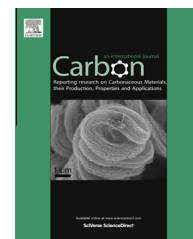


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Orientation dependence of the fracture behavior of graphene

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ABSTRACT

Graphene has unique mechanical properties in that it is simultaneously very strong and stretchy, which severely hampers the prediction of its orientation-dependent fracture behavior based on conventional theories used for common brittle or ductile materials. For the first time, by exploring the entire range of available tensile orientations, this study reveals the unique anisotropic fracture response of graphene using molecular dynamics simulations. We found that, as the uniaxial tensile direction rotates from armchair (0°) to zigzag orientation (30°), both the tensile strength and strain remain almost constant up to an orientation angle of ~12°, then they rapidly increase (exponential growth), resulting in a remarkable degradation of the tensile strength compared to brittle fracture counterpart (inverse-sinusoidal growth). This typical fracture pattern holds for 100–700 K. We propose a model that can explain its physical origin in good agreement with the simulation results. We also found that the elastic behavior of graphene is quasi-isotropic for all tensile orientations, in contrast to its anisotropic fracture behavior. Using indentation simulations of graphene, we showed that the anisotropic/isotropic features of fracture/elasticity are also well-preserved in the two-dimensional tensile systems but its fracture anisotropy is greatly attenuated due to the inherent sixfold symmetry of graphene.

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1. Introduction

Graphene, a single layer of carbon atoms arranged in a honeycomb structure, has attracted great attention after its experimental discovery, owing to its many exceptional properties such as ultrahigh electronic mobility, superior thermal conductivity, and excellent mechanical strength [1–7]. It is thinner and stronger than any other material ever discovered. Naturally, such superlative properties of graphene have triggered its active application to a wide range of engineering fields. For instance, there have been numerous studies to improve the mechanical strengths [8–10], thermal properties [11–13], and energy conversion efficiencies [14–16] of materi-

als by incorporating graphene into them. One of the most featured applications is the use of graphene as a supporting film for a liquid cell in transmission electron microscopy (TEM) studies [17]. In this application, the graphene membranes stay structurally intact while encapsulating the liquid tightly and allowing very feasible electron transmission for high-resolution probing of the reaction occurring in the inside liquid, which basically benefited from the high tensile strength, flexibility, and ultrathin nature of graphene. With the growing demand for such graphene-based devices and composite materials, it becomes increasingly important to understand the mechanical characteristics of graphene at a greater level of depth.

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A number of studies have been performed to explore the mechanical fracture phenomena of ceramics and metals, and their mechanisms are well explained by Griffith's brittle fracture theory [18,19] and the ductile fracture models for soft metals [20,21], respectively. However, graphene is neither brittle nor ductile and essentially differs from either quality. Graphene is both very strong and very stretchy, and owing to these peculiar characteristics, the orientation-dependent fracture behavior of graphene cannot be dictated by any single mechanism proposed earlier.

Great efforts have been made in characterizing the mechanical properties of graphene [5,22], including those of its defective [23–25] structures as well, where various structural defects such as Stone Wales Throwing defects [26,27] and grain boundaries [28] were examined. By nanoindentation using atomic force microscopy, Lee et al. measured Young's modulus and the intrinsic breaking strength to be 1.0 ± 0.1 TPa and 130 ± 10 GPa, respectively, assuming the thickness of graphene to be 0.335 nm [5]. Meanwhile, most of preceding studies on the mechanical properties of graphene have predominantly relied on computational methods such as ab initio calculations [29–31], tight-binding models [32,33], and molecular dynamics simulations [34–36] due to the tremendous experimental difficulties in controlling a monoatomic film and developing appropriate measurement techniques. From these theoretical approaches, we have been able to understand many principal characteristics of graphene, such as Poisson's ratio, the temperature effect, and the grain boundaries effect which had been extremely elusive to determine using experimental methods.

