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ORIGINAL PAPER

Stability of the thin partitioned carbon nanotubes

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Abstract We report on the research of the stability of partitioned (bamboo-like) carbon nanotubes with different diameters. The stability of the partitioned carbon nanotubes of the smallest diameter were determined by the tight-binding method. For the prediction of the destruction regions of the bamboo-like nanotubes atomic framework subjected to strain the new original method of the calculation of the local stress of atomic network was developed. Using this method it was shown that partitioned carbon nanotubes with a diameter of 2.02 nm are stable. These partitioned carbon nanotubes with chirality (15,15) are the most stable partitioned carbon nanotubes with the smallest diameter.

Keywords Atomic structure · Bridge · Local stress · Partitioned nanotubes · Stability

Introduction

Since the discovery of fullerenes structures in 1985 investigation of carbon and carbon-based materials is one of the most actual directions in fundamental and applied science. In recent years, significant progress in the synthesis, investigation of the physicochemical properties and theoretical prediction of a whole set of new nanodimensional carbon forms were achieved. Among carbon forms it is allocated such modifications as fullerenes, nanotubes, graphene ribbons, nanocores, nanofibers, nanohorns, nanocrystallites etc. [1]. These structures are often considered as new carbon nanoallotropes. They have unique physicochemical properties, that determinate their significant potential at the creation carbon nanomaterials of many-functional purposes.

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There are various ways that carbon nanoforms could be classified. These include their synthesis conditions, physical properties such as density and internal surface area, or graphitic sheet texture. Recently, a coherent nomenclature for carbon nanoforms based on their morphological differences and the geometrical transformations that relate one form to another was developed [2]. According to current nomenclature sp^2-bonded carbon nanoforms one can divide into some main groups: molecular forms (0D), cylindrical nanoforms (1D) and layered nanoforms (2D). The most multiple group, containing various nanostructures of complex form, is the group of cylindrical nanoforms. Nanotube bundles, graphene nanoscroll, collapsed nanotube, stracked platelets, partitioned nanotubes, partitioned stacked nanocones, X,Y-shaped nanotubes are the structures of the complex shape [3–9]. Each of these structures is characterized by its individual unusual mechanical and electronic properties, which attracts attention of many scientists.

At the present time the intensive investigations in the area of the partitioned nanotubes are performed. Atomic structure of the partitioned nanotubes is characterized by hollow-core nanoform with internal walls orthogonal to the object axis, which divide the core into separate compartments. Another common term in the scientific literature is “bamboo nanotubes” [10], which in some nomenclatures is replaced by terms such as “partitioned nanotubes” and “partitioned stacked nanocones” [2].

There are many works in the area of synthesis of the partitioned nanotubes. For the first time Saito has synthesized nanotubes with the bamboo-shaped structure [11]. The tubes of such structure consist of many long hollow compartments, are capped with needle-shaped metal particles at their ends. Their sizes are typically 30 nm in diameter and a few micrometres in length. Each tube wall consists of several tens of graphite layers. The carbon partitioned nanotubes were synthesized by pyrolysis of iron(II) phthalocyanine under Ar/H_2 at 1000 °C [12]. Also the partitioned nanotubes (bamboo-shaped) can be

Table 1 Values of the parameters

ε_s, eV	ε_p,eV	$V^0_{ss\sigma}$, eV	$V^0_{sp\sigma}$, eV	$V^0_{pp\sigma}$, eV	$V^0_{pp\pi}$, eV	p_1	p_2, nm	p_3, nm	p_4	p_5, eV	p_6
−10.932	−5.991	−4.344	3.969	5.457	−1.938	2.796	0.232	0.154	22	10.92	4.455

obtained from CH_4/H_2 on Ni–Cu/Al_2O_3 nanoparticles at the 720–770 °C [13].

At the present time there are some sythesis processes of the partitioned nanotubes. In particular, bamboo-shaped multi-walled carbon nanotubes of diameter on the order of 50 nm have been grown on carbon black in a fluidized bed in bulk amount [14]. In this work, the activation energy for the synthesis of the product was found out to be around 33 kJ mol^{-1} in the temperature range of 700–900 °C.

