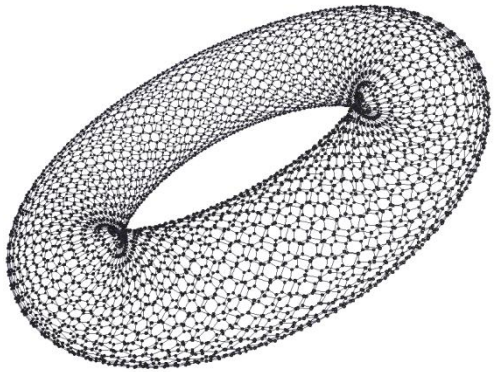
The prediction of defects in the carbon nanostructures based on the analysis of the local stress field for atomic grid



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New IT are used in our own program

- **Implementation** of Platform in **Python and C ++**;
- **Mercurial** Version control system**.**
- **http://nanokvazar.ru/**

Computational methods

Self-consistent charge density functional tight-binding (SCC-DFTB)

Molecular dynamics (MDTB)

Hybrid methods: course-grained (CG)/molecular mechanics (MM); quantum method (QM)/MM

- **MPI programming interface** allows to organize computing clusters;
- **NVidia CUDA** technology allow to perform calculations calculations on display adapters**.**

Applications of the parallel program

- **Simulation** of micro-and nano-devices;
- **Virtual testing** of nanodevices to determine their technical parameters;
- **Virtual testing** of technologies for new materials;
- Study of the **physical and mechanical properties of the element base** in devices of **micro-and nanoelectronics**.

- **http://nanokvazar.ru/**

The local stress field of the atomic grid of nanostructures: original method (Olga Glukhova and Michael Slepchenkov //Nanoscale, 2012, 4, 3335–3344)

It is proposed to carry out the calculation of the local stress field according to the following algorithm.

(1) Optimization of the initial structure by means of the quantum-chemical method.

(2) Calculation of distribution of the bulk energy density per atom using the empirical method.

(3) Search of the atomic configuration of the nanostructure subjected to the external influence as a result of the energy minimization for coordinates, using the quantum-chemical method.

(4) Calculation of the distribution of the bulk energy density per atom in the structure subjected to the external influence, using the empirical method.

(5) Calculation of the local stress in the atomic grid according to the difference between the values of the bulk density of energy for the atoms of the structure subjected to the external influence, and the initial structure.

The bulk energy density w_i of the atom i was calculated by the formula:

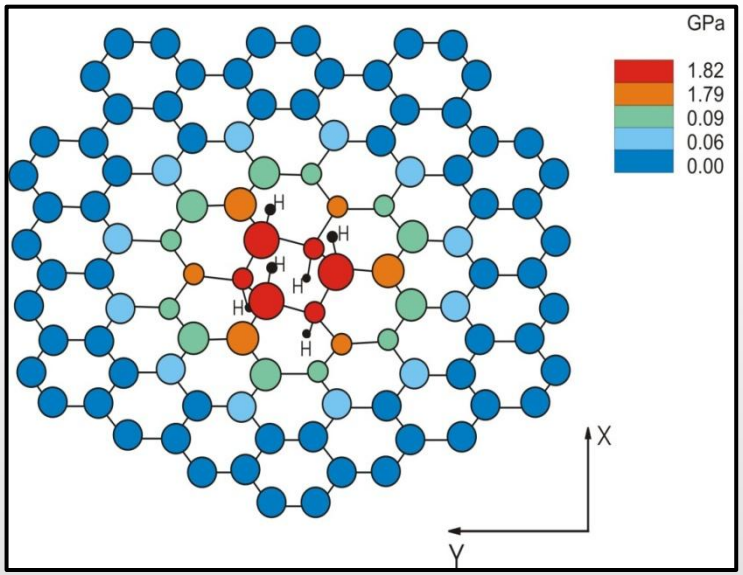
$$w_i = \left(\sum_{j(\neq i)} \left(V_{\mathrm{R}}(r_{ij}) - B_{ij} V_{\mathrm{A}}(r_{ij}) \right) + \sum_{j \neq i} \left(\sum_{k \neq i j} \left(\sum_{l \neq i,j,k} V_{\mathrm{tros}}(\omega_{ijkl}) \right) \right) + \sum_{j(\neq i)} V_{\mathrm{vdW}}(r_{ij}) \right) \Big/ V_i$$

