

Morphology- and dehydrogenation-controlled mechanical properties in diamond nanothreads



Can Feng^{a, b}, Jie Xu^{a, **, *}, Zhisen Zhang^b, Jianyang Wu^{b, c, *}

^a School of Materials Science and Engineering, China University of Mining and Technology, Xuzhou, 221116, PR China

^b Department of Physics, Research Institute for Biomimetics and Soft Matter, Fujian Provincial Key Laboratory for Soft Functional Materials Research, Xiamen University, Xiamen, 361005, PR China

^c NTNU Nanomechanical Lab, Department of Structural Engineering, Norwegian University of Science and Technology (NTNU), Trondheim, N-7491, Norway

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ABSTRACT

Recently synthesized diamond nanothreads (DNTs), collecting desired properties of both inorganic nanostructures and hydrocarbon molecular structures, are an interesting group of carbon-based materials. Using full atomistic first-principles based ReaxFF molecular dynamics (MD) simulations, a comprehensive study on tensile and bending mechanical characteristics of fifteen energy-favorable DNTs is performed. All the DNTs show unique tensile and bending mechanical properties that markedly vary with morphology and arrangement of carbon polygons. A straight DNT composed of purely carbon hexagons shows brittle fracture in the temperature range of 1–2000 K, whereas with regard to another hexagon-dominated DNT and helically coiled DNT with the largest coiled radius, a thermal-induced brittle-to-ductile transition is uncovered at 2000 K. Particularly, the coiled DNT subjected to tensile loading/unloading shows a clear mechanical hysteresis loop. Dehydrogenation does not change the morphologies and stability of DNTs, but significantly affect the tensile mechanical responses; the tensile stiffness, toughness and ductility can be enhanced by approximately 1-fold, 2-folds and 3-folds as much of their pristine counterparts, respectively, however, the failure strain is reduced at any degree of dehydrogenation. Similarly, bending stiffness also closely connects with dehydrogenation. A transition of bending stiffness in two specific dehydrogenation-free DNTs occurring at critical curvatures is detected as a consequence of local bond transformations. Moreover, bending stiffness in different bending directions can differ by around 8-folds, originating from the distinct surface morphologies. The findings provide a critical knowledge of mechanical properties of DNTs for practical applications.

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1. Introduction

Carbon is a unique element that has attracted much interest and has been extensively studied for decades. It is well-known that there exists three naturally occurring carbon allotropes (amorphous, graphite and diamond), containing the sp^2 or sp^3 , or mixed sp^2/sp^3 hybridized carbon atoms. In recent two decades, many artificial nanostructured sp^2 -carbon allotropes, such as zero-

dimensional (0D) fullerenes [1], one-dimensional (1D) carbon nanotubes (CNTs) [2], two-dimensional (2D) graphene [3], three-dimensional (3D) carbon nanocoils [4], have been discovered/fabricated in laboratory settings. Experimental and theoretical studies reveal that those nanomaterials mainly composed of hexagonal carbon rings show outstanding chemical and physical properties. For example, CNTs with diameters in the range between fractions of nanometers and tens of nanometers can be stable at temperature up to 2800 °C in vacuum [5] and can have a room-temperature thermal conductivity of up to 6600 W/m·K [6]. They also exhibit tensile strength and elastic modulus as high as 100 GPa and 1 TPa [7,8], respectively. Moreover, Samsonidze et al. [9] developed the first kinetic approach to predict the strength and yield strain of CNTs as well as the role of chiral symmetry and temperature. Yakobson et al. [10] via MD simulations showed that CNTs are markedly resilient, sustaining large strain with no signs of

* Corresponding author. Department of Physics, Research Institute for Biomimetics and Soft Matter, Fujian Provincial Key Laboratory for Soft Functional Materials Research, Xiamen University, Xiamen, 361005, PR China.

** Corresponding author. School of Materials Science and Engineering, China University of Mining and Technology, Xuzhou, 221116, PR China.