Another method for the synthesis of the partitioned nanotubes is chemical vapor deposition (CVD) method. For example, carbon partitioned nanotubes (bamboo-shaped) were synthesized on a copper foil by catalytic chemical vapor deposition from ethanol [15]. As a result of the investigation by means of the scanning and transmission electron microscopy and Raman spectroscopy it was found that the yield and size of the partitioned nanotubes increased with temperature. Those prepared at 700 °C had a copper droplet tip and those at 800–900 °C had a copper nanopar-ticle inside. Partitioned nanotubes were really grown from the amorphous carbon film consisted of a porous and non-porous layer. The thickness of the carbon film increased from 187 to 900 nm when the duration increased from 5 to 60 min.

Partitioned nanotubes are widely investigated due to their unique structure and properties. Their structures would affect their properties significantly. For example, multi-walled partitioned nanotubes, with a higher ratio of edge-to-plane sites along its surface, have better electrochemical properties than the hollow carbon nanotubes [16]. These properties were rationalized by the presence of end-caps located at regular intervals along the walls of partitioned nanotubes, which introduce edge planes of graphene all along the walls. Heng et al. [17] demonstrated the advantages of partitioned nanotubes over hollow single walled carbon nanotubes for the biosensing of guanine and adenine.

Also it was established that the partitioned nanotubes (single-walled carbon bamboo nanotubes) are very perspective material for emission electronics. In particular, it was found that the ionization potential of these nanotubes decreased by 0.1 eV in comparison with the hollow nanotubes [18]. It was revealed that the emission properties of partitioned nanotubes were improved by inserting the potassium atoms in the atomic structure. Therefore, one can design a high-effective nanoemitter based on the partitioned nanotubes.

For the expansion of the application areas for partitioned nanotubes it is necessary to determine the stability configuration of the atomic structure of partitioned nanotubes. At the present time, there is no definite criterion for determination of the stability of partitioned nanotubes. The aim of this article is the theoretical investigation of the stability of partitioned carbon nanotubes (bamboo-like) with the smallest diameter. Stable partitioned nanotubes with the smallest diameter were determined using the tight-binding method. For the prediction of the destruction regions of the atomic framework for partitioned nanotube, subjected to the strain, the original method of the calculation of the atomic network local stress was used. This method was successfully applied to the theoretical investigation of the influence of the curvature for the atomic grid on the graphene adsorption capacity and hydrogen process [19].

Computational methods

Tight-binding method

The total energy is calculated by the formula

$$E_{tot} = E_{bond} + E_{rep} \quad (1)$$

where E_{bond} is the bond structure energy calculated as the sum of energies of the single-particle occupied states. E_{rep} is the phenomenon energy (repulsive potential).

The bond structure energy is determined by the formula

$$E_{bond} = 2\sum_n \varepsilon_n \quad (2)$$

Table 2 The values of the stress of different nanotubes

Location of the nanotube atoms	E_i, eV	w_i, GPa	σ_i, GPa
The tube (5,5) with diameter of 0.66 nm			
Central area	−7.41	−57.74	0.86
Edge area	−5.28	−41.12	0.42
The tube (10,10) with diameter of 1.36 nm			
Central area	−7.5	−58.39	0.21
Edge area	−5.32	−41.44	0.1
The tube (15,15) with diameter of 2.024 nm			
Central area	−7.52	−58.51	0.09
Edge area	−5.33	−41.5	0.04

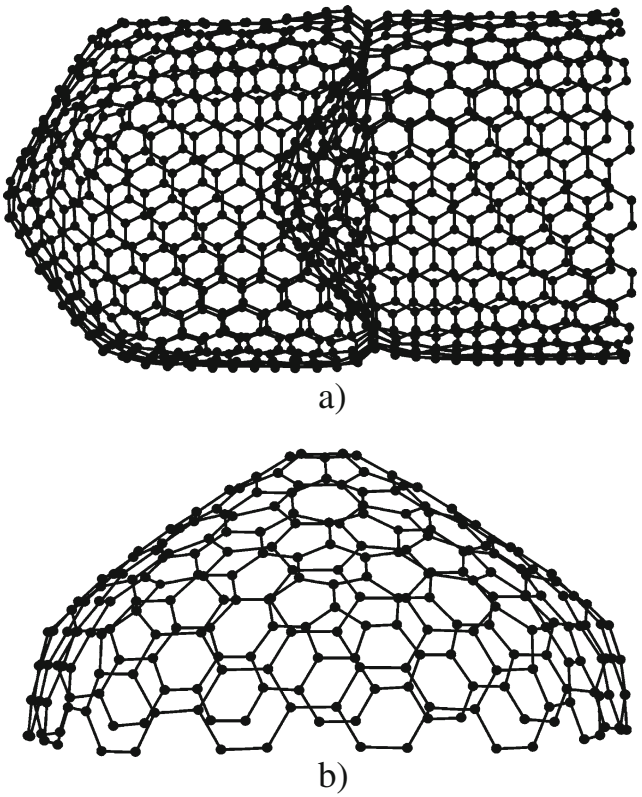

Fig. 1 Partitioned carbon nanotube (15,15): **a**) a general form; **b**) atomic structure of bridge

