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MECHANICS

Deformation and Fracture Processes in Graphene Nanoribbons with Linear Quadrupoles of Disclinations

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Abstract—The deformation and fracture processes in graphene nanoribbons containing linear quadrupoles of disclinations are investigated by the method of molecular dynamics. Special attention is given to estimating the effect of the curvature formed by disclinations and free boundaries in graphene nanoribbons with linear quadrupoles of disclinations on their mechanical characteristics (the stress–strain curve, the strength at the single-axis tension, and the degree of plastic deformation).

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Graphene is characterized by excellent mechanical characteristics, which have a huge potential for technological applications [1–3]. For example, it was revealed experimentally in [1] that the strength of defect-free graphene achieves a record value of ≈130 GPa and exceeds the values for all other world-known materials. In this case, the highest degree of elastic deformation of ideal graphene $\varepsilon_{el} \approx 25\%$ and Young's modulus $E \approx 1$ TPa [1] are also extremely high.

In addition, graphene shows excellent electronic properties owing to its 2D hexagonal crystalline structure and the presence of charge carriers similar to massless particles [2]. An efficient approach to modifying and controlling the electronic properties of graphene is its fabrication in the form of nanoribbons—narrow graphene ribbons with a width less than 20 nm [4, 5]. In this case, the effects of graphene free boundaries (edges) on its properties manifest themselves pronouncedly. As a consequence, graphene nanoribbons with their unique properties and controllable effects of free boundaries are considered as a new generation of base elements for nanoelectronic devices and nanoelectromechanical systems. This viewpoint is supported by computer calculations, which testify to the high mechanical characteristics of graphene nanoribbons (see [6]) making it possible that such nanoribbons can serve as reliable structural blocks in nanoelectronics.

In addition to boundary effects in nanoribbons, the curvature of a flat configuration generated by disclinations, which is similar to buckling of plates under local thermal loading [7, 8], and the corresponding elastic distortions in graphene also affect its electronic properties significantly [9, 10]. At the same time, the investigations of the effect of curvature on the mechanical properties of graphene are at the most initial stage [11]. The influence of cooperative effects of free boundaries and curvature of graphene on its mechanical characteristics, as far as we know, was previously not investigated at all. In this context, the study of the deformation and fracture processes in curved graphene nanoribbons in which such effects operate seems to be urgent and important both for the fundamental science about graphene and for the development of its technological applications. The basic purpose of this study is the modeling of such processes by the method of molecular dynamics for graphene nanoribbons containing linear quadrupoles of topological disclinations, which bend the nanoribbons. In this case, special attention is given to investigating the effect of curvature and free boundaries of graphene nanoribbons with linear quadrupoles of disclinations on their mechanical characteristics (the stress–strain curve, the strength at the single-axis tension, and the degree of plastic deformation).

The choice of the linear quadrupole is caused by the configuration of the ribbon—any other quadrupole would be cramped in a ribbon. In addition, the combined effect of the "global" curvature generated by a linear quadrupole in the entire ribbon and the free edges of the ribbon on its mechanical characteristics is efficiently studied in this configuration. The quadru-

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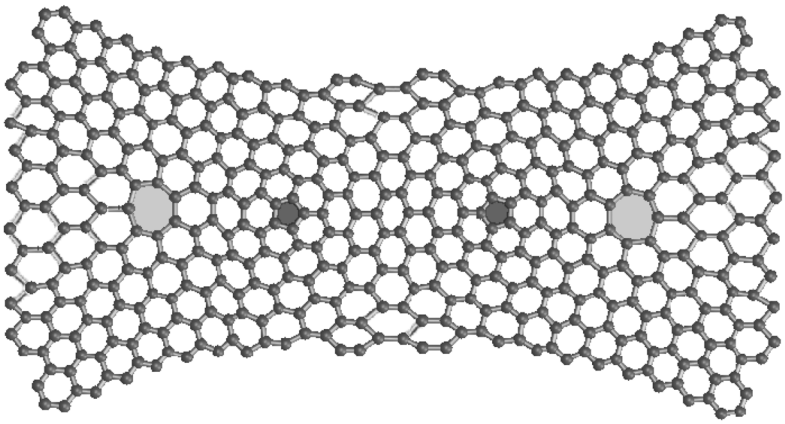

Fig. 1. Flat graphene ribbon with a linear quadrupole of disclinations.

poles of other conventional configurations generate only local curvature.

In this study, we used the molecular-dynamics package "Large-scale Atomic/Molecular Massively Parallel Simulator" for modeling the structural configuration of graphene nanoribbons and the process of their tension. In this case, for describing the characteristics of interatomic bonds, we used the pair interatomic potential AIREBO, which is usually applied in computer models of deformation of graphene structures. The technique of our computer calculation is described in detail in [12].

