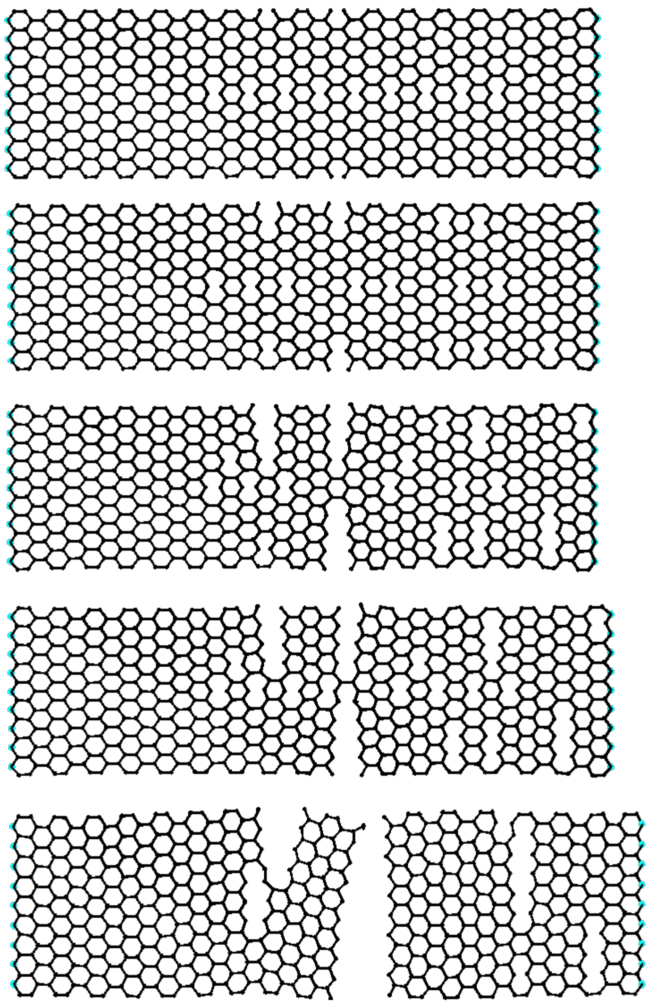
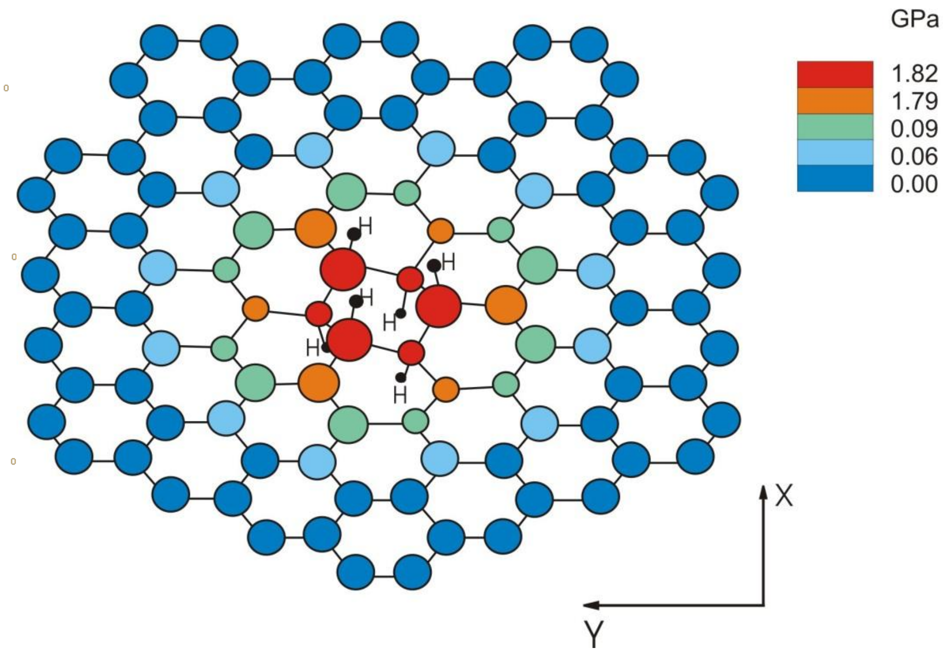
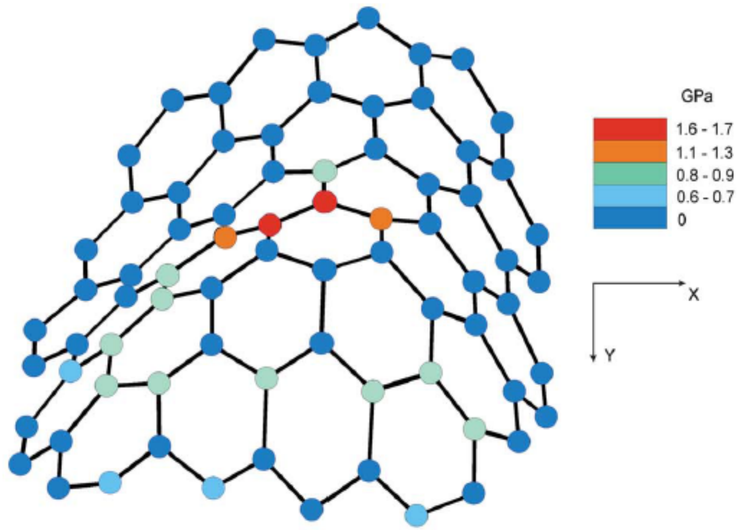
Prediction of defects in nanostructures

Olga E. Glukhova, Michael M. Slepchenkov Influence of the curvature of deformed graphene nanoribbons on their electronic and adsorptive properties: theoretical investigation based on the analysis of the local stress field for an atomic grid // Nanoscale 2012. Issue 11. Pages 3335-3344.

