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Anisotropic and Temperature-Dependent Mechanical Properties of TPDH-Graphene

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***Abstract*—TPDH-graphene is a newly predicted two-dimensional carbon material with exceptional physical properties, positioning it as a promising candidate for nanoelectronics applications. Using classical molecular dynamics simulations, we investigated the anisotropic properties of the material and assessed how temperature influences its mechanical behavior. The results demonstrate that TPDH-graphene shows significant mechanical anisotropy, displaying superior tensile toughness and fracture strength along the zigzag direction in comparison to the armchair direction. At high temperatures up to 1200 K, the material exhibits a certain degree of tensile toughness in the armchair direction.**

Keywords—TPDH-graphene; MD; Mechanical property

I. Introduction

Researchers are highly interested in the existence of 2D carbon materials that possess mechanical properties similar to graphene. With advancements in computational power, first-principles methods have been employed to predict the structures of several promising 2D carbon materials with desirable properties [1-3]. In 2021, a novel two-dimensional carbon material named TPDH-graphene was introduced, showcasing remarkable physical properties. These include dynamic and thermal stability, selective UV light absorption, and unique current regulation behavior, as revealed by first-principles calculations. These attributes make TPDH-graphene a promising candidate for applications in nanoelectronics [4].

Molecular dynamics (MD) simulations were utilized to investigate the tensile mechanical properties of TPDH-graphene. The analysis focused on the effects of stretching in both principal directions and examined how temperature variations influence its mechanical behavior. These findings are expected to serve as a valuable reference for the material's future practical applications.

II. Materials and Methods

Fig. 1 presents the fundamental structural details of the material, with C-C bond lengths varying between 1.41 Å and 1.5 Å. Its space group is identified as Pmmm(47) [4]; A simulation box with dimensions of 14 nm × 14 nm × 10 nm was constructed, containing a single-layer model of thickness 3.34 Å at the center and a total of 6,720 carbon atoms. The time step used for the simulation was 1.0e-4 ps.

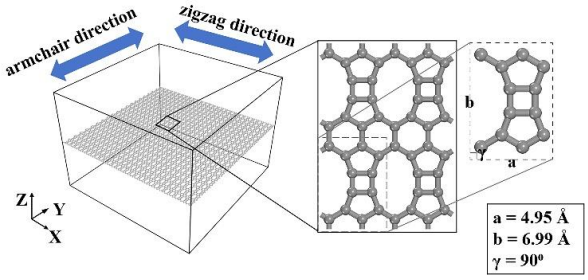

Fig. 1. The structure of TPDH-graphene.

MD simulations were conducted utilizing the LAMMPS [5], and OVITO was used to visualize the trajectory files generated during the simulations [6]. The Tersoff potential function was selected for use in this study [7]. The reasons for choosing the Tersoff potential function will be described in detail later.

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III. Results and Discussions

A. Selection of Potential Functions

In recent years, with the prediction of novel graphene-like materials by machine learning, the simulations of these two-dimensional carbon materials with the latest structure has brought greater challenges to traditional potential functions. The existing potential functions are often difficult to accurately describe the structure of the latest carbon materials.

We use three potential functions to optimize the structure of TPDH-graphene. The structure of material after structural optimization by DFT method is shown in Fig. 2. The structures after relaxation of all three potential functions are displayed by the OVITO software with the same displayed options (cutoff = 2.0 Å).

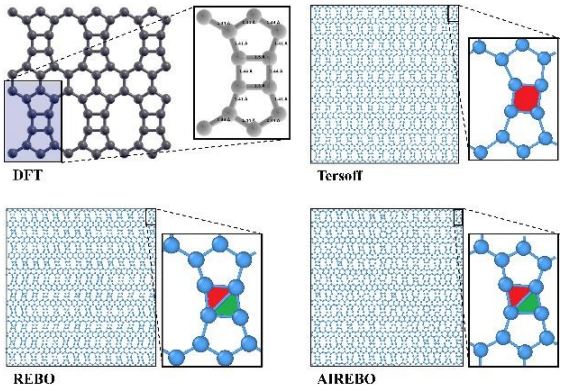

Fig. 2. DFT structure optimization and structure of TPDH-graphene after relaxation using three potential functions

The descriptions of the quaternary ring by the REBO and the AIREBO potential functions seem to be more biased towards describing a quaternary ring as two ternary rings, whereas the structure obtained by relaxation with the Tersoff potential function does not have this problem.