E-mail addresses: fengcan@cumt.edu.cn (C. Feng), j.xu@cumt.edu.cn (J. Xu), zhangzs@xmu.edu.cn (Z. Zhang), jianyang@xmu.edu.cn (J. Wu).

brittleness, plasticity, or atomic rearrangements, and their unique behavior beyond Hooke's law can be well described by a continuum model. Those studies indicated the mechanical properties of CNT exceeds those of diamond. Motivated by the fantastic studies, a number of experimental and theoretical studies focusing on various aspects of diamond on the nanoscale have been performed [11,12]. It was revealed that diamond nanorods have desirable mechanical properties and are energetically competitive with CNTs [13,14]. However, quest for 1D carbon nanomaterials with expected properties is still of great interest in improvement and development of advanced technology.

Recently, bulk production of exceptionally long and stable carbyne chains composed of over 6000 carbon atoms was achieved [15]. It was reported that this 1D carbyne can exhibit either metallic or insulating electronic behaviors, depending on the number of valence electrons of carbon atoms, and possess nominal Young's modulus and effective shear modulus of 32.7 and 11.8 TPa, respectively [16]. Additionally, a newly structural form of carbon, termed as diamond nanothread (DNT), was successfully synthesized from benzene precursors under high-pressure solid-state reactions [17]. This DNT is a close-packed sp^3 -bonded tubular carbon structure in which carbon atoms are arranged in a diamond-like tetrahedral motif, and is surface-functionalized by hydrogen atoms in a 1:1 stoichiometry [18]. Apart from the experimental discoveries, several scholars performed systematic theoretical studies searching possible atomic structures of DNTs. From a different perspective, three structures of 1D sp^3 C–H DNTs, named as hydrogenated tube (3,0) [19], polymer I [20], and polytwistane [21] respectively, have been constructed. Furthermore, based on various stacks of benzene molecules, Xu et al. [22] have identified 50 topologically distinct sp^3 C–H DNTs with small unit cells. However, among them, only 15 structures, including tube (3,0), polymer I and polytwistane, are within 0.48 eV/(CH)₆ of each other.

Notable thermal properties of specific DNTs have been identified by theoretical calculations. It was reported via MD simulations with the adaptive intermolecular reactive bond order (AIREBO) potential that tube (3,0) DNT with Stone-Wales (SW) defects shows a uniformly decreasing and then increasing profile in thermal conductivity with respect to the number of poly-benzene rings as a result of the transition from wave-dominated to particle-dominated transport region, and exhibits both propagating and diffusive vibrational modes [23]. Calculations also showed that DNTs possess outstanding mechanical properties comparable to graphene and CNTs. Using AIREBO force field, it was predicted that tensile strength, Young's modulus and bending stiffness of specific DNTs are in the ranges of 79–141 GPa, 290–1090 GPa, and 1480–2030 kcal/mol Å, respectively. Intriguingly, brittle to ductile transition characteristic in tube (3,0) DNT with SW defects is identified as the length of the number of SW defects increases, originating from the hardening process of the SW defect region under stretching. By employing ReaxFF force field, axial stiffness of tube (3,0) DNT with SW defects varying from around 665–850 GPa or 131–167 nN, depending on SW defect density, is determined. This corresponds to specific strength of 3.94×10^7 – 4.13×10^7 N/m/kg. By introducing a virtual sticky surface to deform along with tube (3,0) DNT with SW defects into curved configurations of various diameters, its out-of-plane bending stiffness is determined to be ~770 kcal/mol Å [18]. Using density functional theory (DFT) calculations, it was also predicted that DNTs exhibit ideal strength and stiffness ranging from 15.7 nN and 2.6×10^7 N/m/kg to 168 nN and 2.8×10^8 N/m/kg, respectively, and the hydrogenated tube (3,0) DNT shows a negative radial Poisson's ratio. Moreover, because intrinsically irregular surfaces of DNT with SW defects can significantly enhance the non-covalent interfacial load transfer, DNTs could be a new reinforcement for nanocomposites [24].