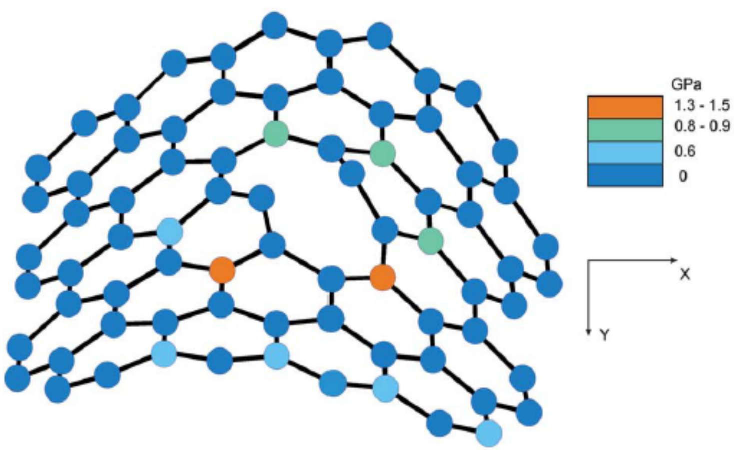




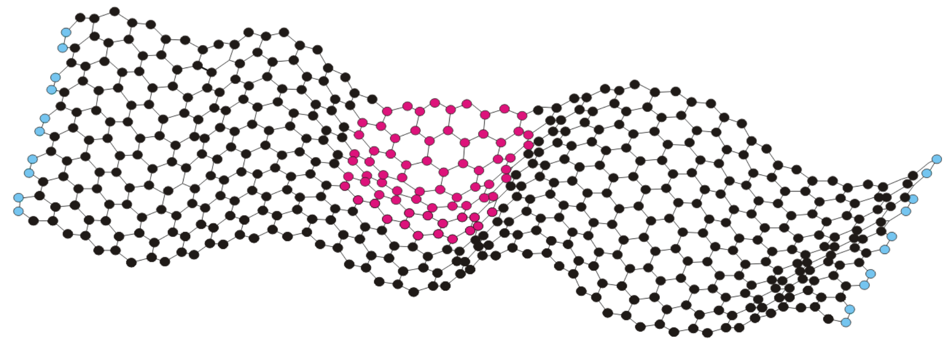
Prediction of the defects appearance

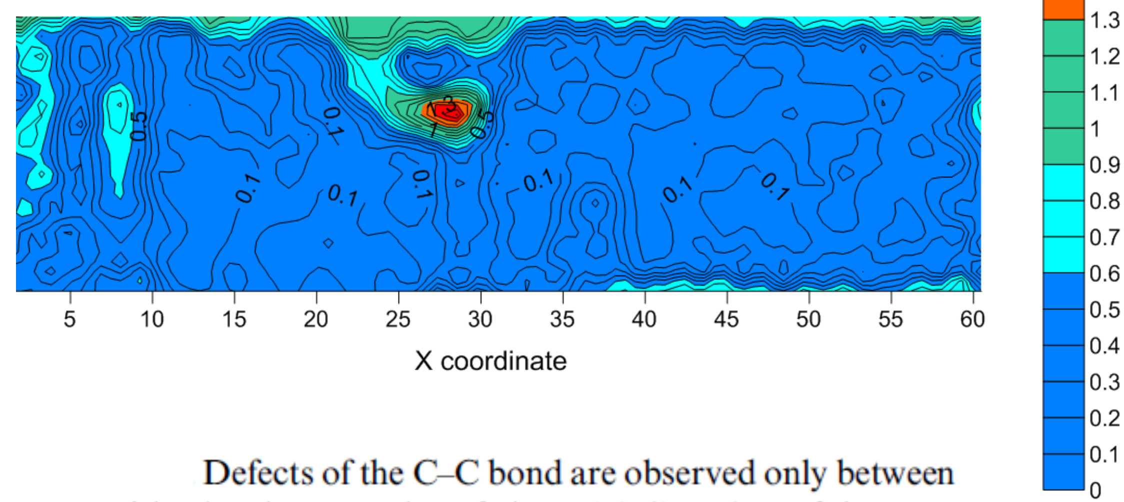


(a)



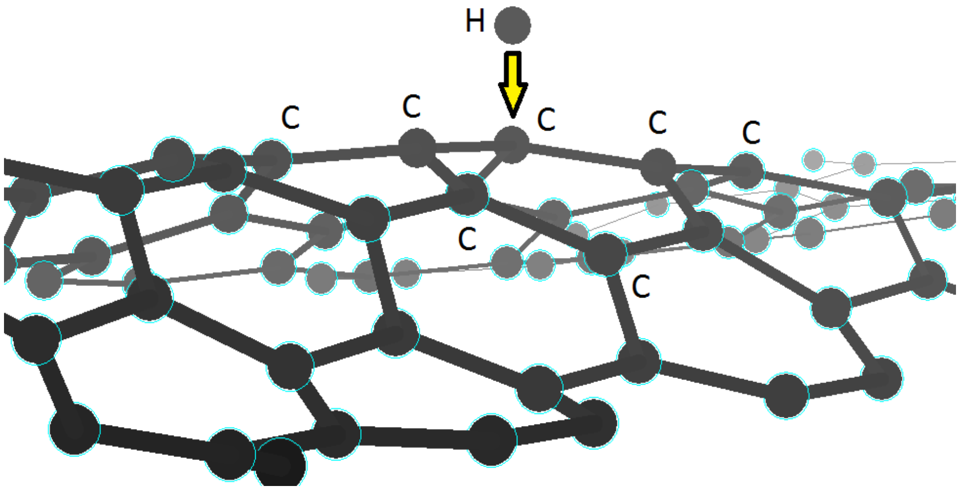
(b)





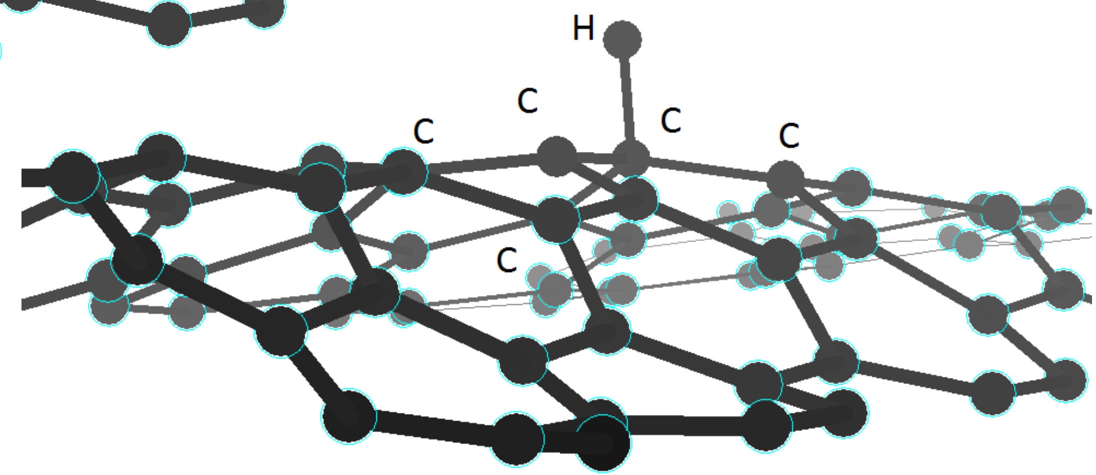
Defects of the C–C bond are observed only between atoms with a local stress value of about 1.8 GPa. One of the most stressed sections of the atomic grid containing a defect is presented in Fig. 4. From the Figure it is clearly seen that after C–C-bond breaking the atomic grid reconstructs and the stress decreases. The enthalpy of the defect formation equals 163.5 kcal mol^{-1}.