This expression is the sum of energies of the molecular orbitals obtained by diagonalizing the Hamiltonian. n is the number of the occupied orbitals, and ε_n – the energy of the single-particle orbitals.

The phenomenon energy can be expressed as a sum of two-body potentials as

$$E_{rep} = \sum_{1<j} V_{rep}\left(\left|r_i - r_j\right|\right) \tag{3}$$

where i, j are the number of the interaction atoms; r_i, r_j are the Cartesian coordinates.

The overlap matrix elements are calculated by the formulas which take into account four types of interaction: $ss\sigma$, $sp\sigma$, $pp\sigma$ and $pp\pi$ and the pair repulsive potential:

$$v_{ij\alpha}(r) = v^0_{ij\alpha}\left(\frac{p_3}{r}\right)^{p_1} \exp\left\{p_1\left[-\left(\frac{r}{p_2}\right)^{p4} + \left(\frac{p_3}{p_2}\right)^{p_4}\right]\right\}, \tag{4}$$

$$v_{rep}(r) = p_5\left(\frac{p_3}{r}\right)^{p_6} \exp\left\{p_6\left[-\left(\frac{r}{p_2}\right)^{p4} + \left(\frac{p_3}{p_2}\right)^{p_4}\right]\right\}, \tag{5}$$

where i and j are the orbital moments of wave function, α presents the bond type (σ or π). The atomic terms ε_s, ε_p are the atomic orbital energies of carbon which are found on the main diagonal of the Hamiltonian. The values of the ε_s, ε_p atomic terms, the parameters p_n (n=1,2,3,4,5,6) and the equilibrium overlap integrals $V_{ij}^{\ 0}$ ($V^0_{ss\sigma}$, $V^0_{sp\sigma}$, $V^0_{pp\sigma}$, $V^0_{pp\pi}$) are given in Table 1. The coefficients p_4, p_1, p_6 are the power exponents, the coefficients p_5 and p_3 are determined by the overall shape and steepness of the function, and the parameter p_2 is a cutoff distance for the hopping matrix elements and repulsive interactions. Tight-binding parametrization was performed in the following way. Modification of the atomic terms and equilibrium overlap integrals was carried out so that the values of the bond lengths and ionization potential correspond to analogous experimental values and ab initio values for fullerene C_{60}.

The geometric and energy parameters for the carbon nanotubes and fullerenes obtained by the tight binding method are in a good agreement with experimental data [20, 21] and ab initio data [22]. The distance between carbon atoms and ionization potential are equal to 0.14 nm and 7.61 eV.

The calculation method of the local atomic stress

We have developed a new method of the local stress of atomic network calculation for more detailed study of the destruction process and prediction of areas of the chemical bonds break possible locations. The following idea is based on the aforementioned method.

Since nanotubes, fullerenes and other carbon nanostructures can be formed using graphene sheet, the stress on atoms of the graphene sheet is assumed to be zero. This graphene sheet is in ground state at the temperature of 0 K. The atoms of the graphene sheet are in sp^2-hybridization state.

The value of stress on atom of framework is determined as a difference between the bulk density energy of atom of the investigated structure (in our article the partitioned carbon nanotubes) and the bulk density energy of the graphene atom. The bulk density energy of atom is calculated by one of the known empirical methods. Its value is a pressure which the atom within the structure experiences from environment. Of course, the internal atoms and the edge atoms will differ by energy, therefore it is necessary to take this fact into account during the stress calculation.