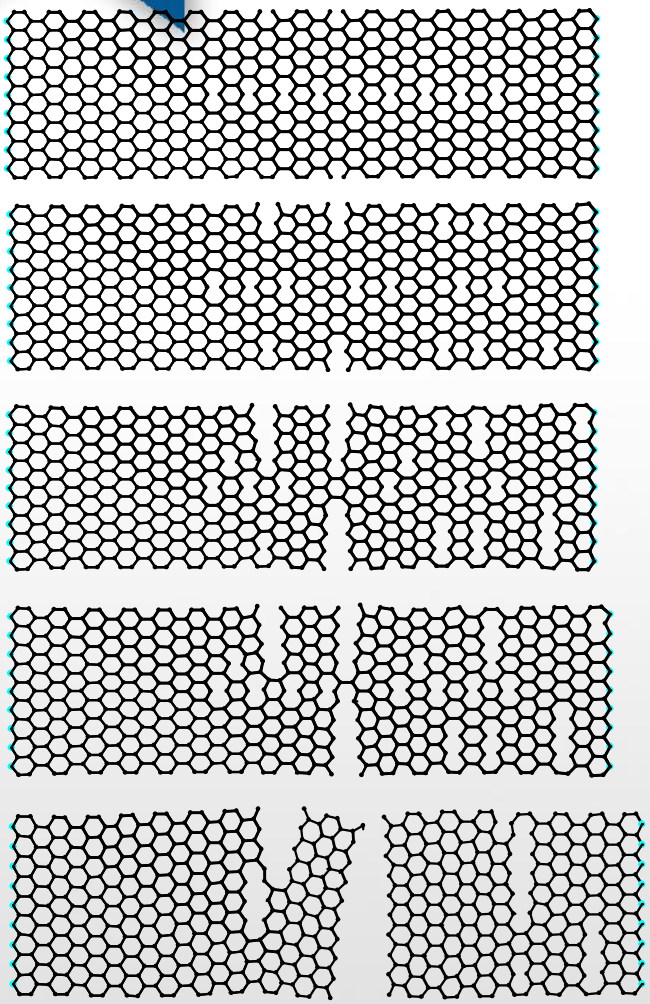
The stress of the atomic grid near the atom with number i is calculated as:

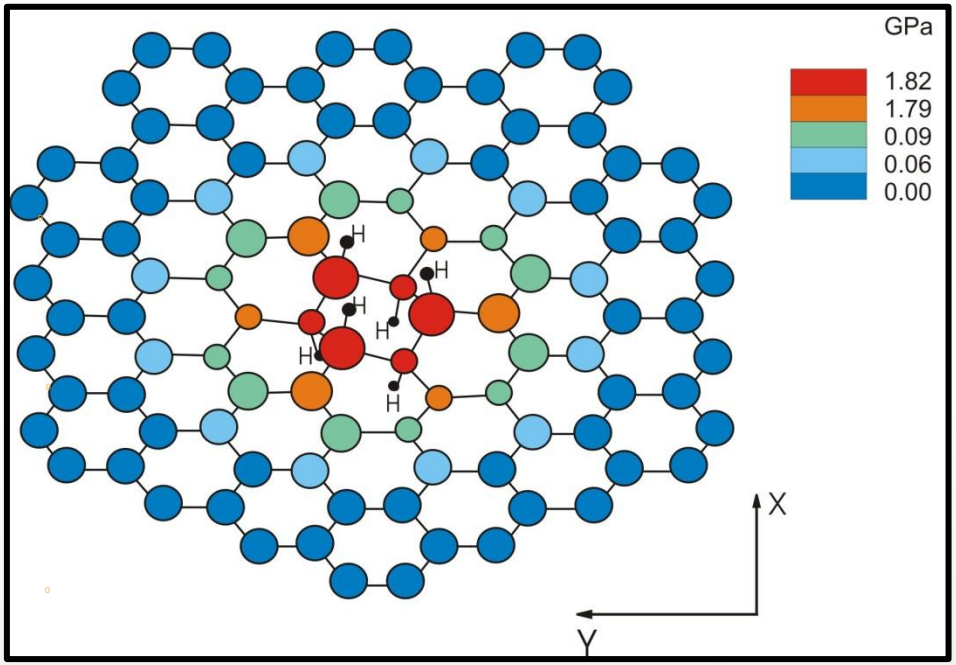
$$\sigma_i = |w_i - w_i^0|$$

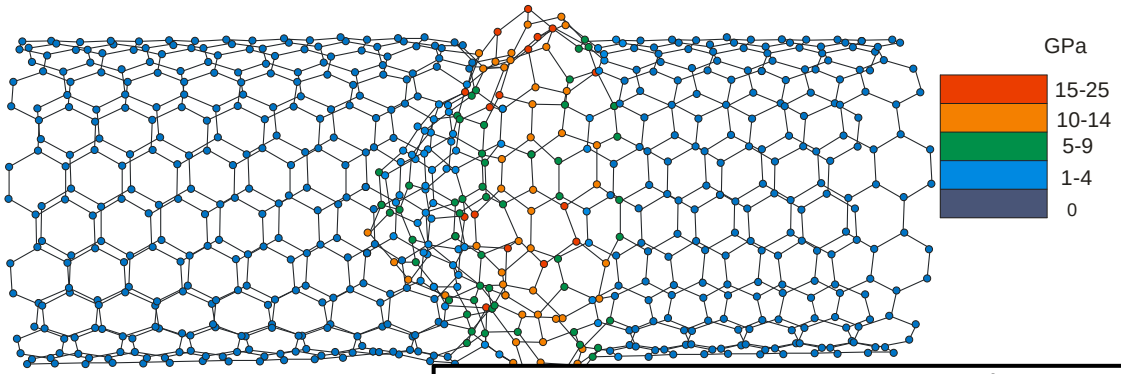
where w_i^0 is the bulk energy density of the i^{th} atom of the graphene sheet which is in equilibrium; w_i is the bulk energy density of an atom of the graphene sheet subjected to the external influence (deformation, defect formation, *etc.*). The value of w_i^0 in the centre of the graphene sheet is equal to −58.60 GPa. At the edges of the graphene sheet the 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 on an armchair edge and on the zigzag edge is equal to −40.64 GPa. It is suggested that without an external influence the stress equals to zero for the atoms in the centre and at the edges of the graphene sheet.