The influence of a curvature on the properties of nanostuctures



The absorption of H-atom on the atomic

network

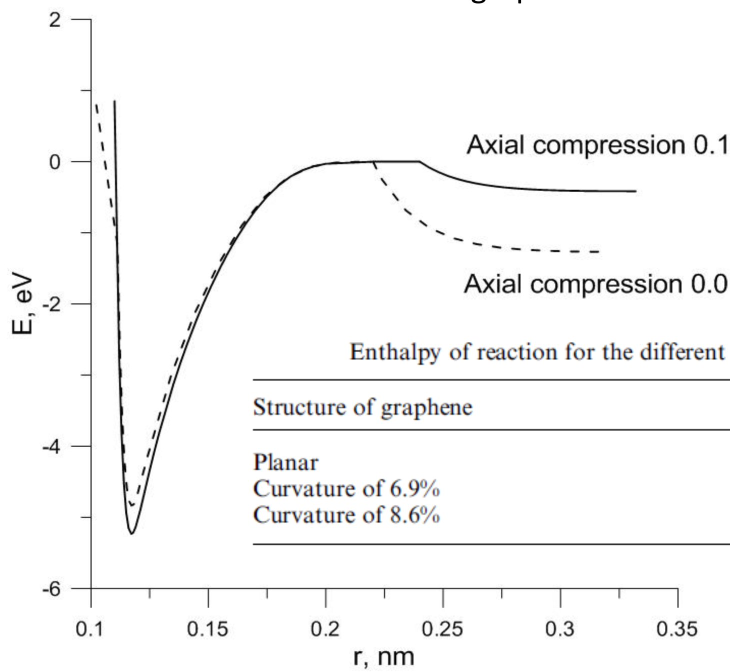


O.E. Glukhova, I.V. Kirillova, M.M. Slepchenkov The curvature influence of the graphene nanoribbon on its sensory properties // Proc. of SPIE. 2012. Vol. 8233. P. 82331B-1-82331B-6.

Olga E. Glukhova, Michael M. Slepchenkov Influence of the curvature of deformed graphene nanoribbons on their electronic and adsorptive properties: theoretical investigation based on the analysis of the local stress field for an atomic grid // Nanoscale 2012. Issue 11. Pages 3335-3344. DOI:10.1039/C2NR30477E.

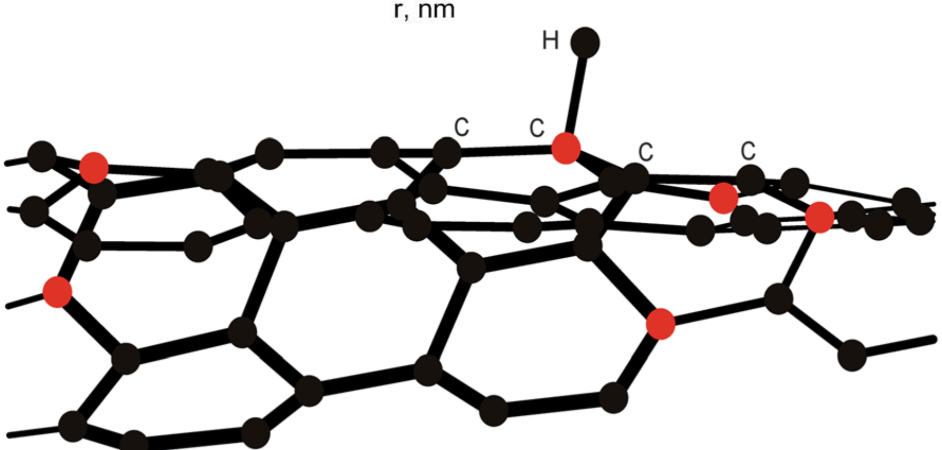
The total energy of the structure depends on the distance between the hydrogen atom and the carbon atom.

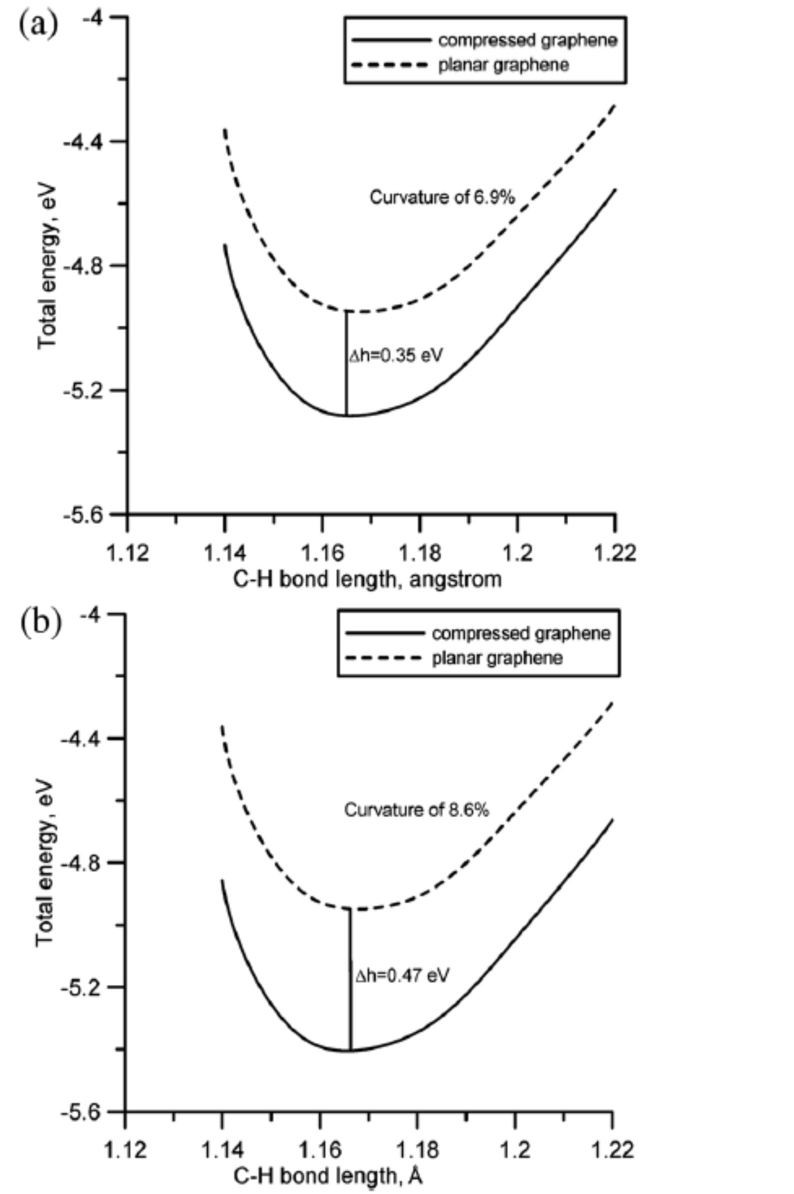
(The dashed line is the interaction of the hydrogen atom with planer graphene nanoribbon; the solid line is the interaction of the hydrogen atom from wave-like graphene nanoribbon)



