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Investigation of crack propagation and existing notch on the mechanical response of polycrystalline hexagonal boron-nitride nanosheets

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ABSTRACT

In this paper, we investigate the effect of temperature and grain size on the mechanical response of atomistic polycrystalline structures through classical molecular dynamic (MD) simulations. Five samples with different grain sizes in the range of 2–20 nm are examined under different temperatures. In addition, the effect of the crack size on the crack speed and orientation is studied for samples with an initial edge crack of different crack lengths. We also determine the effect of the initial crack lengths on the tensile strength. Our results show a drop in the tensile strength and elastic modulus with decreasing grain size while the failure strain is increasing. The failure pattern shows an opposite trend in the sample with a grain size higher than 14 nm. An existing initial center crack reduces the tensile strength and failure strain as well, and this reduction is independent of the initial crack length. The impact of the initial notch on the mechanical properties depends furthermore on the location of the notch in the samples.

1. Introduction

Graphene [1], a sp^2-bonded carbon atom sheet, is one of the most promising materials due its unique properties [2,3]. Its extremely high mechanical [4], thermal [5] and electronic properties [6] makes it interesting for electronic devices and robust membranes [7–9]. Unfortunately, graphene has a zero band gap [10]. This issue restricts controlling electrons to move through graphene [10]. As a result, it prevents direct application of graphene in the field of transistors [11]. Many approaches have been proposed to open a band gap in graphene [12–15], but the gap problem has been not completely solved [16,17].

Hexagonal boron-nitride (h-BN) [18] is an attracted alternative to graphene due to its wide band gap of $\sim 5.5\ ev$[7]. It makes boron nitride a perfect material for electrical application such as developing memories, gate dielectrics and capacitors [19]. Other advantages of boron nitride over graphene include its more stable chemical and thermal properties at high temperature (up to >900 °C) [20]. Hexagonal boron-nitride also possesses high thermal conductivity of 390 W/m-K [20], deep ultraviolet photon emission [21], and considerable piezoelectricity [22]. These properties make hexagonal boron-nitride a promising alternative to graphene especially under extreme conditions.

2D crystalline materials contain various types of disorders and fluctuation that hinder a high-quality mass production. These defects affect the mechanical and thermal properties. Chemical vapor deposition (CVD) technique is commonly employed to synthesize large-scale-grown binary compound such as graphene and boron-nitride [23,24]. However, during the CVD process, growing crystals form grain boundaries [25,26] and defects along the grain boundaries, known as topological defects. These topological defects are pentagon-heptagon (5/7) and square-octagon (4/8) shaped [27], generated by a 90° rotation of two atoms with respect to the midpoint of the bond [28]. A recent study of transmission electron microscopy reveals hexagonal boron nitride mostly consists of pentagon-heptagon (5/7) defects along grain boundaries [29]. Studying the effect of defects on the mechanical response of materials is fundamental.

Recently, several researchers have studied the effect of topological defects on the mechanical and thermal response of hexagonal boron-nitride nanosheets. Most of the studies have been devoted

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to pristine hexagonal boron-nitride nanosheets and models with a single grain boundary through classical molecular dynamic (MD) simulations and density function theory (DFT). As expected, the results show that increasing the density of defects along the grain boundary leads to a reduced tensile strength, elastic modulus and failure strain. [30–32] also suggest that a decreasing trend in tensile strength and failure strain could be observed by rising the temperature [33,30]. The thermal and mechanical response of *large* nanometer molecular models of boron nitride polycrystals with random grain configurations are investigated by several researchers. For example, Mortazavi et al. [34] studied the mechanical response of ultra-fine grained polycrystalline h-BN specimen with different grain sizes (ranging from 2 nm to 10 nm) at room temperatures. They reported that decreasing the grain size leads to a reduction in the elastic modulus and tensile strength. Becton et al. [35] studied the grain size effect on the mechanical response of polycrystalline boron-nitride. They showed that the grain size highly affects the mechanical properties, such as Young's modulus, tensile strength and fracture toughness. In another study [25], a decreasing thermal resistance and conductivity of hexagonal boron-nitride models has been observed by increasing the grain size, and if the grain size is larger than 500 nm, the hexagonal boron nitride model behaves similar to pristine boron nitride.

While there are several contributions on crack propagation in graphene, to our best knowledge, crack propagation in polycrystalline boron-nitride nanosheets has been studied neither theoretically nor experimentally. For example, Budarapu et al. [36] studied the crack initiation and growth mechanisms in a graphene nanosheet through MD simulation testing the influence of the time steps on the crack speed. They also showed that the crack speed changes with the crack length. In another study, Budarapu et al. [37] investigated the effect of the lattice orientation and crack size on the mechanical properties of graphene. The simulations include 13 different crack lengths in 10 different lattice orientations of graphene. A sudden reduction in tensile strength is observed in the models with crack sizes less than 10 nm, while larger crack sizes showed a linear trend. Three particular patterns of graphene fracture are also detected in all lattice orientations. Datta et al. [38] revealed the crack length and orientation effect on the mixed-mode fracture behavior on graphene.

