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Tensile mechanical properties of c-BN thin layers under tension: A molecular dynamics simulation

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ABSTRACT

Molecular dynamics simulations were performed to investigate the axial tension properties and fracture mechanisms of the c-BN nano thin layers. It is found that thin layers display a linear stress-strain relationship firstly at $\varepsilon < 0.054$, and then a quasi-linear response at $0.054 < \varepsilon < 0.302$, and finally the stresses decrease gradually until entire fracture occurs. Fracture stresses are 76, 49, 33 and 21 GPa, respectively, for 100 K, 300 K, 500 K and 700 K, and Young's modulus decreases gradually with the increasing of temperature. The deterioration in mechanical properties derives from the formation of major defects that B—N bond, tetragonum and octagon with broken bonds, and two-hexagon by the sharing of the nitrogen atom. The results not only clear the outstanding property of c-BN nano thin layers but also built relevance between the mechanical behaviors and loading conditions such as side length, temperature and strain rates.

1. Introduction

c-BN, as a kind of artificial superhard materials among the III-V compounds, has motivated tremendous amounts of theoretical and experimental investigations of its fundamental properties for a long time [1]. Because of excellent properties such as extreme hardness, high melting points, high resistivity, high thermal conductivity and stability, the scope of applications mainly include high temperature abrasive, cutting and machining operation [2]. Simultaneously, 2D boron sheets have also attracted wide attention. Mortazavi et al. investigate the mechanical properties and thermal conductivity of h-BN sheets and obtained remarkable results, establishing relations between the properties and atomic structures [3–5]. In addition to their physical characteristics, c-BN ceramics also demonstrate unique chemical property of wide indirect band gap semiconductor, which makes them attractive candidates for electron, light, film and other fields. Recently, motivated by the surge and the discovery that the distinguished strength and ductility of nanostructured ceramics and nanosized whiskers are greater than that of microsized block, the synthesis and study of cubic BN in nano-scale have swallowed a large number of sweats and been a subject in a number of experimental and theoretical studies [6,7]. However, for the mechanical properties of c-BN crystals, the absence of the samples of nano-sized crystals used in the experimental measurement does not currently allow a direct observation of the deformation during mechanical loading. In this present paper, molecular dynamics simulations are performed to investigate a theoretical tensile experiment on c-BN thin layer, shown in Fig. 1.

2. Computational methods

The software packages Lammps is used for the MD simulation, and program atomeye is used for visualization. All the thin layers models are approaching square with the thickness of 1.085 nm and side lengths of about 10.12, 15.18 and 20.24 nm, respectively. Free boundary condition is applied in all models in the planar directions therefore the obtained results reflect the finite layers. The interatomic potential used is the effective potential proposed by Tersoff [8,9], which has been parameterized and used to investigate the mechanical properties of carbide and nitrides [10,11]. Prior to loading, three different sizes of initial thin layers, containing 6272, 42,336, and 75,264, respectively, are fully relaxed to an equilibrium minimum energy using the steepest descent algorithm so as to obtain stable configurations and then thermally equilibrated to 300 K for 200 ps using Nose-Hoover thermostat ensemble with a time step of 0.5 fs. Uniaxial tensions are carried out in

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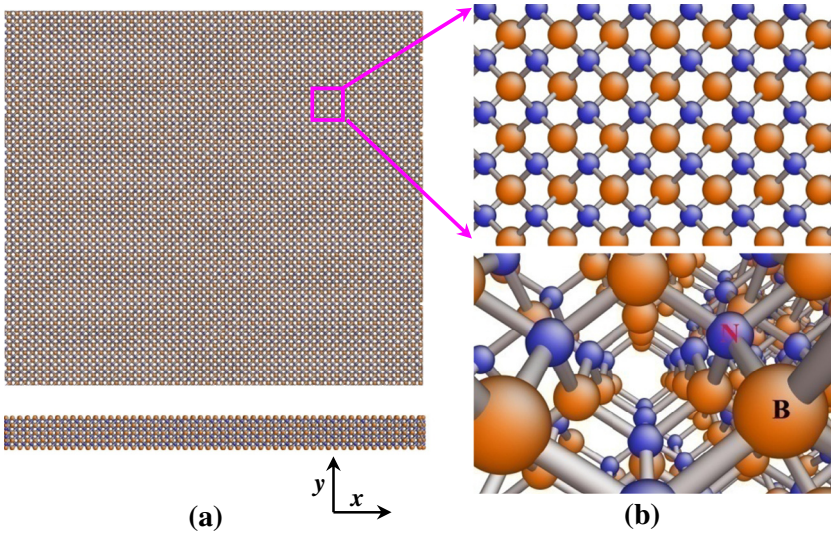

Fig. 1. The simulation configuration of c-BN thin layer: (a) top and side views of the integrated layer and (b) the interior bonding structure. B: orange atoms; N: blue atoms. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

the x direction by applying different velocities and temperatures. Based on the applied velocities and box size, the strain rates are calculated. The simulated elongation steps were repeated until the thin layers were fully ruptured and well separated.