Enthalpy of reaction for the different graphene structures

Structure of graphene	Enthalpy of reaction
Planar	−23.31 kcal mol^{-1}
Curvature of 6.9%	−28.13 kcal mol^{-1}
Curvature of 8.6%	−31.59 kcal mol^{-1}

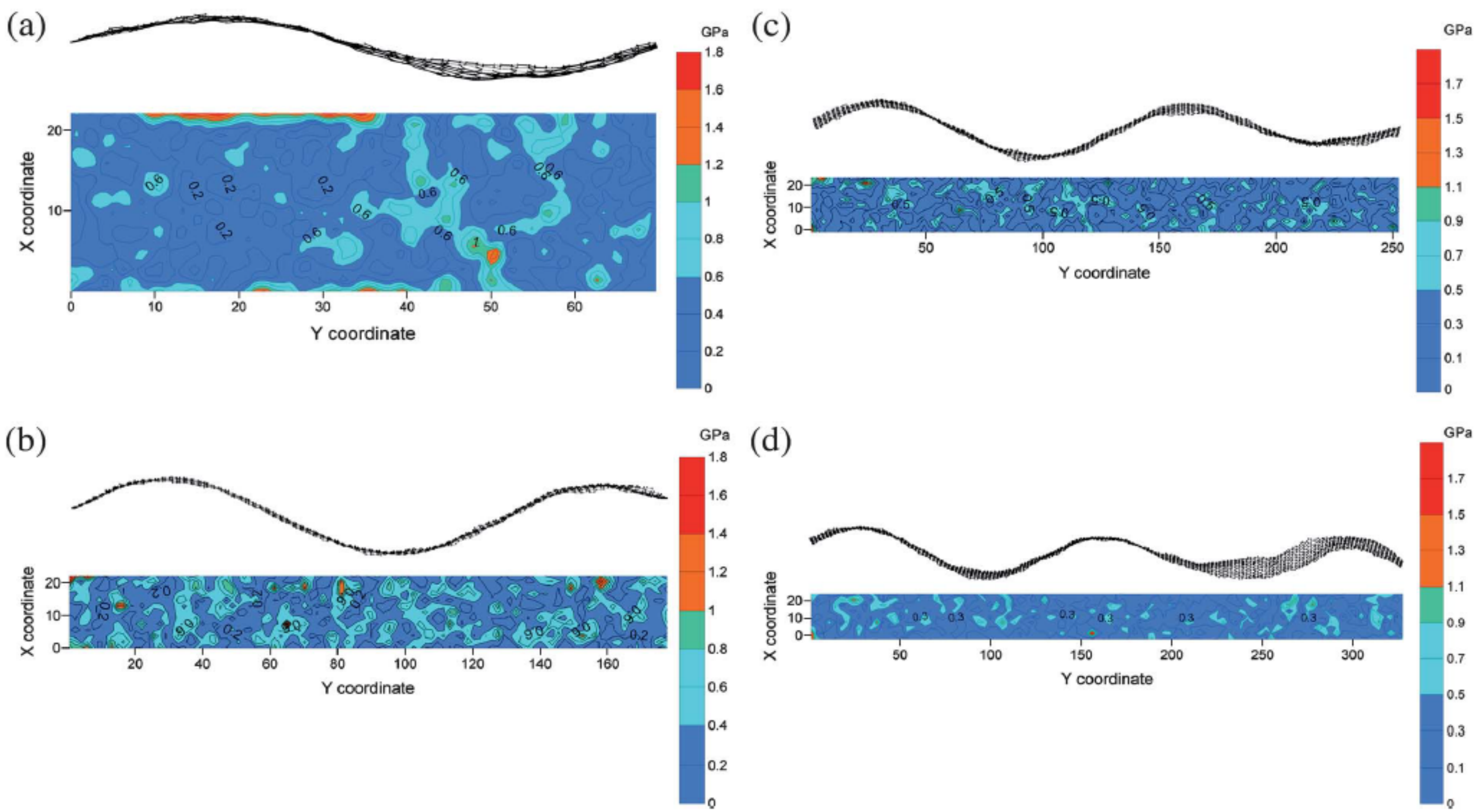




The dependence of the chemical C–H interaction energy on the length of the C–H bond for the planar and compressed graphene nano-ribbon: (a) with curvature of 6.9%; (b) with curvature of 8.6%.