Table 3 Value for diameters of the considered carbon nanotubes

Type of tube	Diameter of tube, nm
(5,5)	0,66
(7,7)	0,94
(8,8)	1,08
(9,9)	1,22
(10,10)	1,36
(11,11)	1,49
(13,13)	1,76
(15,15)	2,02

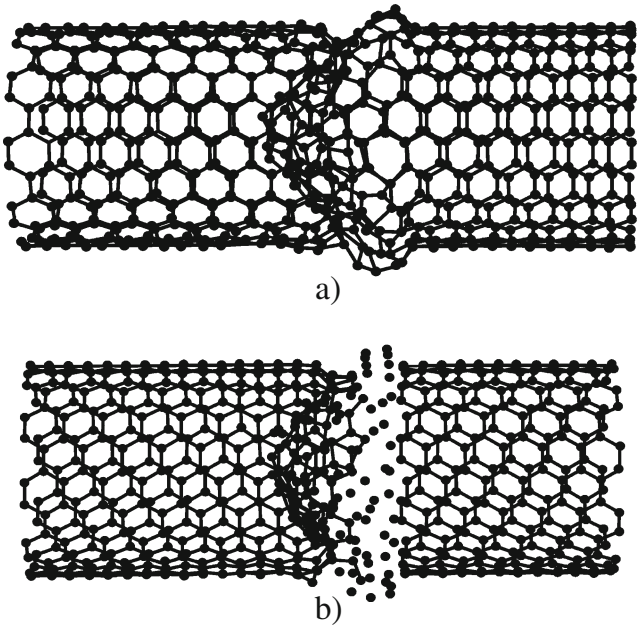

Fig. 2 The partitioned carbon nanotube (10,10) before (**a**) and at the time (**b**) of the destruction

The methodology of the calculation of the atomic network local stress of the partitioned carbon nanotube includes the following steps:

1. optimization of the atomic structure of the stable unstrained graphene sheet by the minimization of the total energy by the coordinates of atoms;
2. calculation of distribution for the bulk energy density of the stable unstrained graphene atoms;
3. atomic structure optimization for partitioned nanotube by the minimization of the total energy calculated for atoms coordinates;
4. calculation of distribution for the bulk energy density on atoms of the partitioned nanotube;
5. calculation of the atomic framework local stress map as a difference of the bulk energy density for the partitioned nanotube atoms and the bulk energy density for the planar graphene sheet atoms.

Optimization of structure was carried out by the minimizing of the structure total energy (1) for coordinates of all atoms by the tight-binding method. The calculation of distribution of the bulk energy density on atoms was performed by the empirical method. This method is based on the Brenner's potential with the introduced torsion interaction energy and van der Waals interaction energy in polynomial of energy function [23]. The bulk energy density of the partitioned carbon nanotube was calculated by the formula:

$$w_i = \frac{\left(\sum_{j\ (\neq i)} \left(V_R(r_{ij}) - B_{ij} V_A(r_{ij})\right) + \sum_{j\neq i} \left(\sum_{k\neq i,j} \left(\sum_{l\neq i,j,k} V_{tors}(\omega_{ijkl})\right)\right) + \sum_{j(\neq i)} V_{VdW}(r_{ij})\right)}{V_i} \quad (6)$$

where V_R (r_{ij}) and V_A (r_{ij})– the pair of potentials of repulsion and attraction between chemically bonded atoms which is determined by the atoms type and the distance between them. r_{ij} is the distance between atoms i and j, i and j are the numbers of interaction atoms; B_{ij} is the multiparticle term correcting interaction energy of the atoms pair $i-j$ considering specificity of interaction of σ- and π-electron clouds; V_{tors} (ω_{ijkl}) is the torsional potential, which is the function of the linear dihedral angle ω_{ijkl} constructed on the basis of atoms with an edge on bond $i-j$ (k, l are the atoms forming chemical bonds with i, j). V_{VAW} (r_{ij}) is the van der Waals interaction potential between the chemically unbounded atoms; $V_i = \frac{4}{3}\pi r_0^3$ is the occupancy volume of the atom i, r_0 is the van der Waals radius of the carbon atoms which is equal to 1.7 Å.

