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Size effect on brittle and ductile fracture of two-dimensional interlinked carbon nanotube network

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ABSTRACT

The mechanical properties of two-dimensional (2D) interlinked carbon nanotube (CNT) network are investigated using ab initio calculation and molecular dynamics simulations (MD) with Reaxff force field. The simulation results show that bulk 2D interlinked CNT network has good mechanical properties along the axial direction which can be comparable to that of single-walled CNT and graphene, but has better ductility along the radial direction than single-walled CNT and graphene. In addition, the mechanical properties of 2D interlinked CNT network ribbon along the radial direction depend strongly on the size of the ribbon. The Young's modulus and Poisson's ratio decrease as the size increases while the fracture strain increases with the size increasing. By analyzing the atomic structural (both bond length and atomic von Mises stress) evolution of the ribbons, the mechanism of a brittle-to-ductile transition is revealed. The exploration of the mechanical properties of the 2D interlinked CNT network paves the way for application of the relevant devices that can benefit from the high Young's modulus, high tensile strength, and good ductility.

1. Introduction

CNTs have attracted great research interest for various potential applications since their discovery [1] due to their inherent outstanding mechanical, electronic, and thermal properties [2,3]. In the previously both experimental and theoretical work, it has been reported that CNTs possess extremely high axial tensile strength and Young's modulus values of about 150 GPa and 1 TPa [4–6], respectively. However, for larger-scale potential applications, the CNT networks do not exhibit expected mechanical properties because of the relatively weak van der Waals interactions between CNTs. Owing to weak interactions, individual CNTs can easily slide on each other, which results in little load transfer [7,8]. This hinders the wide range of application of CNT networks. Pressure is not only important method to study the structural and physical properties of materials, but also is an effective means to tune or modify the physical properties of materials. In order to maintain their curvature (i.e., C-C-C bond angles), small diameter CNTs have higher reactivity of surface atoms with only three bonds which are similar to the tetrahedron sp3 bonds in diamond [9]. Therefore, pressure may induce the transformations of bond state from the sp2 hybridized to sp3 bonds and produce some novel carbon based materials.

Single-walled CNTs (SWCNTs) covalent interlinking under pressure have been reported both experimentally and theoretically during the past decade. The earlier experimental studies [10] have indicated that the covalent C-C bonds interlinking between CNTs can be formed under high pressures and temperatures. In other experimental high-pressure studies, the quenchable superhard carbon phase has been synthesized by compression of CNTs under a non-hydrostatic pressure of 24 GPa [11] at room temperature. These superhard carbon allotropes have higher bulk modulus (465 GPa) than that of diamond (about 440 GPa) and high hardness (62–150 GPa) which is in the range between cubic BN (46–80 GPa) [12] and diamond (175 ± 5 GPa) [13]. These observations are supported by other obtained quenchable superhard carbon phase by compressing CNTs [14,15]. The determined bulk modulus is 447 GPa [14] and the measured hardness is 58 ± 6 GPa [15].

At the same time, variously pressure-induced 2D and 3D interlinked CNTs networks have been revealed according to the theoretical calculations. The theoretical predications of one- and two-dimensional (2D) networks of interlinked small diameter zigzag single-wall CNTs at higher external pressures are performed [16]. The small nanotubes are covalently boned to each other by sp3 hybridized carbon. However, at ambient pressure, the spontaneous cross linking is also found in the bundle of small-diameter zigzag CNTs based on density functional

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theory (DFT) calculations [17]. The recent DFT calculations also find that the novel quasi-2D sheets of interlinked single-wall CNTs are formed at hydrostatic pressure [18]. The strong bonds are formed between the atoms in adjacent CNTs according to electron localization function (ELF) analysis. In addition, the transition pressure is dependent on the size and chirality of CNTs. The resulting 3D interlinked CNTs networks possess high thermodynamic stability, mechanical, and electronic properties. For example, these 3D interlinked CNTs networks can be metallic or semiconducting with wide direct/indirect gaps ranging from 0 to 3.45 eV [19,20]. Based on semi-empirical formula and DFT calculations, the Young's modulus (about 1 TPa) and tensile strength (can be larger than 100 GPa) can be comparable to that of CNTs [19,21].

Compared to the 3D interlinked CNTs networks, the 2D interlinked CNT networks can have more potential application because of large surface area to volume ratio in nanotechnology. Recent studies have shown that 2D CNTs networks with various junctions (e.g. X- and Y-junction) can find a number of applications, for example, sensors and actuators [22,23], optoelectronics [24,25], and energy devices [26,27]. The new interlinked 2D materials consisting of single-wall CNTs should have novel mechanical and electronic properties. It is therefore highly desirable to systematically investigate the mechanical properties of 2D interlinked CNT networks. However, to the best of authors' knowledge, investigation on the mechanical properties and fracture process of 2D interlinked CNT networks has not been studied in the literature up to now.

In this work, ab initio calculations are performed to obtain robust predictions of structures and mechanical properties of the 2D interlinked CNT networks, and then we investigate the elastic properties and tensile behavior such as Young's modulus and fracture strain using molecular dynamics (MD) simulations. Additionally, the size effect on the elastic properties and fracture strain is studied.

