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Investigation of the mechanical properties of multilayer graphene helicoids with different geometric characteristics using molecular dynamics simulation

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ABSTRACT: Graphene helicoid is a man-made spiral structure that has recently been created with the advent of nanotechnology inspired by nature. In this study, the mechanical properties of multi-layer graphene helicoid with different geometric characteristics are studied using molecular dynamics simulation and the relationship between several layers, geometric properties, and mechanical properties of nanoparticles are investigated. The results show that the unique geometric properties of these nanoparticles produce interesting mechanical properties that are highly dependent on their structure. The stages of the tensile behavior of these nanoparticles are altered by increasing the number of layers corresponding to the geometric characteristics of the nanoparticles. One of the most important characteristics of these nanoparticles is their high stretchability, even for some specimens, up to 3000%, which, with the addition of a layer to their structure, decreases sharply. The results also indicate a strong increase in force in the small strain range with the onset of the stretching process due to the strong Van der Waals forces between the adjacent layers. The spring constant for these nanoparticles is calculated in this initial area of the tensile test and, decreases with the addition of the layers. Identifying the properties of multilayered graphene helicoid can lead to an increase in their efficiency and their optimal performance in nanoscale devices and even improve multiscale performance.

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1. INTRODUCTION

With regards to advancement in the domain of nanotechnology, and the methods of producing nanomaterial, and by patterning the substances available in nature, the researchers have proposed a spiral model based on the nanomaterial. Coiled carbon nanotubes, were studied in experimental [1] and theoretical forms and in molecular model [6-2]. The interesting properties of the coiled carbon nanotubes are due to carbon bonds with sp^2 hybridization, as well as its spiral structure. Enjoying its spiral geometry, this structure can result in a more energy attraction in nano-composites [7]. Nowadays, new forms of spiral structures have been made experimentally based on 2D materials such as graphene [9,8], or MoS_2 [10]. Through another research Sharifian et al. [11], reviewed the mechanical properties of the net and functionalized spiral graphenes. They Figured out that by functionalizing the nanostructures in different percentages, and various distributions, we can achieve some completely different mechanical properties.

Despite the studies conducted in the domain of mechanical properties of spiral graphene nanostructures, the influence of the change of geometric characteristics of this spiral structure alongside increase of layers of spiral Graphene, have not yet been reviewed. In this research, we study the mechanical properties of the multilayer spiral graphene with different geometric characteristics. The influence of the increase of layers in these nanostructures from one to three layers has been reviewed in three different samples. The spring's stability, elasticity, final fracture strength, and the mechanical response procedure under the tensile testing in multilayer spiral Graphene are studies.

2. RESEARCH METHOD

All the calculations have been conducted based on the molecular dynamic method through the LAMMPS Open-source software. The AIREBO Potential [12] was used for the simulation of multi-interactions. This potential has the ability of constituting and breaking the covalent bonds of C-C and C-H, and is made of three parts:

$$E=\frac{1}{2}\sum_{i}\sum_{j\neq i}\left[E_{ij}^{LJ}+\sum_{k\neq i}\sum_{l\neq i,j,k}E_{kijl}^{TORSION}+E_{ij}^{REBO}\right] \quad (1)$$

where the E_{ij}^{REBO} represents the REBO potential, E_{ij}^{LJ}, represents the long-distant interactions and $E_{kijl}^{TORSION}$ represents the spiral interactions. To remove the nonphysical effects, the cut-off radius for the REBO 2 part was taken as 2 angstroms. [13, 14]. Initially, the structure's energy was optimized through the conjugate gradient method. And then, the structure was balanced under the fixed pressure – fixed temperature ensemble (NPT), based on Nosé–Hoover thermostat and Nosé–Hoover

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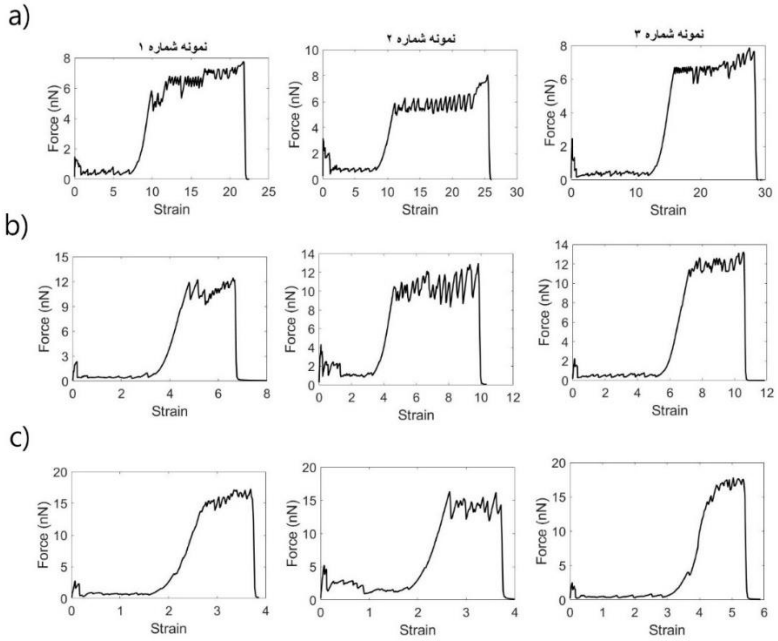

Fig. 1. The tensile behavior of spiral graphene for samples No. 1, 2, and 3 in the forms of (a) single-layer (b) dual-layer and (c) triple-layer

barostat at zero pressure for 400 to 700 ps. The 1K temperature was chosen to review the structures to decrease the influence of thermal fluctuations [4,5].