At the first stage of preparation for modeling, a flat graphene ribbon with a linear quadrupole of disclinations (Fig. 1) was formed as the initial region. The quadrupole represents the configuration of the 7-gon ($-\pi/3$ disclinations), the 5-gon ($\pi/3$ disclinations), and the 5-gon and 7-gon located along the central axis of the nanoribbon in the hexagonal crystalline lattice of graphene (Fig. 1). The model nanoribbon for simulation consists of 468 atoms of carbon and is of 39 Å in length and of 17 Å in width, which corresponds to 23 elementary crystal-lattice cells of graphene in length and to 7 cells in width. The disclinations (5-gons and 7-gons) generate high internal stresses in a flat nanoribbon, which, as a consequence, contains strongly distorted 6-gon crystal-lattice cells (Fig. 1). For the model under consideration, the periodic boundary conditions in the direction of tension (along the nanoribbon long axis) and the free boundary in other directions are set. Short and long nanoribbon edges have a mixed configuration; i.e., they have both chair-like and zigzag fragments (with domination of the latter, Fig. 1).

At the second preparatory step, we simulated the thermal vibrations on the nanoribbon at a temperature of 100 K using the Nose–Hoover thermostat after which the model accepted a steady curvilinear shape (Fig. 2). In this case, the dipoles of 5- and 7-disclinations (Fig. 2) were formed near the nanoribbon edges in its medium portion. Such disclination dipoles represent dislocations, which are the carriers of plastic strains in graphene [13] by analogy with disclination dipoles in conventional 3D nanomaterials [14, 15]. Thus, the local plastic deformation accompanies the formation of the curved configuration of the nanoribbon in the situation under consideration (Fig. 2).

The nanoribbon curvature is set by the values of elastic energies corresponding to flat and curved configurations of graphene with disclinations. In short, without the external mechanical loading, the elastic energy of the curved state (Fig. 2) of the graphene nanoribbon with disclinations is much lower than the elastic energy of the flat configuration (Fig. 1).

The nanoribbon curved by disclinations (Fig. 2) represents a characteristic example of the graphene nanostructure in which the effects of curvature and free boundaries operate simultaneously. For the identification and description of such effects, we carried out the computer modeling of the single-axis tension of the curved nanoribbon with a linear quadrupole of disclinations. The nanoribbon was extended in the direction of the long axis with the rate of 0.0005 fs^{-1}. During the tension, the nanoribbon began partially to straighten out (Fig. 3), the consequence of which is its increased elastic energy. Also during the nanoribbon tension, an intense formation of new n-disclinations occurs, where $n = 4$, 5, 7, 8, and 9 (Fig. 3.). In this case, the n-disclinations with $n > 6$ nucleate more often than those with $n < 6$.

During further tension, further formation of n-disclinations is observed in the middle portion of the ribbon. Then the disclinations coalesce with the subsequent formation of cracks or pores, which separate two large fragments of the nanoribbon. In parallel, one-atom carbon strings connecting the large fragments of

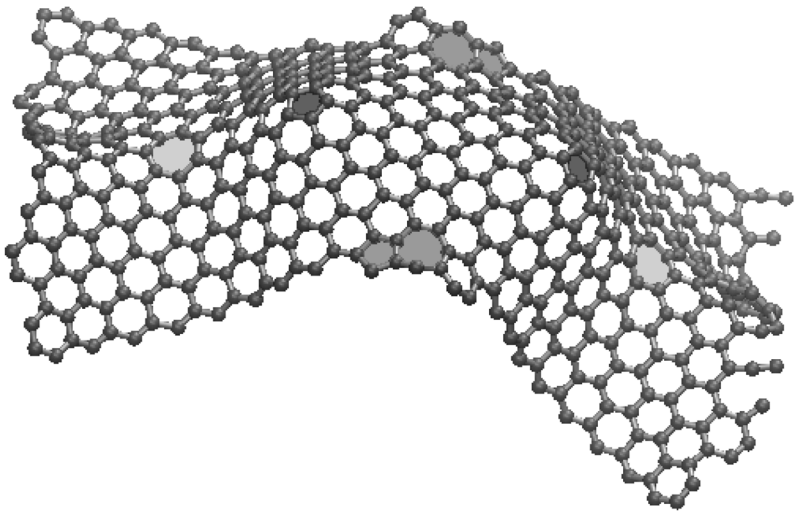

Fig. 2. Curved graphene nanoribbon with a linear quadrupole of disclinations in the absence of loading.