2. Simulation details

Ab initio calculations are mainly performed with the Spanish Initiative for Electronic Simulations with Thousands of Atoms (SIESTA) code with atomic orbitals [28]. Some ab initio calculations are also performed using the Vienna Ab Initio Simulation Package (VASP) with projector augmented wave method [29,30] in order to obtain robust predictions and check different empirical potentials' accuracy. In the SIESTA calculations, the double zeta plus polarization (DZP) basis set is used. The 32 × 1 × 32 or 1 × 1 × 32 Monkhorst Pack grid [31] is used for k-point sampling, together with a meshcutoff of 600 Ry for the system are used in the calculation. In the VASP calculations, the projector-augmented wave (PAW) method is used. The 1 × 1 × 16 Monkhorst Pack grid is used for k-point sampling and an energy cutoff of 850 eV is used. In both ab initio calculations, the Perdew-Burke-Ernzerhof (PBE) formulation of the generalized gradient approximation (GGA) for the exchange and correlation functional is used in the calculation to account for the electron-electron interactions. To avoid interactions between species, neighboring structures are separated by more than 10 Å in the tetragonal supercells. For the bulk 2D interlinked CNT networks tension, stress-control method is performed and small stress is applied along tensile direction of the system. For the 2D interlinked CNT network ribbons tension, strain-control method is performed and the applied strain is 0.2% at each time. And then relax the geometry until the forces on each atom are less than 0.02 eV Å−1.

In the MD simulations performed herein, the reactive potentials including ReaxFF [32] and AIREBO [33,34] are used to describe carbon-carbon and carbon-hydrogen interactions. Due to provide accurate descriptions of dynamic bond formation and breaking, these two potentials have been widely used in a variety of MD simulations of carbon systems and provide better representations of mechanical properties and phonon thermal transport in carbon related systems [35–38]. All MD simulations are performed using the Large Scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) package [39]. All molecular systems are equilibrated at a constant pressure of 1 atm and a temperature of 300 K using NPT (constant number of particles, pressure, and temperature) for 100 ps with a time step of 0.1 fs. The temperature is controlled by employing the Nosé-Hoover thermostat [40]. The Velocity-Verlet algorithm is employed to integrate the equations of motion. And then the strain is applied along the uniaxial direction to perform uniaxial tensile tests. The applied strain rate is 0.005 ps-1. The pressure component vertical to the loading direction is controlled to maintain the uniaxial tensile condition. The strain increment is applied to the structure after every 10,000 time steps with the step size of 0.1 fs. During this process, we monitored the total energy and temperature of the entire system and found that the total energy conserved very well, and the temperature remained constant with small fluctuations around 300 K, which meant that the system had reached the equilibrium state.

3. Results and discussions

As shown in Fig. 1a, the 2D interlinked CNT network is composed of single-walled (5,0) zigzag CNTs. The structure is optimized based on ab initio calculations. In order to determine the bonding type between CNTs, the local environment of the carbon atoms in the optimized 2D-linked (5,0) CNTs network is investigated using ab initio calculation, as shown in Fig. 1b (left). It can be seen that the bond length between CNTs in the 2D interlinked CNT network is about 1.56 Å which is comparable to that in diamond (1.55 Å calculated using ab initio calculation), indicating sp^3 hybridization. In addition, the electron localization function (ELF) [41] is calculated. For comparison,

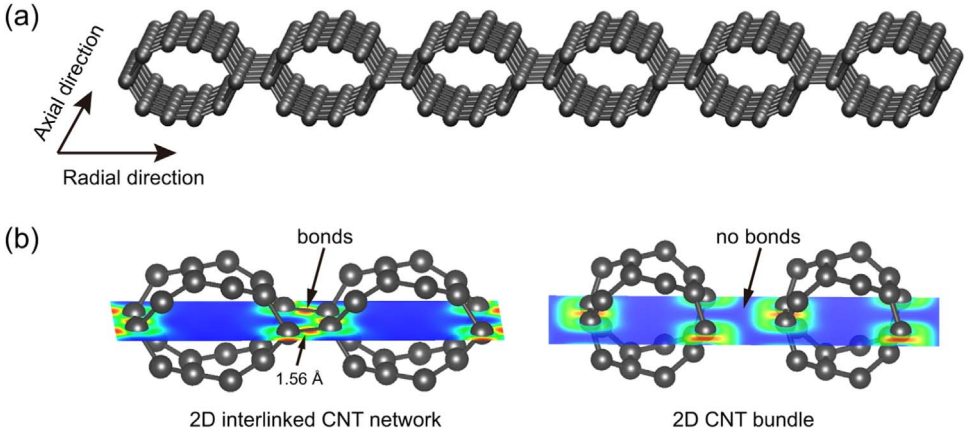

Fig. 1. (a) Optimized 2D-linked (5,0) CNTs network. (b) Electron localization function (ELF) for the 2D interlinked CNT network (left) and 2D CNT bundle (right).