The Tersoff potential function effectively captures the interactions of the four carbon rings present in TPDH-graphene. As illustrated in Fig. 3, the potential energy of the TPDH-graphene structure rapidly stabilized.

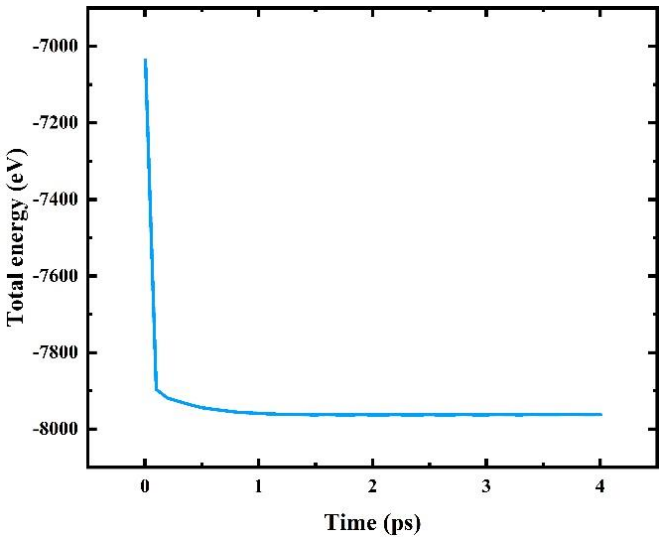

Fig. 3. Total energy of the system during relaxation of TPDH-graphene using Tersoff potential function

The differences in the structures for the same display settings raise concerns about the applicability of the AIREBO potential function. But considering that the AIREBO potential function is currently recognized as the most suitable potential function for simulation of graphene materials, we also did uniaxial stretching tests on TPDH-graphene using the AIREBO potential function.

B. Effects of System Size

Selecting an appropriate number of atoms for the simulation model is essential to balance computational efficiency with the accuracy of the results. A system with too few atoms may fail to accurately capture the mechanical behavior of the material, while an overly large system unnecessarily increases computational demands.

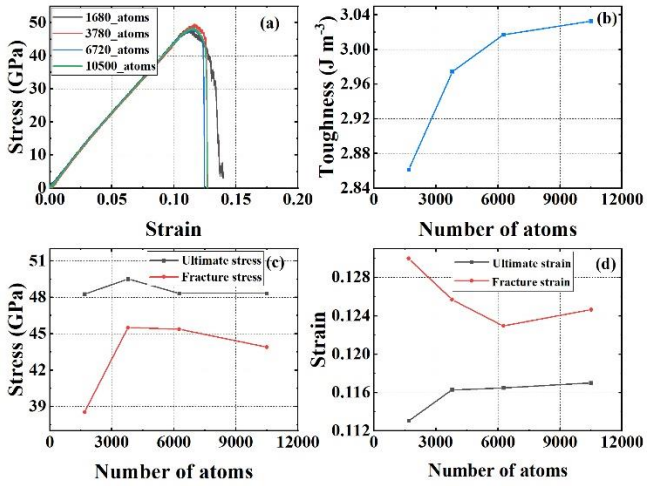

Fig. 4. Convergence test for simulating system size in the armchair direction. (a) Stress-strain curve (b) Fracture toughness (c) Ultimate and fracture stresses (d) Ultimate and fracture strains.

Figure 4 demonstrates that as the system size grows, the stress-strain curves become progressively smoother. In comparison, a system with only 1,680 atoms does not accurately represent the material's mechanical behavior. In general, systems with insufficient atom numbers fail to capture the mechanical properties of TPDH-graphene, while further increasing the atom count beyond a certain point has minimal impact on the results. Based on these observations, this study opted for a system consisting of 6,720 atoms.

C. Effects of Strain Rate

The results presented in Fig. 5 reveal that increasing the strain rate from 0.0005 to 0.01, a rise of two orders of magnitude, leads to a noticeable enhancement in the mechanical properties of TPDH-graphene during tensile testing. At lower strain rates, atoms have more time for thermal vibrations, increasing the likelihood of surpassing energy barriers and breaking C-C bonds. These findings align with prior studies investigating the impact of strain rate [8-10].