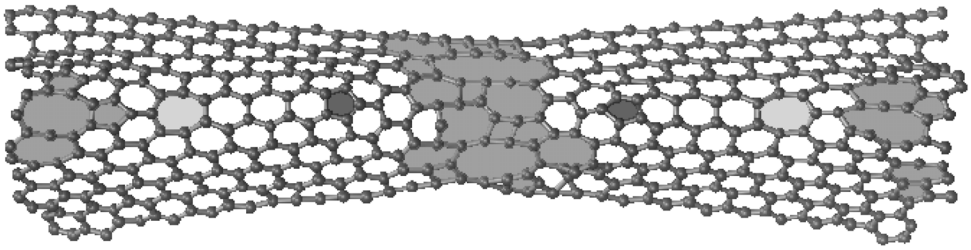

Fig. 3. Plastic deformation and fracture of a graphene nanoribbon during tension.

the nanoribbon are formed. Subsequently, the carbon strings are serially ruptured, which results in the final fracture of the nanoribbon, i.e., in its separation into two fragments isolated from each other.

We also calculated the stress–strain curve for a graphene nanoribbon with a linear quadrupole of disclinations (Fig. 4). In the curve, it is possible to single out a strongly nonlinear elastic portion characterized by the deformation-degree interval from 0 to 19.6%. The nonlinear character of the elastic stage of nanoribbon deformation is caused, first of all, by decreasing its initial space-nonuniform curvature under tension.

The plastic-deformation stage of the nanoribbon is implemented in the deformation-degree interval from 19.6 to 33% (where 33% is the degree of deformation at which complete fracture occurs). In other words, the graphene nanoribbon with an initial linear quadrupole of disclinations is characterized by a reasonably high plasticity with a degree of deformation of about 13.4%. In the majority of cases, graphene (in particular, defect-free graphene) demonstrates fragile behavior with zero plasticity [1, 3]. The nanoribbon plasticity in the case under investigation is explained by the cooperative effect of its free boundaries and the initial disclinations (the curvature source), which provide an efficient screening of stress fields of new (nucleating during the plastic deformation) disclinations and,

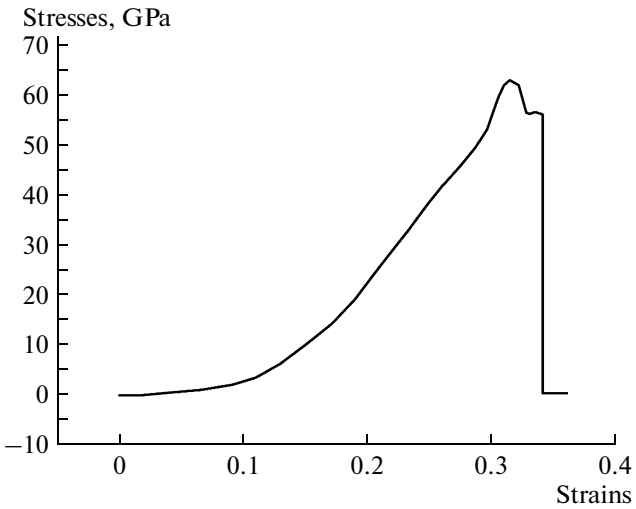

Fig. 4. Stress–strain dependence for the graphene nanoribbon containing a linear quadrupole of disclinations.

thus, a substantial decrease in their elastic energies in the nanoribbon. As a consequence, the cooperative effect of its free boundaries and initial disclinations in the nanoribbon set an "easy" nucleation of disclinations—the carriers of plastic deformation and, consequently, a sufficiently high plasticity of the nanoribbon.

The strength of the nanoribbon with a linear quadrupole of disclinations amounted to 65 GPa. This very high value, however, is significantly (approximately twice) lower than 130 GPa characterizing the strength of the defect-free graphene.

Thus, in this study, the processes of deformation and fracture of graphene nanoribbons containing the linear quadrupoles of disclinations were investigated by the method of molecular dynamics. It was revealed that the presence of the linear quadrupole of disclinations in the graphene nanoribbon sets an appreciable curvature of the nanoribbon in its initial unloaded state, and results in a significant decrease in the nanoribbon strength (approximately two times) in comparison with the strength of defect-free graphene under single-axis tension. The graphene nanoribbon with a linear quadrupole of disclinations demonstrates a strongly nonlinear elasticity and a sufficiently high plasticity characterized by the degree of plastic deformation $\varepsilon_{pl} \approx 13.4\%$. The nonlinear character of the elastic stage of nanoribbon deformation is caused, first of all, by decreasing its initial space-nonuniform curvature under tension; i.e., it represents the manifestation of the effect of the initial curvature of the nanoribbon on its behavior under tension. The nanoribbon plasticity in the case under investigation is explained by the cooperative effect of its free boundaries and the initial disclinations (the curvature sources), which determine the "easy" nucleation of disclinations—the carriers of plastic deformation—and, consequently, a sufficiently high nanoribbon plasticity.

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