Geometrical characteristics of the curved armchair graphene nanoribbons compressed up to 98% of initial length

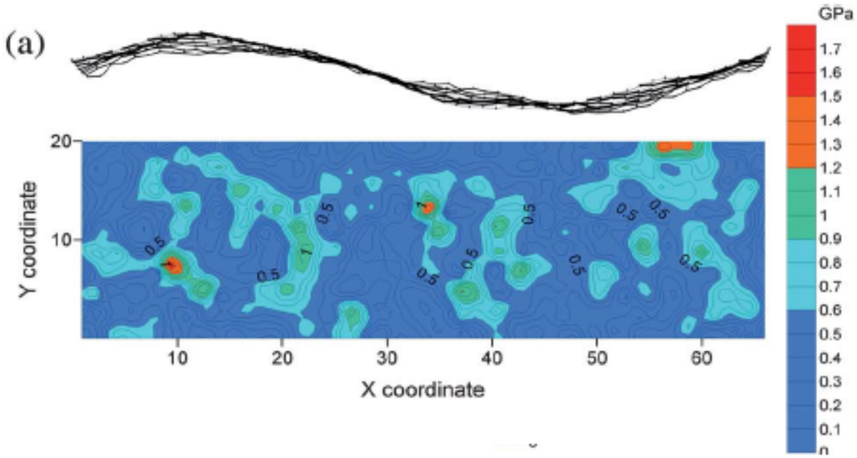
Number of half-waves	Number of atoms in structure	Length of nanoribbon/Å	Length of half-wave/Å	Amplitude of half-wave/Å	Number of hexagons in half-wave	Width of nanoribbon/Å
2	646	71.0	35.5	2.2	9	22.4
3	1634	181.7	60.5	5.3	14	
4	2318	258.4	64.6	5.65	15	
5	3002	335.12	66.2	5.4	15	

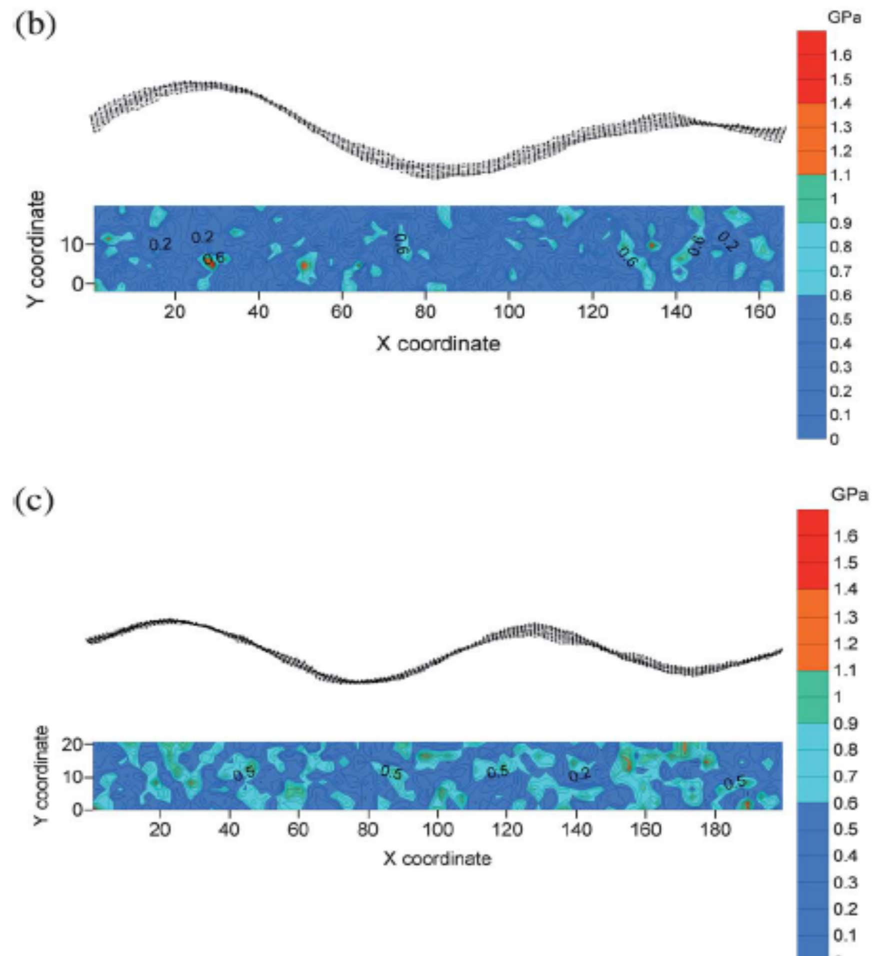


Map of distribution of the local stress for the nanoribbon armchair: (a) in the case of two half-waves; (b) in the case of three half-waves; (c) in the case of four half-waves; (d) in the case of five half-waves.

Geometrical characteristics of the curved zigzag graphene nanoribbons compressed up to 98% of the initial length

Number of half-waves	Number of atoms in structure	Length of nanoribbon/Å	Length of half-wave/Å	Amplitude of half-wave/Å	Number of hexagons in half-wave	Width of nanoribbon/Å
2	550	65	32.5	2.8	12	19.88
3	1390	165.18	55.06	5.4	20	
4	1670	198.7	49.6	5.6	20	