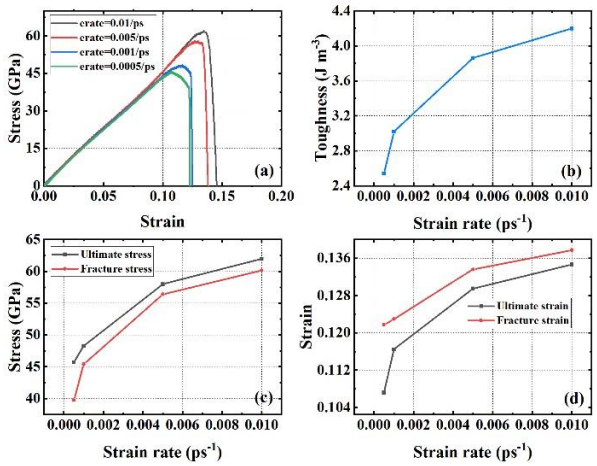

Fig. 5. Effect of strain rate. (a) Stress-strain curve; (b) Fracture toughness; (c) Ultimate and fracture stresses (d) Ultimate and fracture strains.

D. Mechanical properties in different directions

This portion of the simulation was conducted at a temperature of 300 K, a pressure of 0 Pa, and a strain rate of 1.0e-3 ps-1. Figure 6 shows the stress-strain curves of TPDH-graphene in both directions.

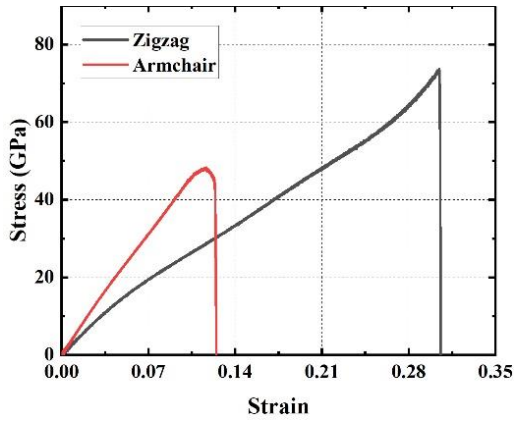

Fig. 6. Stress-strain curves of TPDH-graphene stretched in x(zigzag) and y(armchair) directions

Table I summarizes the mechanical properties obtained from the tensile tests. The tensile test results reveal differences in fracture behavior.

TABLE I. MECHANICAL PROPERTIES OF TPDH-GRAPHENE

Tensile direction	Ultimate tensile stress (GPa)	Ultimate tensile strain	Fracture stress (GPa)	Fracture strain	Toughness ($J\ m^{-3}$)
Along Zigzag	**73.75**	**0.3046**	**73.12**	**0.3049**	**11.0**
Along Armchair	**48.31**	**0.1165**	**45.39**	**0.1229**	**3.02**

The fracture patterns are depicted in Fig. 7. For the zigzag direction (Fig. 7(a)), cracks initiate at a strain of 0.305 from the edges of the structure, propagating inward until complete failure. In the armchair direction (Fig. 7(b)), cracks begin at a strain of 0.123, initiating at the center and spreading outward until the structure fully breaks.

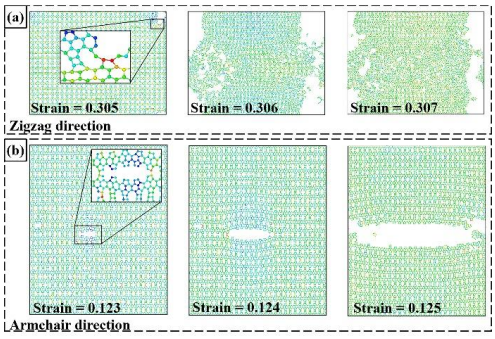

Fig. 7. Fracture process of TPDH-graphene under uniaxial stretching. (a) Zigzag direction; (b) Armchair direction.

We further provide a theoretical analysis of the mass density of carbon atoms and further explain the anisotropic behaviour of the material based on its fracture behaviour.

