfacial continuity with the lateral BN domain. By studying the dynamic failure process of heterostructure with varying hybridization intervals and GB tilt angles, two different local failure types are noticed. Coupled effects of *h*-BN hybridization and GB tilt angle on the tensile strength of heterostructure are revealed. For heterostructure with graphene GBs of evenly spaced 5–7 defects, the tensile strength is insensitive to the *h*-BN hybridization and increases anomalously with the defect density. For heterostructure with graphene GB of unevenly spaced 5–7 defects, lateral *h*-BN hybridization enhanced the tensile strength of the heterostructure. Such strength enhancement effect is contributed to the bond length mismatch between graphene and *h*-BN, and deteriorates with the increase of hybridization interval. Our results give helpful insight into the strength characteristics of hybrid two-dimensional nanomaterials based electronic and optical devices.

1. Introduction

Graphene and hexagonal boron nitride are both two dimensional nanomaterials consisting of a single layer of hexagonally arranged atoms. Graphene has attracted tremendous research attention over the last decade [1–3] with exceptional properties in terms of chemical [4,5], thermal [6], electrical [7–9], mechanical [10], and optical characteristics [11]. Hexagonal boron nitride has the similar hexagonal lattices as well as outstanding properties [12,13], and stimulates great interests about the properties of hybrid CBN material. Heterostructure with seamlessly stitched graphene and *h*-BN, such as CBN films [14,15] and CBN nanotubes [16,17], has been synthesized with interesting electronic applications [18]. In-plane heterostructure of graphene and *h*-BN with controlled and patterned domain sizes has also been successfully created by growing graphene in lithographically patterned *h*-BN atomic layers [19]. Studies about the electrical [20], thermal [21] and mechanical [22] properties of hybrid CBN sheet have been reported. To give an example, graphene has zero band gap [23] while the *h*-BN is electrically insulating with a band gap of ~5.8 eV [24–26], graphene-BN lateral heterostructure exhibits tunable band gap from 0 eV to 5.8 eV by varying the ratio of composition [27]. More interesting properties are expected in the CBN in-plane heterostructure.

Currently, Chemical Vapor Deposition is the most common fabrication techniques for the production of large-area graphene [28,29]. However, grain boundary defects are unavoidable in the fabricated graphene because each grain in metallic substrate could be a nucleation site for individual grains of graphene [30,31]. What's more, GB as a typical defective graphene structure alters its physical and chemical properties. Grantab et al. investigated the effect of GBs on the mechanical strength of graphene and reported that graphene sheets with large-angle tilt GBs turned out to be stronger than those with low-angle GBs, and even as strong as the pristine graphene [32]. Wei et al. discovered the key roles of the arrangement of pentagon-heptagon defects in the strength of graphene [33], and a series of relevant studies on the mechanical property of defective graphene have been carried

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out [34–37]. Even though the strength of graphene GBs has been studied extensively, investigations about graphene GBs in graphene-BN hybrid nanostructures have not reported before.

In this work, the mechanical properties of in-plane heterostructure with alternating graphene GB and *h*-BN stripes are studied using classical Molecular Dynamics (MD). The graphene GB contains an array of 5–7 defects. The hexagonal honeycomb lattices are continuous across the interface between graphene and *h*-BN stripes [38]. The stress distribution and the failure process of heterostructure with varying hybridization intervals and GB tilt angles are studied using the MD simulations. Effects of the *h*-BN hybridization and the GB tilt angles on the tensile strength of heterostructure are revealed. The results provide useful insight into the lateral hybridization manipulated graphene strength as well as the design of CBN sheets based nanodevices with tunable strength.

2. Computational details

We use the Tersoff potential with parameters adopted from Kınacı et al. [39] in LAMMPS [40] package for MD simulations. The size of the simulated CBN nanosheets is approximately 80 Å × 80 Å. Tilt graphene GBs are constructed in the middle of these heterostructure along *y*-direction, as shown in Fig. 1. Lateral BN stripes are constructed symmetrically on both sides of the graphene domain. The honeycomb lattices are continuous across the C/BN interface which parallel to the GB. During simulation, the models are fully relaxed by energy minimization before applying uniaxial tension along *x*-direction. A 3 Å wide ribbon at each end of the hybrid sheet along *x*-direction is fixed by specifying the velocity and the force of atoms equal to zero along *x*- and *z*-direction, as depicted by the red arrows in Fig. 1. With these constraints, the hybrid sheet is stretched along *x*-direction at a strain rate of 0.01%/*ps* by scaling all atomic coordinates accordingly. Each stretching step is accompanied with a relaxation of 100 steps. Such procedure of stretching and relaxation is repeated at time step $\tau = 1fs$ until complete failure. All sets of MD simulations are performed at room temperature under NVT ensemble.