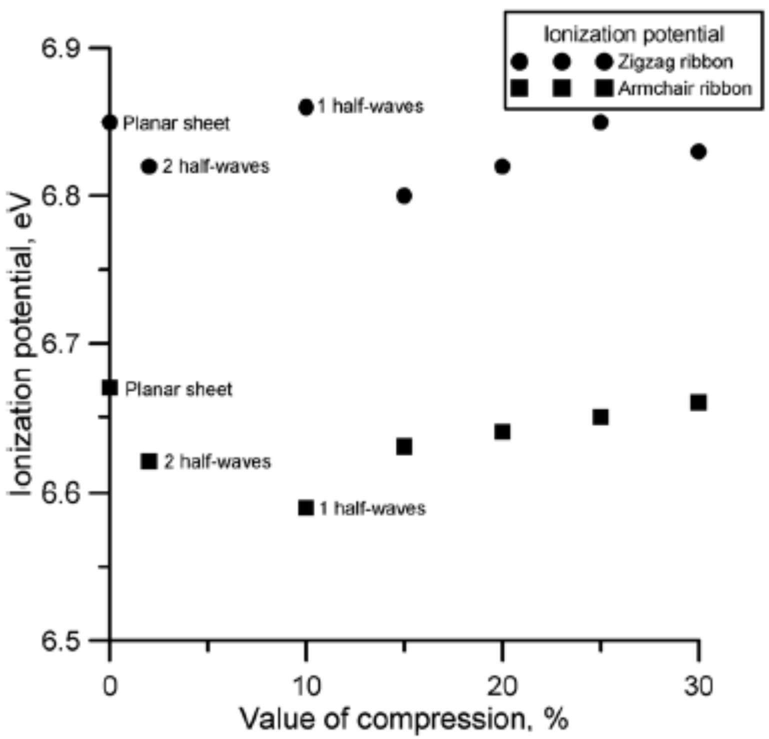


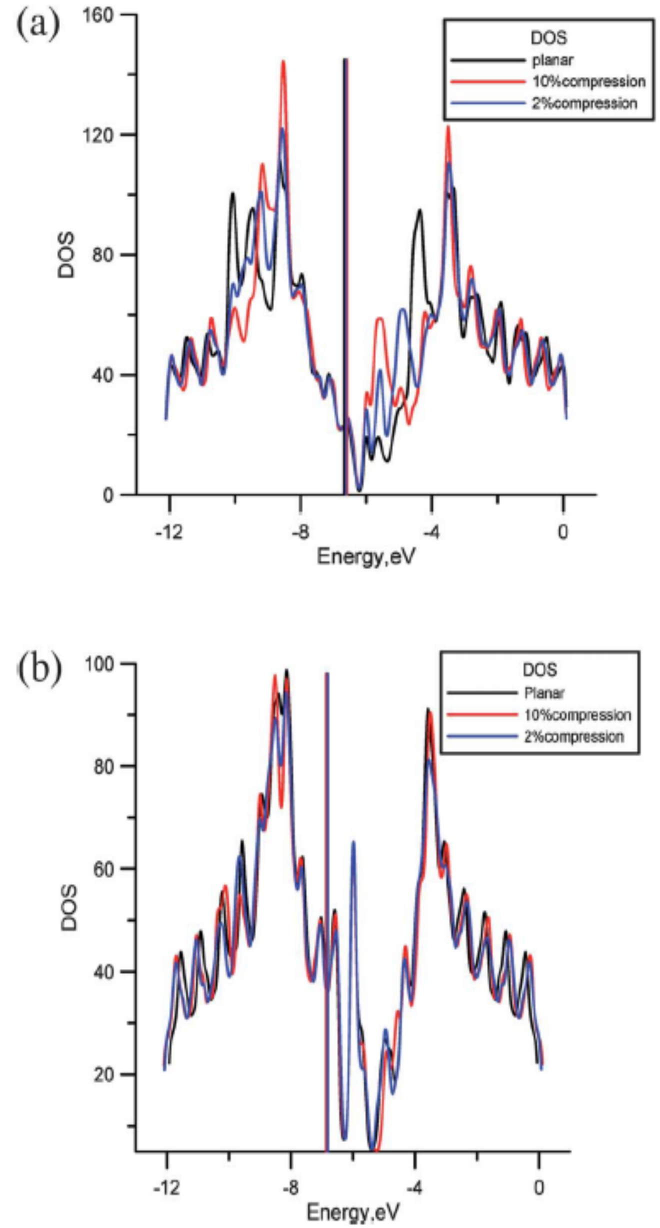


Map of distribution of the local stress for nanoribbon zigzag: (a) in the case of two half-waves; (b) in the case of three half-waves; (c) in the case of four half-waves.

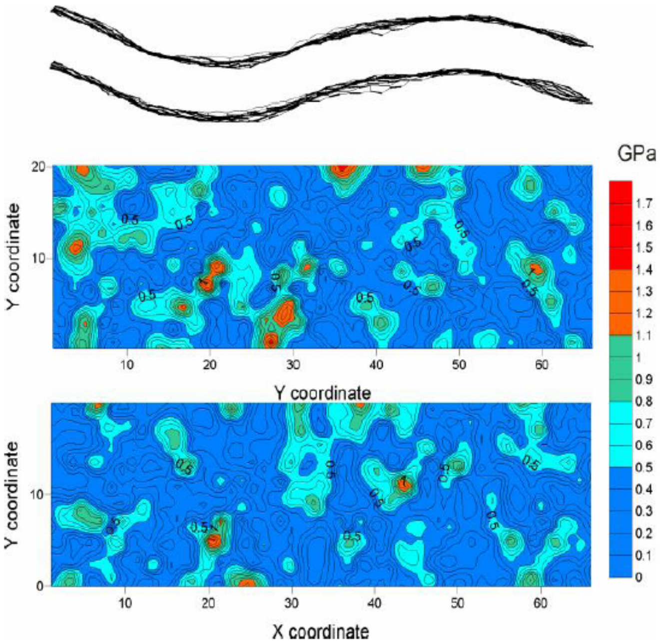
Some parameters of the electronic structure of nanoribbons

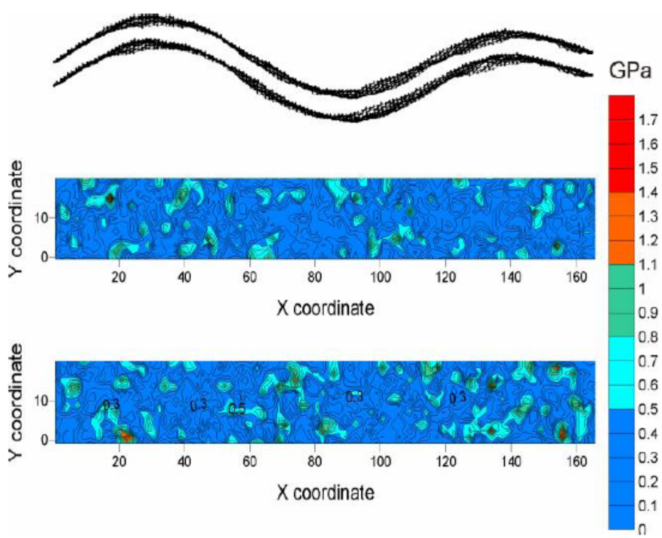
Number of half-waves	Length of half-wave/Å	IP/eV	E_{gap}/eV
Armchair ribbon of width 22.4 Å			
2	71.0	6.63 (6.65)	0.04 (0.03
3	181.7	6.50 (6.53)	0.04 (0.03
4	258.4	6.44 (6.47)	0.02 (0.01
5	335.12	6.41 (6.44)	0.04 (0.02
Zigzag ribbon of width 19.88 Å			
2	65	6.82 (6.84)	0.04 (0.02
3	165.18	6.79 (6.81)	0.01 (0.01
4	198.7	6.80 (6.81)	0.01 (0.01