Under certain conditions, DNTs may be capable of being dehydrogenated to yield well-ordered mixed sp^2/sp^3 carbon nanomaterials [25,26]. Previous studies showed that dehydrogenation of diamond nanowires leads to a reduction in the band-gap, indicating that diamond nanowires may be semiconducting to semi-metallic or metallic by a combination of dehydrogenation, surface morphology and reduction in diameter [27]. However, mechanical properties of dehydrogenated DNTs are unexplored so far. Thus, it is of both scientific interest and technological significance to understand how the morphology and dehydrogenation affect the tensile and bending mechanical properties of DNTs. Herein large-scale MD simulations are performed to systematically investigate the mechanical properties of both hydrogenated and dehydrogenated DNTs. This study provides a well-rounded perspective on mechanical performance of DNTs.

2. Models and method

In order to systematically understand the influence of morphology on the mechanical characteristics of DNTs, all the 15 lowest-energy DNTs proposed by Xu et al. [22] are taken into investigation in this study. All those DNTs are comprised of specific carbon polygons ranging from pentagon, hexagon, heptagon to octagon carbon rings. As suggested by Xu et al., all 15 DNTs are classified into three kinds, named as achiral (DNT-I), stiff-chiral (DNT-II), soft-chiral (DNT-III), respectively. Fig. 1 shows both side and top views of atomistic lattices of those carbon nanostructures. The DNT-I, DNT-II and DNT-III contain six, four, and five molecular models, respectively. Apparently, DNT-III show helically morphological features. The pitch and diameter of the helices are

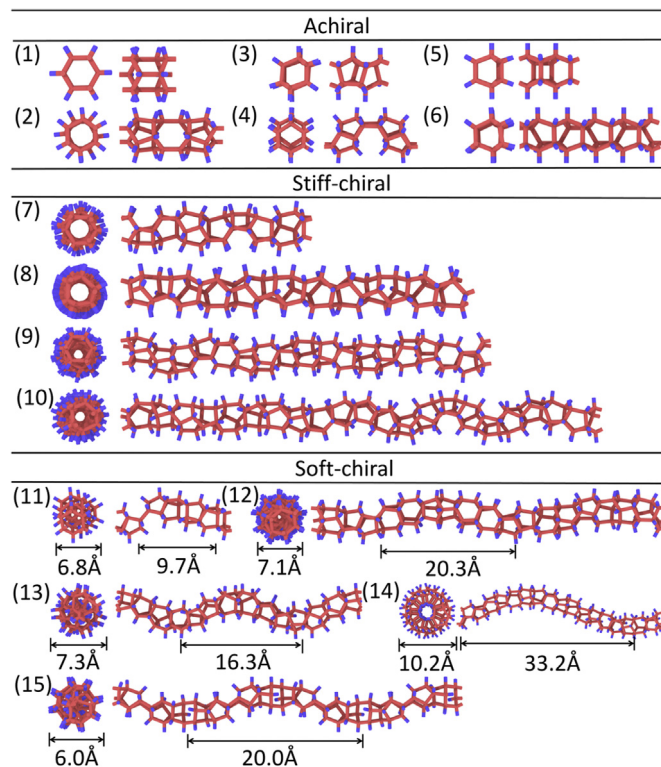


Fig. 1. Atomic configurations of unit cell of various hydrogenated DNTs. (1)–(6) Achiral DNT-I. (7)–(10) Stiff-chiral DNT-II. (11)–(15) Soft-chiral DNT-III. Left and right show the top-view and side-view snapshots. The arrow labels in (11)–(15) show the pitch and diameter of helically coiled DNTs. Red and red-blue sticks represent carbon-carbon and carbon-hydrogen bonds in the DNTs system. (A colour version of this figure can be viewed online.)

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