3. Results and discussion

3.1. The side length dependence of thin layer tension

The calculated stress-strain curves of the thin layers subjected to axial tension in x direction is depicted in Fig. 2. Note that the strain is defined as the percentage of extension of the entire thin layer in the loading direction. The fracture stress is determined as the peak stress in the elastic stage and the corresponding strain is the fracture strain. From Fig. 2, it is observed that the thin layers display a linear response stage when the strain is in the range of 0–0.054 and subsequently the stress displays a quasi-linear increase with the strain until fracture occurs. In the elastic phase, the calculated fracture stresses and fracture strains of the thin layers increase with the increasing of side lengths, as indicated in Table 1. The Young's moduli of the thin layers can be calculated from the stress-strain data in Fig. 2 by using the Hooke's law $\sigma = E\varepsilon$ at

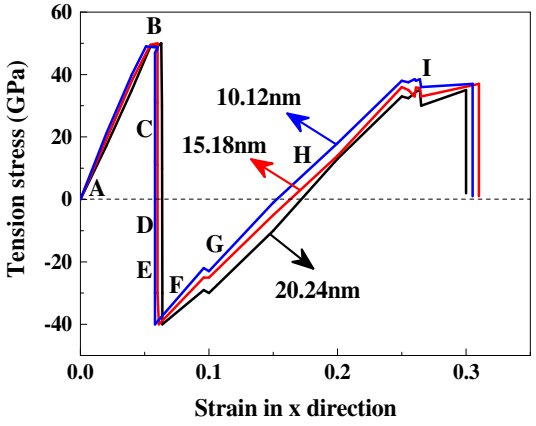

Fig. 2. Stress-strain curves of c-BN thin layer with different side lengths subjected to axial tension in x direction. The snapshots of deformations at the point A-I are shown in following Fig. 3, respectively.

Table 1
Fracture stresses, fracture strains and Young's moduli of the c-BN thin layers.

Number of atoms	Fracture stress (GPa)	Fracture strain	Young' modulus (TPa)
6272	46.58	0.022	0.975
42,336	48.09	0.027	0.976
75,264	50.15	0.031	0.978

$0 < \varepsilon < 0.04$, where the structures are fully in the linear deformation region and the law is suitable for the determination of the Young's modulus. The Young's moduli of the thin layers are listed in Table 1. The calculated values are well in accordance with the theoretical values obtained by Nagakubo [12] and Guo et al. [13]. In the subsequent quasi-linear phase, the tensile stresses increase with the strains increasing in three cases and the thin layer with side length of 10.12 nm has the maximum value of 37 GPa. The sudden drops in stress at a strain of 0.054 showed that the thin layers exhibit a brittle fracture.

Fig. 3 illustrates the fracture morphologies of the thin layer with a square side length of 10.12 nm in the y direction. Different colors indicate different potential energy values, which in turn represents atoms in distinctive local structures such as surface, stacking faults, defects or simply deformed regions, as demonstrated in the corresponding potential energy distribution spectrum in Fig. 3. At a strain of 0.054 (shown in Fig. 3b), the initial B—N bond breaking defect in the center position of the thin layer can be observed as indicated in the red box. The broken bond defect weakens the fracture property under tension and becomes the origin of the crack, thus leading to the sharp drop in stress. Simultaneously, the yellow of boron atoms located at fracture means the highest potential energy value. Fig. 3c displays the evolution of the configuration at a strain of 0.056. It is clearly found that the crack spreads to all the directions on further loading. In addition to the B—N broken bonds, the emerging defects such as B—N—B bond breaking defects (red triangle) and hexagon defects with broken bonds (pink ellipse) can be seen, and the thin layer begins to fracture. When the strain comes to 0.061 (see Fig. 3d), the crack spreads further and the emerging octagon defects with broken bonds can be observed (rounded rectangle), which is responsible for the energy consumption. When the strain increases to 0.068 (see Fig. 3e), a large number of octagon defects with broken bonds