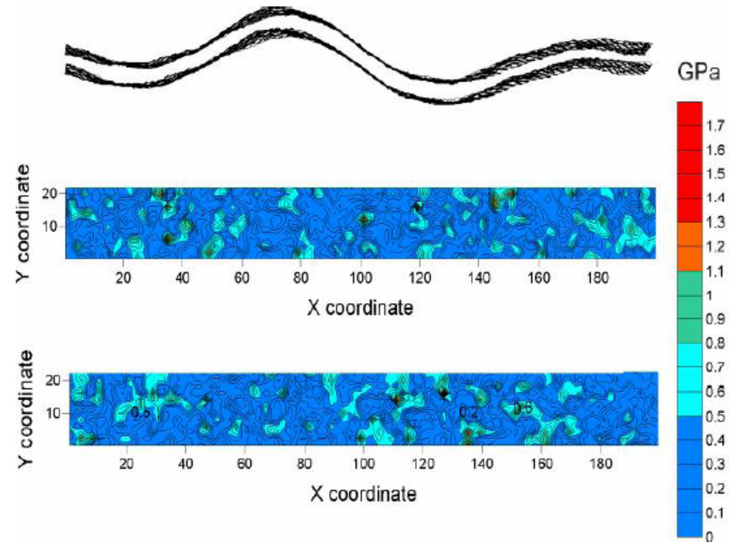




The compression process of bi-layer graphene

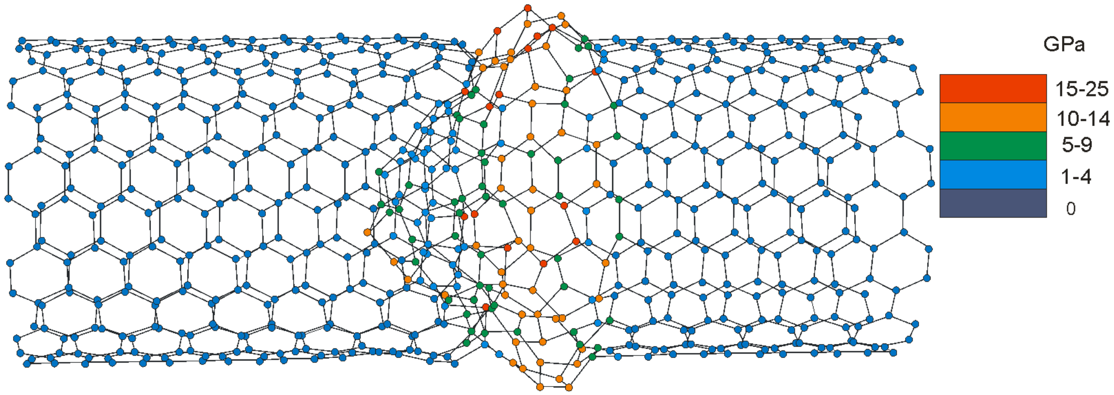


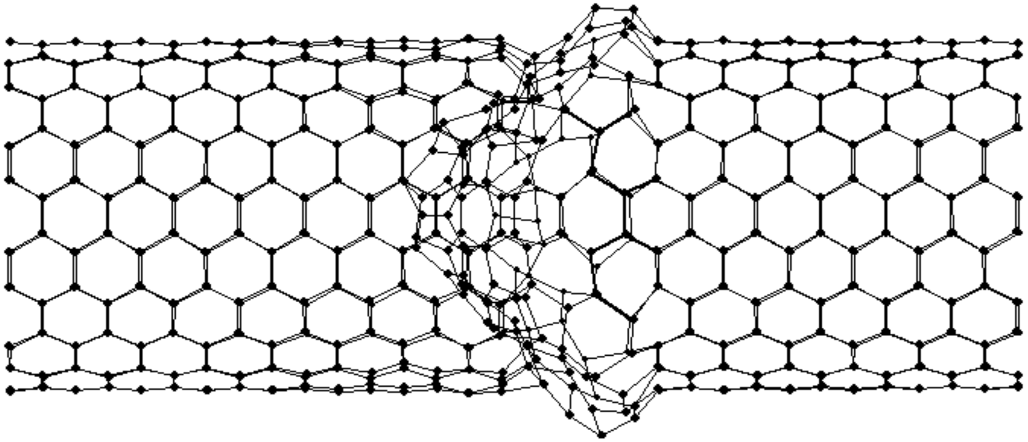




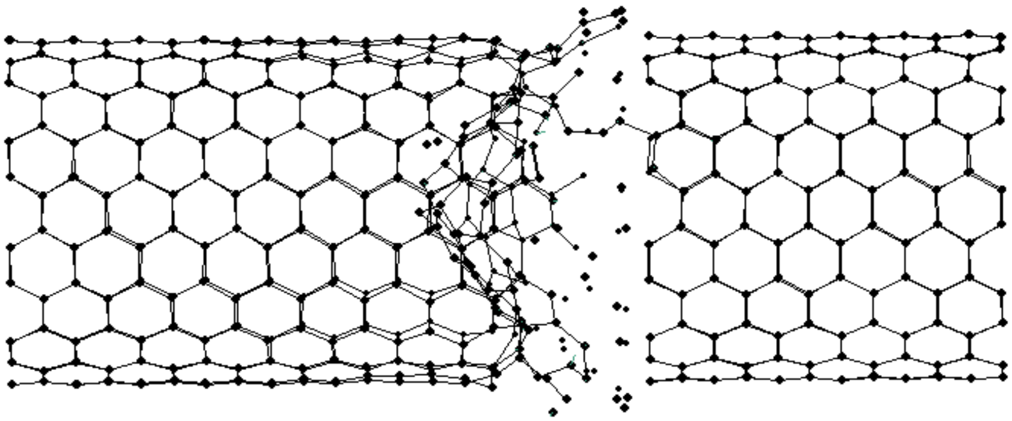
Geometrical characteristics of the curved zigzag bi-layer graphene nanoribbons compressed up to 98% of the initial length

Number of half-waves	Number of atoms in structure	Length of nanoribbon, Å	Length of half-wave, Å	Amplitude of half-wave, Å	Number of hexagons in half-wave	Width of nanoribbon, Å
2	1100	65	32.3	3.1	13	
3	2780	165.18	55.4	5.48	20	19.88
4	3340	198.7	49.8	5.55	20	