The strain of the atomic framework near the atom with number i is calculated as:

$$\sigma_i = \left|w_i - w_i^0\right| \quad (7)$$

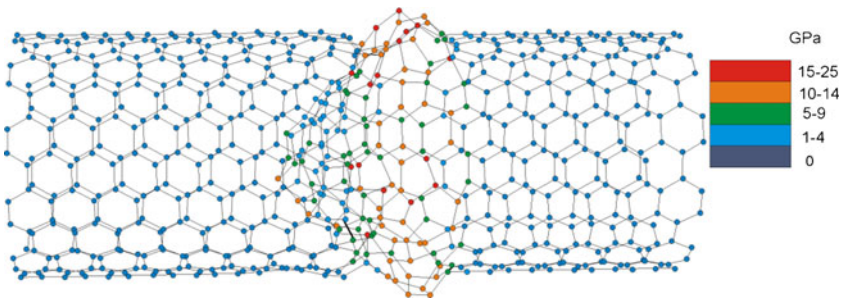

Fig. 3 The distribution of the stress on the atoms of the partitioned nanotube (10,10)

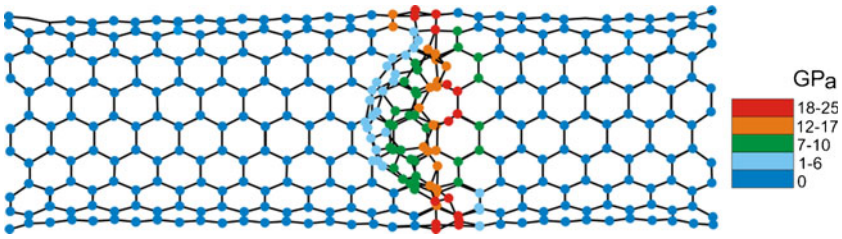

Fig. 4 The distribution of the stress on the atoms of the partitioned nanotube (9,9)

where w_i^0 is the bulk energy density of *ith* atom of the graphene sheet which is in equilibrium; w_i is the bulk energy density of the partitioned carbon nanotubes. The value of w_i^0 in the center of the graphene sheet is equal to −58.60 GPa. At the edges of the graphene sheet bulk energy density is higher since the atoms of the edges have only two links with other carbon atoms. It is equal to −41.54 GPa. It is suggested that stress is equal to zero for the atoms in center and at the edges.

Let us demonstrate a validity of our method of the stress calculation on an example, which is calculation of the stress map for the hollow carbon nanotube of different diameter. It is known that the tubes of the large diameter are the most stable and the tubes of subnanometer diameter are unstable and exist only inside the other tube of larger diameter. Thus, as a result of our calculations, we can conclude that while the tube diameter is increasing the stress decreases, therefore approaching to zero, which is the stress of the planar graphene.

We have investigated open-ended tube of subnanometer diameter (5,5), an open-ended tube of nanometer diameter (10,10) and an open-ended tube of greater diameter (15,15). All tubes have identical length of 36.96 nm. The diameters, the values of energy per atom (calculated by the Brenner method) E_i, the values of the energy density w_i, the stress σ_i are indicated in Table 2.

From the table data it is obvious that the stress of the atoms of the largest tube tends to zero. This fact confirms a validity of our method of calculation of the local atomic stress.

Table 4 Value for diameters of the considered carbon nanotubes

Type of tube	Maximum stress values, GPa
(5,5)	31,62
(7,7)	28,94
(8,8)	26,14
(9,9)	25,38
(10,10)	24,78
(11,11)	21,35
(13,13)	18,18
(15,15)	14,61

Results and discussion

Most of the partitioned carbon nanotubes that have been discussed in the literature have closed caps. However, open-ended partitioned carbon nanotubes with dangling bonds have also been reported [24, 25]. In the current work the model of partitioned carbon nanotubes with closed cap and the model of open-ended partitioned carbon nanotubes are considered. The investigation of the partitioned carbon nanotubes is carried out for models of the armchair nanotubes. The partitioned carbon nanotubes are modeled by the connection of the fullerene fragment to the inner surface of nanotube by the chemical bonds. The fragment of the partitioned carbon nanotube model, constructed on the basis of tube (15,15), is shown in Fig. 1a. The bridge of the partitioned carbon nanotube is shown separately in Fig. 1b. We have considered the set of partitioned carbon nanotubes with different diameter. Values for diameters of the considered partitioned carbon nanotubes are presented in Table 3.

In the first step of the calculations we optimized the geometry of the atomic structure for partitioned carbon nanotube by minimization of the total energy (1) using tight binding method. As a result of the calculations it was found that the increase of the distance between atoms in structure within the range from 0.16 to 0.2 nm is observed for tubes of subnanometer and nanometer diameter. The partitioned carbon nanotube (5,5) with the diameter of 0.66 nm has a maximum bond length of 0.2 nm. Thus the partitioned carbon nanotubes with the diameter of less than 0.66 nm cannot exist. The partitioned carbon nanotubes (7,7), (8,8), (9,9), (10,10), (11,11), (13,13) are metastable. In particular, the partitioned carbon nanotubes (9,9) and (10,10) are destroyed under little external influence such as the tension/compression within a few percent. The tube (10,10) is shown in Fig. 2 for the timing close to the destruction (see Fig. 2a) and at the moment of the destruction itself at the region near the bridge (see Fig. 2b).