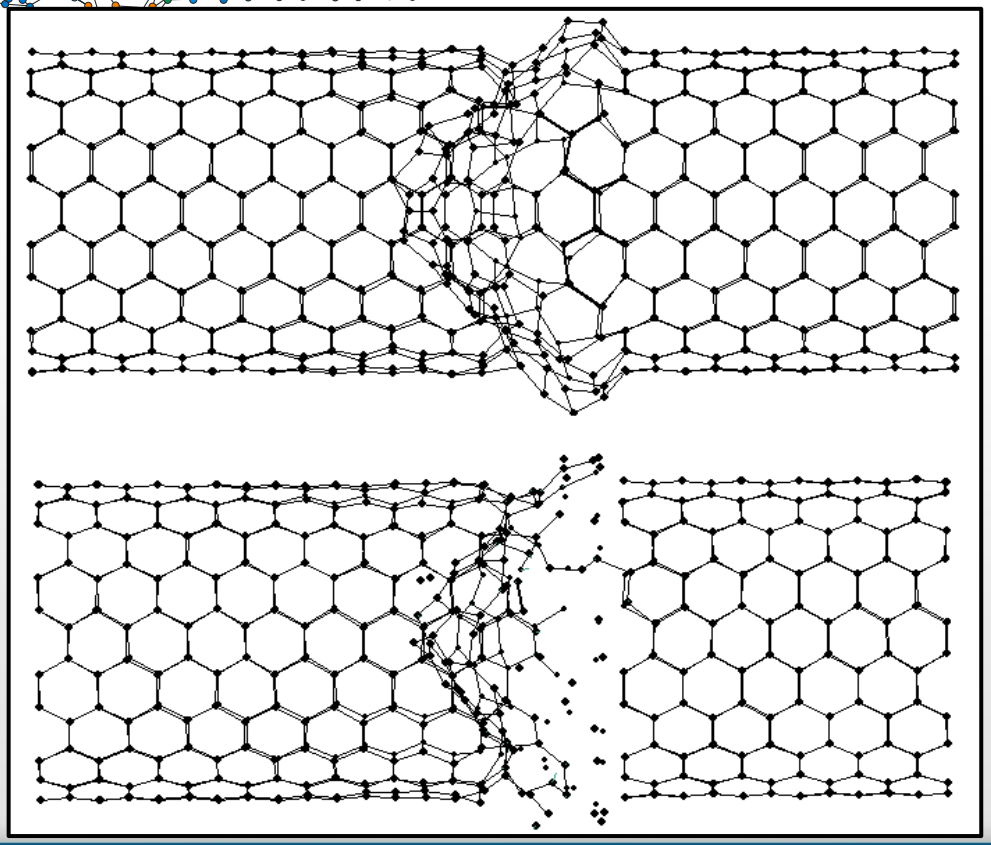
$$V_i = \frac{4}{3}\pi r_0^3$$





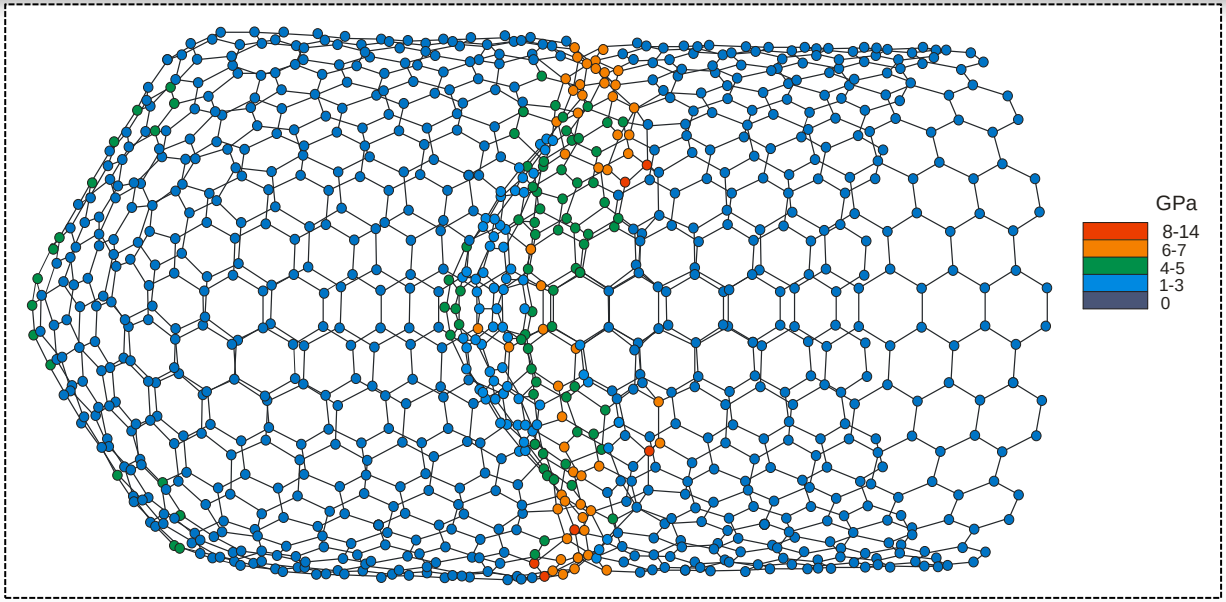


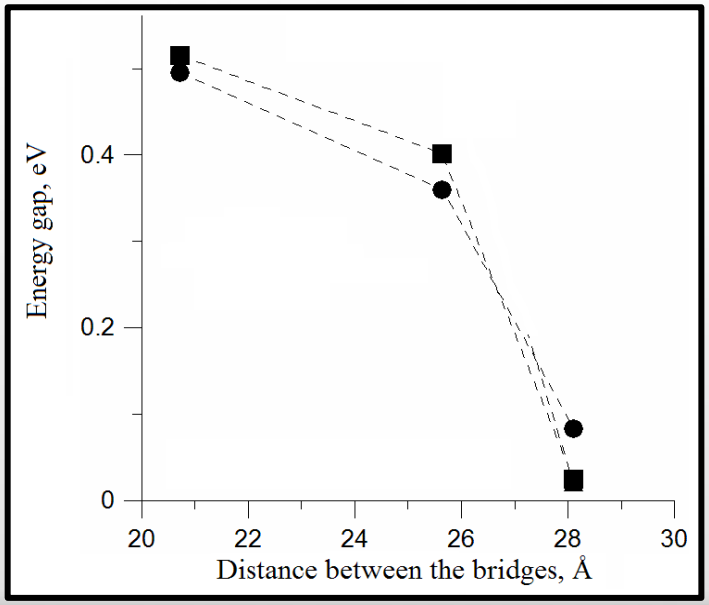


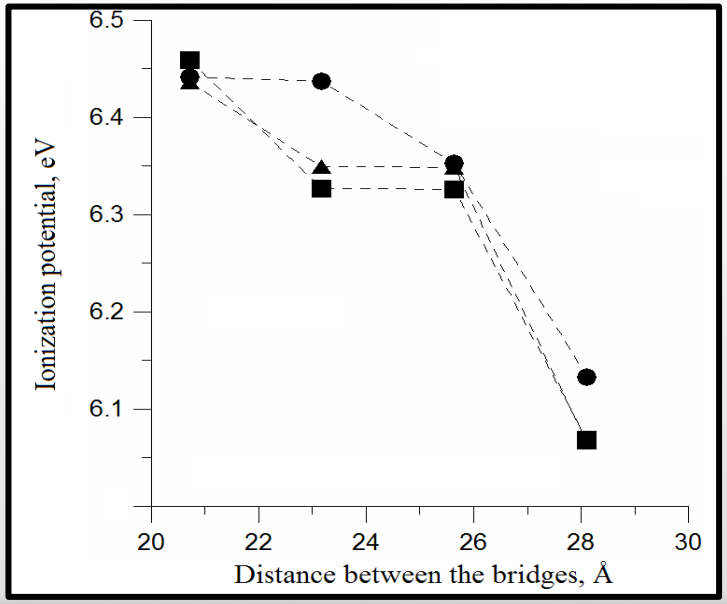