In all the single-layer structures, seven loops have been used. After balancing, the tensile testing was done to prevent the influences of the number of layers with given the periodic boundary condition. The appropriate strain rate i.e. $10^8 \frac{1}{s}$ is applied allover the tension. This part of the simulation was made through the fixed-temperature ensemble (NVT) under the Nosé–Hoover thermostat. The time step of 1fs is used for all the simulations. To calculate the stress-strain curve, the viral stress relation was used [18]:

$$\sigma_{ij}^{\alpha} = \frac{1}{V^{\alpha}}\left(\frac{1}{2}m^{\alpha}v_i^{\alpha}v_j^{\alpha} + \sum_{\beta=1,n} r_{\alpha\beta}^{j} f_{\alpha\beta}^{i}\right) \quad (2)$$

where the β and α represent the atoms and the *i* and *j* represent the components of the Cartesian coordinate. *m* and *v* indicate the velocity and mass of the atoms respectively. $f_{\alpha\beta}$ and $r_{\alpha\beta}$ respectively indicate the energy and distance between the β and α atoms.

3. RESULTS AND DISCUSSION

Study of the tensile behavior of different spiral Graphene structures for three samples with different geometrical particulars (internal radius, external radius, and nanostructure thickness) were studied with one, two, or three layers. The simultaneous effect of changing the geometrical particulars of the structures and increase of layers were studied. The geometrical particulars have been chosen such that it would be possible to compare the influence of geometrical changes over the tensile behavior of nanostructures.

First, the tensile behavior of the single-layer spiral graphenes are reviewed and then the influence of the increase of layers for each structure is studied. As can be deduced from Fig. 1, the tensile behavior of the single-layer spiral graphenes is divided into four parts. In the first part that is highly influenced by the Van der Waals forces, the sudden increase of energy was observed. In this part and a strain of 0 to 0.8%, a linear behavior was observed and in this area the spring constant for instances No. 1, 2, and 3 were respectively calculated as 23.5 $\frac{nN}{pm}$, 49.5 and 18.97. In the second area, and after the emancipation of a layer, severe energy loss happens and subsequently, the layering process takes place; such that first of all a layer is separated and the separation process is done gently. Therefore, under a fixed process, the tensile test process continues, up to a level wherein the third area, the layering process is completed and the energy increases particularly in the internal area of the spiral graphene.

In phase No. 4, the bonds rupture begins. The phase continues following a Sawtooth pattern. In fact, by increase of strain and subsequently by increase of energy, the bonds rupture happens. By the end of this phase, the monoatomic carbon chain is created within the structure. By the increase of internal radius in spiral graphene, the increase of elasticity is also observed; while, there are not that much changes in the final energy. Another remarkable point is the little increase of strain in the fourth phase alongside of severe increase of thickness of the spiral nanostructures (increase for 2 times).

By increase of the number of layers in sample No. 1, a remarkable change in tensile behavior is observed. The tensile behavior of spiral graphene in sample No.1, enjoying from two layers, just like its single-layer sample has four samples; though some tangible differences can be seen.

By increase of the number of layers in sample No. 1, the tensile behavior of the triple-layer sample was encountered several changes. The initial phase, just like the former samples was followed by a severe energy increase. The end of phase No.2 seems to have a smaller strain, by an increase of the number of layers. Further, the layers' separation in this phase is in a triple form, and the Van der Waals forces

remain between the three adjacent layers. In the third phase, the layers in a triple form, are almost completely open and the energy increase happens. The remarkable point in the triple-layer sample is the deletion of the fourth phase.

4. CONCLUSION

In this research, the mechanical properties of single-layer and multilayer spiral graphene with geometric characteristics have been reviewed. The change of the number of layers for each structure with special geometric characteristics, has a different influence on the phases of tensile behavior. A number of the most important influences of a change in the number of layers, in proportion to geometric characteristics of the spiral graphenes are listed as follows:

- For all the structures, by an increase of layers of strain limitation in the test, their tension decreases, and the maximum level of energy borne by the nanostructure increases.

- Various phases have been observed in the tensile behavior of nanostructures, which in a comprehensive categorization, they include: 1. The initial phase, including severe energy increase arising from the Van der Waals forces; 2. The second phase, including gentle separation of single-layers from each other; 3. The third phase begins after the complete separation of the layers and in this phase, the energy is highly increased. 4. The fourth phase where the bonds rupture happens at almost a fixed force and creates a Sawtooth pattern.

- The phases mentioned in the former section depend on geometric characteristics and the number of layers and even part of this feature results in deletion of a phase.

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