In the next step we calculated the local stresses on the atoms of the partitioned nanotubes using the original calculation method described above. As a result of the calculations it was found that for tube (10,10) the maximum stress is observed in the region of the bridge (see Fig. 3), therefore the metastable tube (10,10) can be easily destroyed under the external load only in this region. Thus, our results of the calculations of the local stress distribution for nanotube

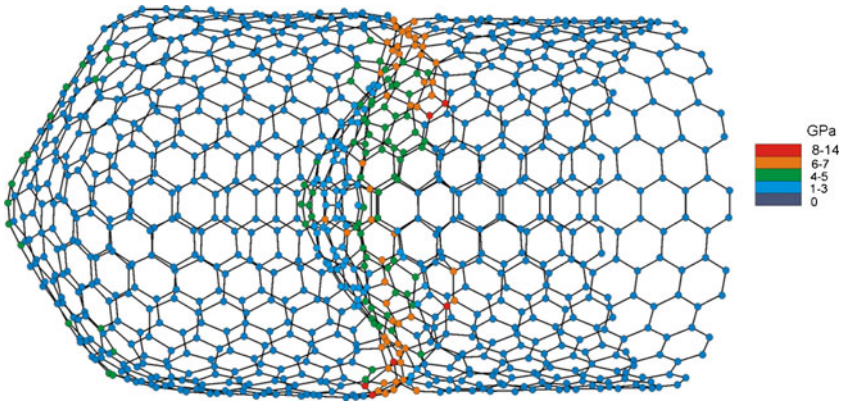

Fig. 5 The distribution of the stress on the atoms of the partitioned nanotube (15,15)

(10,10) with diameter of 1.36 nm clearly explains the process of destruction of this tube (10,10) in the area of bridge as shown in Fig.2b.

The distribution of the stress on the atoms of the partitioned nanotube (9,9) is presented in Fig. 4.

We have calculated a distribution of the stress on the atoms for all considered partitioned nanotubes. Maximum stress values on the atoms of the nanotubes are presented in Table 4.

As results of calculations it was found that the partitioned carbon nanotube (15,15) with a diameter of 2.02 nm is stable. This tube is characterized by the uniform distribution of stress along the bridge and the nanotube. The distribution of stress of the atoms for this tube is presented in Fig. 5. As a result of the calculations it was found that the highest stresses of the partitioned carbon nanotube are obtained in the area of the junction of the tubes and bridge.

Part of the atoms of the partitioned carbon nanotubes is sp^3 hybridized in comparison to the atoms of the usual tubes. In the sp^3 hybridization state each atom has four chemical bonds with nearest-neighbor environment. In the partitioned nanotubes all atoms have $sp^{2+\Delta}$ hybridization beside atoms connecting nanotube and bridge. In this region atoms have sp^3 hybridization similar to the diamond atoms. We carried out calculation of the diamond fragment where all atoms were in sp^3 hybridization and established that they have a bulk energy density equal to 63.70 GPa. This value exceeds the bulk energy density of graphene sheet by 5.1 GPa. Therefore, stress within range from 8 to 14 GPa is not critical since it is caused only by nature of sp^3 hybridization. If stress of the atoms in sp^3 hybridization is higher, then it can be considered as critical. For atoms outside the region of the bridge and nanotube junction stress of~7 GPa is a critical one.

Conclusions

We developed method of calculation of the local stress map of the structure. The developed method is based on the empirical approach in calculation of energy for single atom. We can predict regions of the possible destruction of the nanostructure using this method. As a result of the calculations of distribution of the local stress on atoms for partitioned nanotubes it was found that atoms in the area of the bridge and tube wall junction are subjected to the largest stresses. By means of developed method it is found that the partitioned nanotube (15,15) with a diameter of 2.02 nm is a first stable nanotube of the smallest diameter. It is predicted that for atoms of this structure in $sp^{2+\Delta}$ hybridization state stress of 7 GPa is a critical stress, although for atoms in sp^3 hybridization state a stress higher than 14 GPa can be found critical.

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