To obtain the stress-strain curves during deformation, the atomic stress of individual atoms in the hybrid sheet is calculated according to the equation [41,42]

$$\sigma_{ij}^{\alpha} = \frac{1}{\Omega^{\alpha}}\left(\frac{m^{\alpha} v_i^{\alpha} v_j^{\alpha}}{2} + \sum_{\beta=1,n} r_{\alpha\beta}^{j} f_{\alpha\beta}^{i}\right)$$

where *i* and *j* denote indices in Cartesian systems; α and β are the atomic indices; m^{α} and v^{α} denote the mass and velocity of atom α; $r_{\alpha\beta}$ is the distance between atoms α and β; Ω^{α} is the atomic volume of atom α. After the stress of each atom is obtained, the stress of the hybrid BNC sheet is computed by averaging over all the atoms in the sheet. The thickness of hybrid graphene–BN sheet is adopted as 3.35 Å [22], which is the mean thickness of graphene and BN. Young's modulus *E* and ultimate strength σ can be obtained from the simulated stress-strain curves. The Young's modulus is calculated as the initial slope of the stress-strain curve and the strength is defined at the point where the peak stress is reached.

3. Results and discussions

Before calculating the strength of the constructed heterostructure, we first simulate the stress-strain curves of pure graphene and *h*-BN sheet with a size of 80 Å × 80 Å for accuracy verification. The simulated pristine nanosheets and corresponding stress-strain curves under tension are plotted in Fig. S2. The averaged Young's modulus and tensile strength extracted from the stress-strain curves of armchair- and zigzag oriented graphene is 886.5 GPa and 154.4 GPa, which is consistent with the experimental result of 1014 GPa and 130 GPa [10]. For the *h*-BN, the averaged Young's modulus of armchair- and zigzag-oriented *h*-BN obtained from simulations is 711 GPa, which is in good agreement with the experimental result of 811 GPa [12]. The calculated strength of *h*-BN is also consistent with the reported MD simulations based on the Tersoff potential [22].

We now proceed to study the strength of the in-plane heterostructure. Here we focus on the difference between the strength of heterostructure with varying tilt GB angles and

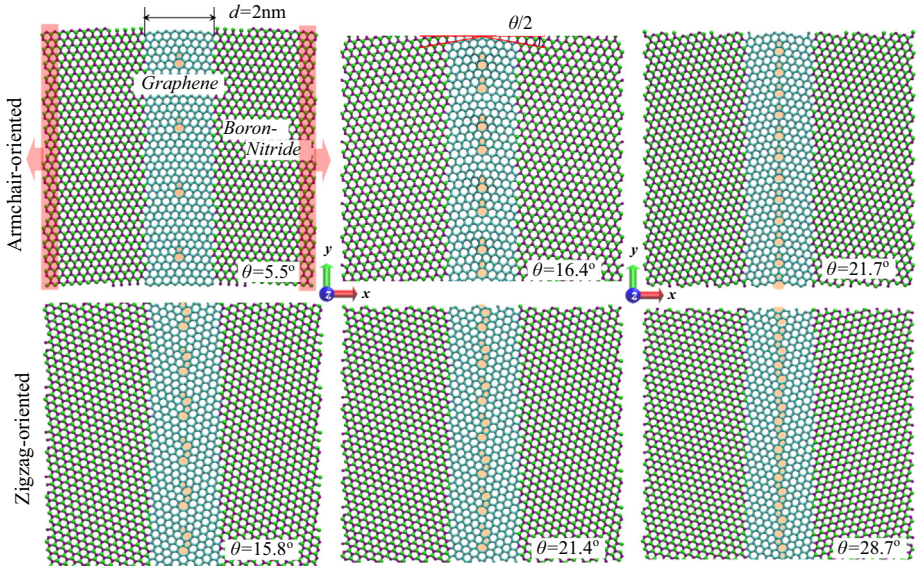

Fig. 1. In-plane heterostructure of graphene GB and *h*-BN with varying hybridization interval *d* and GB tilt angles θ. In-plane strain is applied perpendicular to the armchair- and zigzag-orientated GBs for stress-strain curves. Atoms in blue, purple and green represent carbon, boron and nitride atoms respectively. Pentagon-heptagon defects in armchair- and zigzag-orientated GBs are marked with orange background. (Heterostructures with tilt GB angle θ = 13.2°, 17.9° can be referred in Fig. S1). (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)