In particular, theoretical studies suggested that graphene would exhibit distinct anisotropic fracture behavior in tensile deformation, which has not yet been experimentally observed. For instance, a molecular dynamics study indicated that the tensile strength and strain of graphene are 107 GPa and 0.20 under zigzag-directional elongation while they are 90 GPa and 0.13 under armchair-directional elongation at 300 K [22]. However, all preceding studies on the tensile mechanics of graphene have been devoted merely to the zigzag and armchair directional deformations, and the tensile mechanics of other orientations have never been inspected, although graphene would be likely to deform along various directions in realistic cases.

To address this problem, in the present paper, the tensile fracture and elastic behaviors of graphene were systematically investigated using molecular dynamics simulations as the uniaxial tensile direction rotated very gradually from the armchair to the zigzag direction in the honeycomb crystal lattice of graphene. This rotational range covers the complete range of tensile orientations of graphene due to its sixfold symmetry. Specifically, nine tensile orientations were selected for this study as shown in Fig. 1a, and our uniaxial tensile simulation system is briefly illustrated in Fig. 1b.

2. Computational methods

All calculations were performed using the LAMMPS (large-scale atomic/molecular massively parallel simulator) software package [37] and the simulation systems were

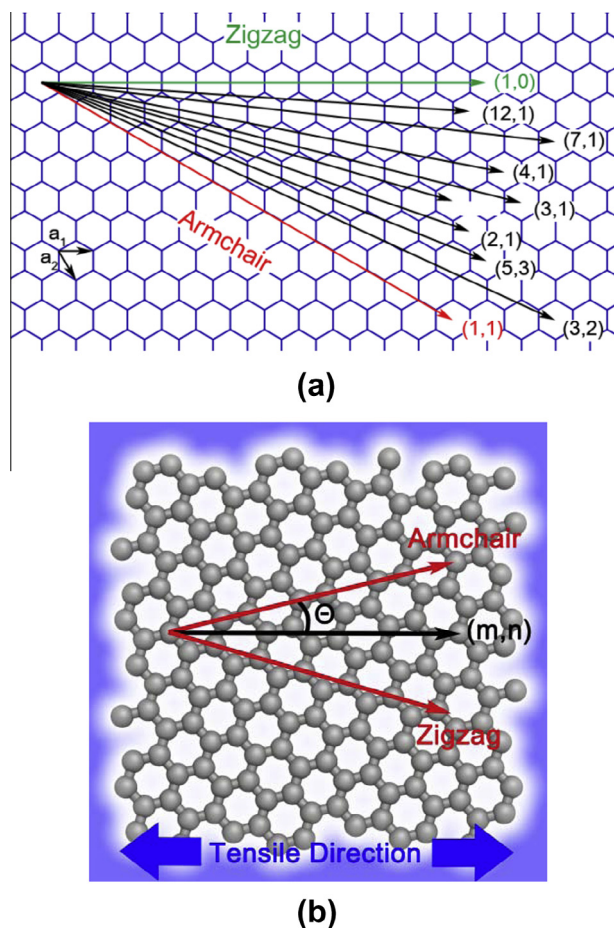


Fig. 1 – (a) The nine tensile orientations selected to investigate the orientation-dependent tensile mechanics of graphene, where the corresponding chiral notations are given in parentheses. (b) The illustrated uniaxial tensile simulation system where the tensile direction has been set to an arbitrary (m,n) chiral direction, and an orientation angle θ is defined as the angle made between the relevant tensile direction and the armchair direction. (A color version of this figure can be viewed online.)

constructed to meet a periodic boundary condition. For interactions between carbon atoms, we employed (AIREBO) adaptive intermolecular reactive empirical bond order potential [38] which has been widely used to study the mechanical properties of carbon materials, such as carbon nanotube (CNT) [39], fullerenes [40], and graphene [24,35,41]. The cut-off radius of the potential was set to be 2.0 Å to avoid spuriously high bond forces and unphysical results near the fracture region [24,35,41]. The dimensions of the simulation system and atomic coordinates were first optimized using a gradient-based minimization method with tolerance criteria of 10^{-8} eV/Å in force and/or 10^{-8} eV in energy. Using the system size obtained above, a canonical ensemble simulation was subsequently performed for 3×10^5 steps by increasing the temperature gradually from zero to the desired temperature and further equilibrated for 7×10^5 steps under isothermal conditions. After equilibrium was reached, the system was finally elongated with a strain rate of 0.1 ns^{-1} in the

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