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Fast crack kinking manipulated by atomic hoop stress in monolayer hexagonal boron nitride strip

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ABSTRACT

A model of monolayer hexagonal boron nitride strip with initial zigzag crack under displacement loading is built in molecular dynamic simulation. The interaction between boron and nitride atoms is modeled by a modified Tersoff potential. The propagation speeds of edge cracks, the crack paths and the stresses around crack tip are analyzed, which show that the crack propagates smoothly and symmetrically at low speed, while rapid crack oscillate and its surface becomes rough when its speed rises up. Moreover, the hoop stress around crack tip calculated by virial stress components varies with the crack speed. Hoop stress reaches its maximum at 60° to the crack tip once the crack moves fast beyond a critical velocity of 8.37 ~ 8.61 km/s (~78% Rayleigh wave speed), and cracks deviate from its original trail, kink along the direction perpendicular to the peak hoop stress.

1. Introduction

Dynamic fracture of materials has long attracted the interest of many researchers, *e.g.* Yoffe [1] studied the stress field around the crack tip in isotropic elasticity using classic continuum, and found that the crack propagates straightly at low velocity, but starts to branch once the hoop stress around crack tip reaches another maximum value at polar angel larger than 0°, especially in cracked glass. Buehler et al. [2–4] carried out pioneering work on the instability of dynamic fracture in harmonic materials by molecular dynamics (MD) methods (for triangular lattices) and continuum mechanics. In the classic linear elastic theories, the crack propagation speed should not be larger than the Rayleigh wave speed in model I cracks. However, hyperelasticity may appear at the crack tip during the crack propagation and affect the crack tip further, resulting in supersonic cracks in hyperelasticity region. Their MD results showed that the hoop stress decreased gradually from 0° to 180° and the crack propagates straightly when the crack propagation speed is low (less than 0.73 Rayleigh wave speed C_R). Furthermore, once the crack propagation speed rise up to 73% C_R, two stress peaks appeared in the hoop stress curves, one is at 60° while another at 150°, which agreed well with Yoffe's study and continuum mechanics theory of fracture. Jia et al. [5] studied the supersonic crack in triangle lattices by finite element (FE) and MD, their results show that crack can propagate faster than the longitudinal wave speed and crack propagation speed is related to the longitudinal wave speed and microstructure geometry. The instability of dynamic mechanics in 2D triangular lattices has been researched extensively, but few attentions is paid to the dynamic fracture of hexagonal lattices, another microstructure geometry.

Hexagonal boron nitride (*h*-BN), as a two-dimensional crystal, possessing excellent mechanical properties similar to graphene [6] for their similar structures of hexagonal lattices. The atoms of B and N bounded by strong covalent bonds arrange alternately in an annular hexagon, which is definitely different from triangle lattices. The Young's modulus of *h*-BN was measured 0.78 GPa by X-ray [7], its in-plane stiffness was 278.3 N/m [8]. In addition to the outstanding mechanical properties, the production of graphene and *h*-BN on large-scale has been promoted a lot in recent years [9,10]. Graphene could reach 1.5 in. in 2.5 h [11], and single crystal *h*-BN could grow to 7500 μm^2 on Cu-Ni substrate [12], which show their potential applications in nanodevices, however, dynamic fracture of two-dimensional crystals, as the primary failure style, has not been explored extensively yet. Therefore, it is of practical significance to study the rapid fracture of two-dimensional crystals, *e.g.* *h*-BN, which could predict active life of devices against catastrophic failure.

In account of the cost and difficulty to conduct experiments at nanoscale, the diverse mechanical properties of two-dimensional crystals are usually examined by atomic modeling, *e. g.* MD. The mechanical properties of graphene and *h*-BN were ever calculated by MD, revealing that the Young modulus of graphene was almost independent of the

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temperature [13]. It was also indicated that the yield strength of the mixtures of graphene and *h*-BN reduced markedly, but the composites showed strong plasticity during the tensile process [14]. The behavior of yield stress as well as yield strain with crack length is studied to be insensitive to the orientation, a constant yield strain ~0.05 can be observed [15]. The yield strength varies as the inverse square of the initial crack length and specimen size [16]. Moreover, Le et al. [17] studied the dynamic fracture of graphene with armchair crack, and explored how the initial crack length and strain rate affected the crack propagation speed. Alireza et al. [18] demonstrated the crack propagation path of *h*-BN under mixed loading, only zigzag crack among the initial five different cracks could propagate symmetrically, the others also tend to propagate along the zigzag direction, which is same as graphene [19]. Graphene strip [20] under uniaxial tension was also investigated by MD and FE, and the results of crack propagation speed were consistent with Buehler's results, but the hoop stress was not considered yet. It's worth noting that the crack branches along edges by 30° (or multiples of 30°), and one of the peaks of hoop stress in triangular lattice is also at 60°, the direction of crack branching and the maximum hoop stress is accordant. The relationship between crack speed and crack branching was studied in PMMA, which shows that the microcrack branching occurs when the speed reaches a critical speed [21]. However, the intrinsic relations between the crack kinking/branching and the hoop stress in hexagonal lattice have not been reported yet.

In this paper, we use LAMMPS to simulate the rapid rupture in *h*-BN strip with initial zigzag crack under tensions. The interaction between boron and nitride atoms is described by a modified Tersoff potential [22]. The crack propagation path, crack speed, hoop stress around crack tip and other variables are calculated and analyzed in details.

