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A molecular dynamics study of nanofracture in monolayer boron nitride

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ABSTRACT

In this paper, we use molecular dynamics (MD) modeling to study the fracture properties of monolayer hexagonal boron nitride (h-BN) under mixed mode I and II loading. We investigate the impact of crack edge chirality, crack tip configuration and loading phase angle on the crack propagation path and critical stress intensity factors. The MD results predict that under all the loading phase angles cracks prefer to propagate along a zigzag direction and the critical stress intensity factors of zigzag cracks are higher than those of armchair cracks. Under mixed mode loading, the h-BN sheets can undergo out-of-plane deformations due to the buckling induced by compressive stresses. The out-of-plane deformations can be significant when mode II loading is dominant. An excessive amount of out-of-plane deformation can induce buckling cracks. Depending on the loading phase angle and crack configurations, buckling cracks can nucleate before or after the propagation of the original cracks.

1. Introduction

The current interest to graphene and the need to introduce an electronic bandgap to the gapless pristine graphene has brought intense interests to other graphene-like two-dimensional materials such as hexagonal boron nitride [1–3]. Hexagonal boron nitride (h-BN) has a honeycomb atomic structure in which boron (B) and nitrogen (N) atoms occupy alternating sites. Despite similar morphology with graphene, the binary atomic structure of hexagonal boron nitride leads to mixed ionic-covalent atomic bonding. Such atomic bonding which is different from the covalent sp^2 bonding of graphene gives h-BN distinct physical and mechanical properties than graphene. Opposed to graphene which displays a zero bandgap and is semimetallic [4], h-BN shows a band gap and is an insulator with a wide band gap of 5.6 eV [5]. Such differences in the physical properties of h-BN and graphene, has motivated the synthesize of hybrid graphene–boron nitride sheets with properties which are complementary to both graphene and boron nitride [3,6].

Besides being complementary to graphene, the remarkable physical and mechanical properties h-BN such as low dielectric constant [7], high temperature stability [8], high thermal conductivity [9] and high strength [10,11] make it appealing for a wide spectrum of applications in its own right. The wide spectrum of applications of h-BN expose it to different thermal, electrical and vibrational loadings. For a reliable usage of h-BN in such sensitive devices it is essential to ensure that h-BN can sustain such loadings. This necessitates a fundamental understanding regarding the mechanical and fracture properties of h-BN.

Opposed to graphene whose mechanical and fracture has been studied in the past [12–14], the studies on the fracture properties of graphene-like two-dimensional materials is scarce. Considering that graphene-like two-dimensional materials such as h-BN have a more complex atomic structure than graphene, their fracture properties can be quite different from graphene. Such differences necessitate a separate study of the fracture of h-BN. Ideally, the fracture and mechanical properties of h-BN should be characterized experimentally, e.g., by uniaxial test. However, designing and conducting test at nanoscales is very complicated; to date no uniaxial test on two-dimensional materials has been reported. Computational studies such as molecular dynamics, on the other hand, can provide valuable insights regarding the behavior of two-dimensional materials. In this paper, we use molecular dynamics simulations using a Tersoff potential [15] to study the fracture properties of single layer boron nitride sheets under mixed mode I and II loading.

2. Tersoff potential

We use molecular dynamics simulations to study the toughness and crack propagation path of monolayer boron nitride under

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mixed mode I and II loading. The molecular dynamics simulations are conducted using LAMMPS package [16,17]. The interatomic interaction between boron and nitrogen atoms in the BN sheets are prescribed using a Tersoff potential [15]. The Tersoff potential can be written as

$$V_{ij} = f_C(r_{ij})\left[f_R(r_{ij}) + b_{ij} f_A(r_{ij})\right], \tag{1}$$

where f_C is a cut-off function defined as

$$f_C(r) = \begin{cases} 1, & r \le R - D \\ 0.5 - 0.5\sin\left(\dfrac{\pi}{2}\dfrac{r-R}{D}\right), & R - D < r < R + D \\ 0, & r \ge R + D \end{cases} \tag{2}$$

The function f_R is a two body term and represents a repulsive pair potential whereas f_A is a three body term and represents the attractive pair potential due to the atomic bondings. The functions $f_R(r_{ij})$ and $f_A(r_{ij})$ are given by

$$f_R(r_{ij}) = A\exp(\lambda_1 r_{ij}) \tag{3a}$$

$$f_A(r_{ij}) = -B\exp(\lambda_2 r_{ij}). \tag{3b}$$

Function b_{ij} represents a measure of the bond order which depends on the local coordination of the neighbors of atoms i and the angle θ_{ijk} between atoms i, j and k. Function b_{ij} is defined by

$$b_{ij} = \left(1 + \beta^n \zeta_{ij}^n\right)^{-1/2n}, \tag{4a}$$

$$\zeta_{ij} = \sum_{k \ne i,j} f_C(r_{ij}) g(\theta_{ijk}) \exp\left(\lambda_3^3 \left(r_{ij} - r_{ik}\right)^3\right), \tag{4b}$$

$$g(\theta) = 1 + \frac{c^2}{d^2} - \frac{c^2}{d^2 + (\cos\theta - h)^2}. \tag{4c}$$

In the above equations, the summation is taken over all neighbors j and k of atoms i which are located within a cutoff distance of $R+D$.