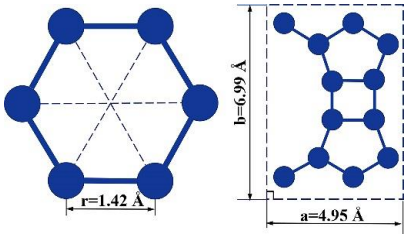

Fig. 8. Structures of graphene and TPDH-graphene

Firstly, we calculated the area of both materials:

$$S_{Graphene} = \frac{3\sqrt{3}}{2} r^2 = 0.052\ nm^2$$

$$S_{TPDH-graphene} = a \times b = 0.495 \times 0.699 = 0.346\ nm^2$$

Next, we determined the surface density by calculating the number of carbon atoms incorporated in the model:

$$\rho_{Graphene} = \frac{m}{S_{Graphene}} = \frac{2 \times 1.993 \times 10^{-20}}{5.2 \times 10^{-20}} = 0.766\ mg/m^2$$

$$\rho_{TPDH-graphene} = \frac{m}{S_{TPDH-graphene}} = 0.691\ mg/m^2$$

Finally, we calculate the line density in the corresponding direction based on the surface density of TPDH-graphene:

$$\rho_{Armchair} = a \times \rho_{Surface} = 0.342 \times 10^{-9}\ mg/m$$

$$\rho_{Zigzag} = b \times \rho_{Surface} = 0.483 \times 10^{-9}\ mg/m$$

TPDH-graphene exhibits a higher carbon atom density along the zigzag direction, resulting in its pronounced anisotropy.

Additionally, analysis of the fracture process reveals distinct differences between the two directions. When stretched uniaxially in the armchair direction, the material fractures by breaking the four-membered carbon rings, forming cracks that propagate along the arrangement of these rings. In contrast, zigzag uniaxial stretching requires the initial fracture of five- and six-membered rings, which are more resilient and difficult to break than the four-membered rings in the armchair configuration. The denser arrangement of carbon rings in the zigzag direction further contributes to its greater resistance to fracture.

E. Effects of temperature

Temperature significantly impacts the mechanical properties of materials [10-12]. As shown in Fig. 9, the temperature-dependent degradation is primarily attributed to the softening of the material at elevated temperatures. The trend aligns with observations from studies on the temperature effects on graphene's mechanical properties [13-15].

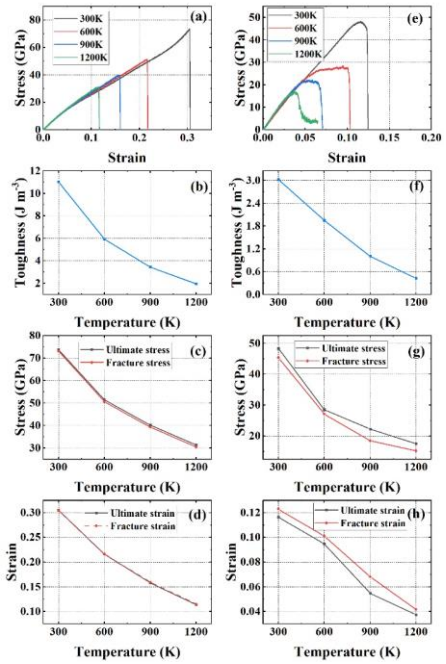

Fig. 9. Impact of temperature on the mechanical behavior of TPDH-graphene. Figures 9(a)~(b) are in zigzag direction and Figures 9(e)~(h) are in armchair direction.

Notably, as temperature rises, TPDH-graphene shows tensile toughness characteristics in the armchair direction.

IV. Conclusions

This study employed MD simulations to evaluate the mechanical properties of TPDH-graphene and investigate the effects of strain rate, tensile direction, and temperature on the test results. The findings reveal that lower strain rates lead to reduced fracture stress and strain. TPDH-graphene exhibits notable anisotropy in its mechanical properties, with significant differences observed between the zigzag and armchair directions. Additionally, higher temperatures cause material softening, which subsequently diminishes its mechanical performance.

These results enrich the understanding of TPDH-graphene nd offer valuable insights into its mechanical behavior. This study lays a groundwork for the potential practical applications of TPDH-graphene in nanoelectronics, highlighting the importance of accounting for orientation-dependent properties and temperature effects during design and implementation

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