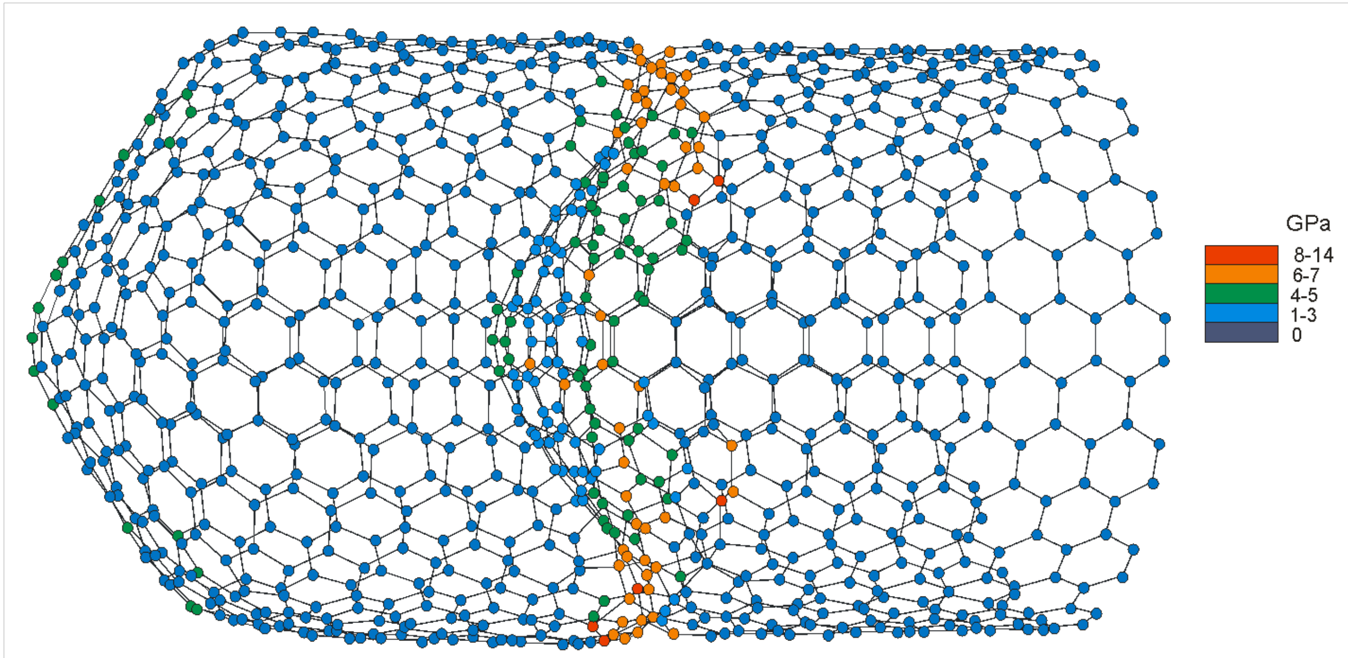


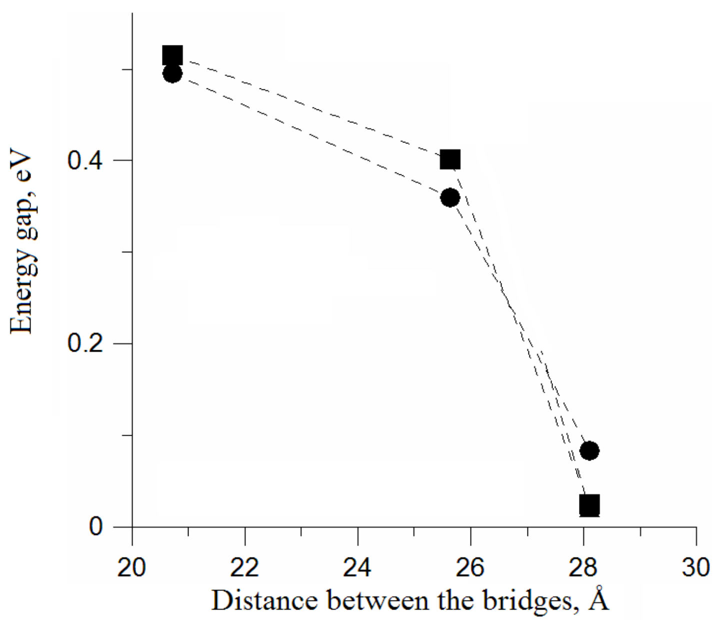


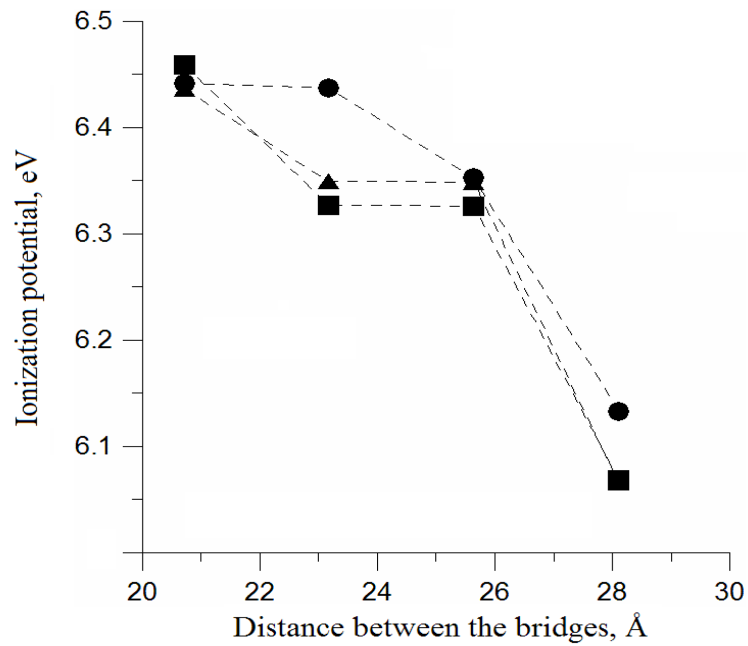
Destruction of the structure of bamboo-like CNT during
the increase of the temperature



O.E. Glukhova, I.V. Kirillova, A.S. Kolesnikova, E.L. Kossovich, G.N. Ten
// Proc. of SPIE. 2012. Vol. 8233. P. 82331E-1-82331E-7.


GPa
8-14
6-7
4-5
1-3
0


Energy gap, eV
0
0.2
0.4
20
22
24
26
28
30
Distance between the bridges, Å


Ionization potential, eV
6.1
6.2
6.3
6.4
6.5
20
22
24
26
28
30
Distance between the bridges, Å