Several sets of Tersoff potential parameters for interaction between boron and nitrogen atoms have been developed in the past [9,18–20]. Sekkal et al. [18] modified the Tersoff set of parameters of carbon [15] to describe the B and N interactions in cubic boron nitride (c-BN) systems. Verma et al. [19] modified this set of parameters to describe the interactions of B and N in hexagonal BN (h-BN) systems. More recently, adjusted set of Tersoff potential parameters for boron nitride are developed by fitting the obtained interatomic forces, bond lengths, cohesive energy and phonon dispersion curves to the experimental and *ab initio* modeling data [9,20,21]. Furthermore, Tersoff potential parameters have been extended to describe the interaction among carbon, boron and nitrogen [20,22]. Such parameters are used to study the thermal transport and mechanical properties of more complex materials such as hybrid graphene-boron nitride [20] or graphitic carbon nitride [22].

In this paper, we use the potential parameters and their corresponding values for BN provided by Çağın et al. [9,20]. This potential parameter set has been successfully used in accurate reproduction of structural, mechanical, vibrational and thermal transport properties of hexagonal boron nitride nanostructures [9] and hybrid graphene-boron nitride nanoribbons [20].

3. Molecular dynamics simulations

Our MD model is a circular domain cut around the crack tip as is shown in Fig. 1. The circular domain is chosen large enough that its boundary falls in the K-dominant zone. The equilibrium configuration of the cracked domain is obtained by first applying the crack tip asymptotic field to all the atoms in the domain and then while the boundary atoms are kept fixed the position of the interior atoms is relaxed. The crack tip asymptotic displacement fields for a linear isotropic material under combined mode I and II loading are given by [23]

$$u_x = \frac{1+\nu}{E}\sqrt{\frac{r}{2\pi}}\left[K_\mathrm{I}\cos\frac{\theta}{2}\left(\kappa - 1 + 2\sin^2\frac{\theta}{2}\right) + K_\mathrm{II}\sin\frac{\theta}{2}\left(\kappa + 1 + 2\cos^2\frac{\theta}{2}\right)\right] \tag{5a}$$

$$u_y = \frac{1+\nu}{E}\sqrt{\frac{r}{2\pi}}\left[K_\mathrm{I}\sin\frac{\theta}{2}\left(\kappa + 1 - 2\cos^2\frac{\theta}{2}\right)\right. \tag{5b}$$

$$\left. -K_\mathrm{II}\cos\frac{\theta}{2}\left(\kappa - 1 - 2\sin^2\frac{\theta}{2}\right)\right] \tag{5c}$$

where r and θ are the polar coordinates shown in Fig. 1, u_x and u_y are the displacement components in the x and y directions, E=925 GPa [24] is Young's modulus of pristine monolayer h-BN, ν=0.23 [24] is its Poisson's ratio and κ is the Kolosov constant which is equal to $(3-\nu)/(1+\nu)$ for plane stress condition. K_I and K_II are the mode I and II stress intensity factors; respectively. The effective stress intensity factor is $K_\mathrm{eff} = \sqrt{K_\mathrm{I}^2 + K_\mathrm{II}^2}$, and the loading phase angle defined as $\phi = \tan^{-1}(K_\mathrm{I}/K_\mathrm{II})$ describes the ratio of the mode I and II loading. Based on this definition a loading phase angle of zero degree corresponds to a pure mode I loading and a loading phase angle of 90° corresponds to a pure mode II loading.

The initial zigzag and armchair cracks are generated by eliminating respectively four and three rows of atoms as are shown in Fig. 2. We investigate the effect of crack edge chirality on the fracture properties by considering both armchair (AC) and zigzag (ZZ) cracks. As are shown in Fig. 2a, the edges of zigzag cracks are not alike; in one of the edges, boron atoms occupy the outermost layer while in the other edge nitrogen atoms are located at the outermost layer. When the loading phase angle is not zero (i.e. loading is not pure mode I), the deformation of the top and bottom edges of the crack is not symmetric, e.g. under pure mode II loading one edge is under compression and the other edge is under tension. To take into account the crack edge unsymmetry the loading phase angle is varied from −90° to 90°. This allows us to consider the effect of tension or compression in either of the edges on the critical stress intensity factor, K_cr.

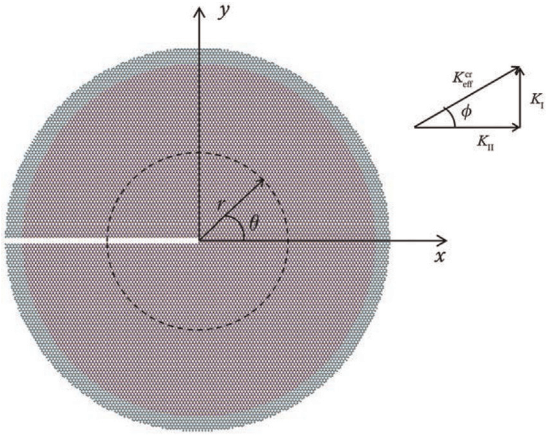

Fig. 1. Molecular dynamic domain. The boundary atoms are shown in cyan. (For interpretation of the references to color in this figure caption, the reader is referred to the web version of this paper.)