2. Molecular dynamic simulation method and models

The interatomic interaction in MD is usually described by atomic potential, such as modified Tersoff potential that is widely used in graphene. Tersoff parameters of the interactions between B and N atoms have been studied, *e.g.* Sekkal [23] modified parameters to fit *c*-BN, and this potential cannot describe the interaction between B and N clearly. Recently, scholars [24,25] developed the Tersoff potential which can be used successfully in *h*-BN by comparing the interatomic force and bond lengths obtained in experiment and theory. The modified Tersoff potential parameter can also be used to describe the interaction of C, B and N atoms. Kinaci [24] studied the change of heat conduction in B, N and C mixed nanostructures with modified Tersoff potential, suggesting that the interface between armchair and zigzag is much larger than that of super lattice, the bending stiffness and atomic distance of hexagonal boron nitride are similar to those of graphene, but the energy of point defect is very different. In this paper, the Tersoff potential developed by Albe [25,26] will be used. Han [25] demonstrated that the young modulus of monolayer *h*-BN in different temperature and strain rate are agreed with theoretical and experimental studies, verifying that the Tersoff potential adjusted by Albe is reliable. Tersoff potential by Albe is written as:

$$v_{ij} = f_c(r_{ij})[f_R(r_{ij}) + b_{ij}f_A(r_{ij})],\ \mathrm{f_R(r)} = Ae^{-\lambda_1 \mathrm{r}},\ \mathrm{f_A(r)} = -Be^{-\lambda_2 \mathrm{r}}$$

$$f_c(r) = \begin{cases} 1, & r \leqslant R-D \\ 0.5-0.5\sin\left(\frac{\pi}{2}\frac{r-R}{D}\right), & R-D < r < R+D \\ 0, & r \geqslant R+D \end{cases} \quad (1)$$

Here f_C is cutoff function, f_R and f_A represent the repulsive and attractive pair potentials respectively. The cutoff parameters R and D are 2 Å and 0.1 Å [25]. The specific parameters are shown in Table 1.

To validate the model and potential, we calculate the Young's modulus of monolayer *h*-BN. Square model (Fig. 1) contains 4850 atoms, and tensile loading is applied quasi-statically along the direction

Table 1
Parameters of modified Tersoff potential [25,26].

	B-B	N-N	B-N
m	3	3	3
γ	1	1	1
λ_3	0	0	1.9925
c	0.52629	17.7959	1092.9287
d	0.001587	5.9484	12.38
h	0.5	0	−0.5413
n	3.9929061	0.6184432	0.364153367
β	0.0000016	0.019251	0.000011134
λ_2	2.07750	2.627272	2.784247
B	1173.197	2563.560	3613.431
R	2	2	2
D	0.1	0.1	0.1
λ_1	2.23726	2.82931	2.99836
A	1404.47520	2978.95279	4460.83397

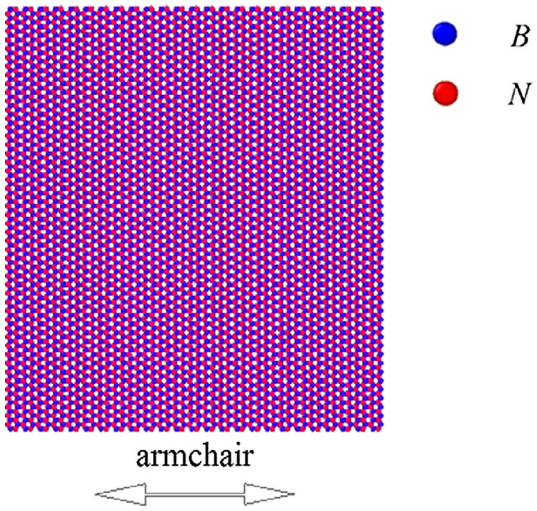

Fig. 1. Verification model of *h*-BN under unaixal tension. Blue dot represents B atom and red dot N atom everywhere.

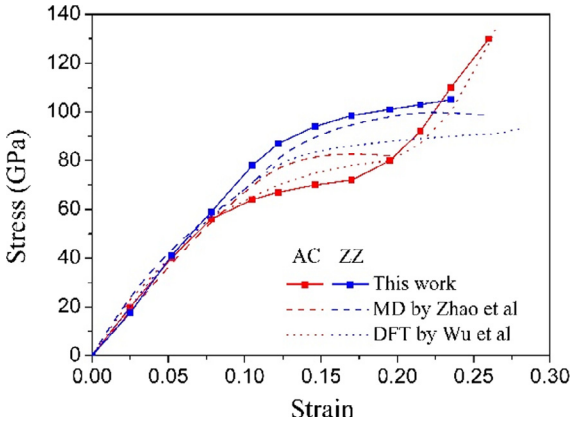

Fig. 2. Stress-strain curves of *h*-BN under uniaxial tensions.

Table 2
Mechanical properties of *h*-BN comparing with other results.

References	Young's modulus (GPa)
This work	720.9 (AC)/767.4 (ZZ) (strain < 10%)
Experiment by Bosak et al. [7]	780 (AC)
DFT by Wu et al. [8]	773 ± 40 (AC)/780 (ZZ)
MD by Zhao et al. [14]	739.9 (AC)/692.7 (ZZ)