Notches or vacancies are among the most common types of defects in materials and can substantially affect the mechanical performance. Therefore, quantifying these effects on the mechanical performance of materials is crucial. To the best of our knowledge, there are no studies on the notch effects on the mechanical properties in hexagonal boron nitride sheets. On the other hand, this topic has attracted attention in graphene. Sha et al. [39] reported that circular notches like grain boundaries create stress concentration zones. They also show that the stress concentrations are highest when the notch and grain boundaries interact.

In this paper, we investigate the grain size effect ranging from 2 nm to 20 nm on the mechanical properties of polycrystalline boron-nitride nanosheet under different temperatures. Futhermore, we study crack propagation for samples with an initial center-crack. The effect of the crack size on the crack speed and mechanical properties are also quantified. And finally, the effect of pre-existing notches on the mechanical response is investigated. Our findings can provide a useful guideline for using boron-nitride under service conditions.

2. Computational models and methods

In this study, MD simulations are performed using the open-source software LAMMPS [40]. The results are visualized with OVITO [41]. The modified Tersoff potential [42] is used for interactions between the boron and nitrogen atoms which is given by:

$$E = \frac{1}{2}\sum_{i}\sum_{j\neq i} f_c(r_{ij})\left[f_R(r_{ij}) + b_{ij} f_A(r_{ij})\right] \tag{1}$$

where, cutoff function is denoted by f_C. f_R and f_A are repulsive and attractive pair potentials, which managed by the b_{ij} bond function. The parameters of the Tersoff potential can be found in Table 1.

In order to verify our method, two polycrystalline boron-nitride nanosheets of different sizes have been constructed. The sizes of the sheets were 50 nm × 50 nm with 25 grains and 25 nm × 25 nm with 144 grains. The tensile strength, failure strain and elastic modulus results agreed well with the obtained results of the molecular dynamic work of Mortazavi et al. [34].

In the present work, five samples of polycrystalline hexagonal boron are examined. They have been constructed by using the Voronoi method. In this method, the atoms along the grain boundary with a distance less than 0.1 nm are removed. After creating the initial atomic positions, MD simulations are conducted to form the grain boundaries. It should be noted that complex grain boundaries could not be formed due to limited reactivity of the Tersoff potential. To overcome this limitation, a similar method as proposed in [32,43] is used to fabricate polycrystalline graphene. Therefore, boron and nitrogen atoms were replaced with carbon atoms, and interactions between carbon atoms are also defined by using second-generation reactive empirical bond order (REBO) [44]. In the first step, the initial structure was relaxed for 10 ps at room temperature using the Nose-Hoover thermostat method (NVT). In the second step, we used the NVT method for 100 ps to heat the structure uniformly to 3000 K. Then, the structure was relaxed at 3000 K for another 100 ps. At this temperature, the position of atoms were rearranged to form the grain boundaries. In the final step, the structure was cooled at room temperature for 100 ps. After these steps, boron and nitrogen atoms are substituted with carbons atoms yielding the desired polycrystalline hexagonal boron nitrite.

Five different models of different grain sizes are studied. All models have a 50 nm × 50 nm square geometry and a thickness of 0.33 nm. The model with 2 nm grain size has the highest density of defects which includes 600 grains. On the other hand, the model with 20 nm grain size includes 6 grains having the lowest density of defects. Other models have 100, 25 and 12 grains with 5, 10 and 14 nm grain size, respectively. The number of atoms in all models are in the range of 96,000–98,500 atoms. The grain size for a square geometry with an equivalent average grain in a polycrystalline sheet is given by [34]:

$$\textit{Grain size} = \sqrt{\frac{L^2}{N}} \tag{2}$$

where L denotes the length of the nanosheet and N is the number of grains in the plane. Fig. 1 illustrates the four samples with equiva-

Table 1
The parameters of the modified Tersoff potential [42].

Parameter	B-B	N-N
m	3.0	3.0
γ	1.0	1.0
c	0.52629	79934
d	0.001587	134.32
h	0.5	−0.9973
n	3.9929	12.4498
β	0.0000016	0.10562
λ_{II}	1.5856	2.5115
B (eV)	183.49	219.45
R (Å)	1.95	2.15
D (Å)	0.15	0.15
λ_I	1.9922	5.7708
A (eV)	277.02	11000