Destruction of the structure of bamboo-like CNT during the increase of the temperature

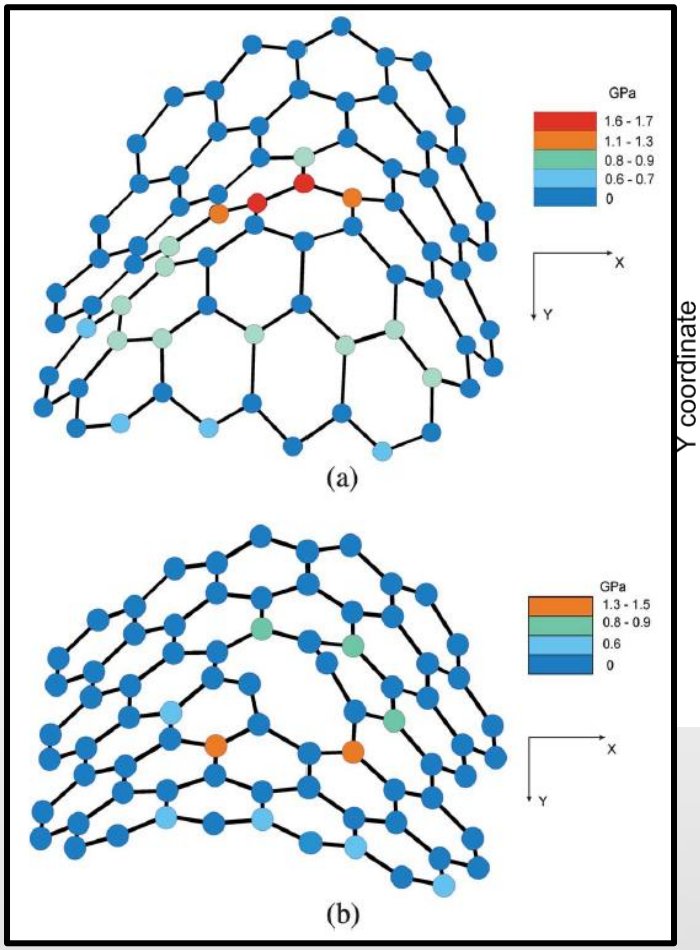
O.E. Glukhova, I.V. Kirillova, A.S. Kolesnikova, E.L. Kossovich, G.N. Ten
// Proc. of SPIE. 2012. Vol. 8233. P. 82331E-1-82331E-7.

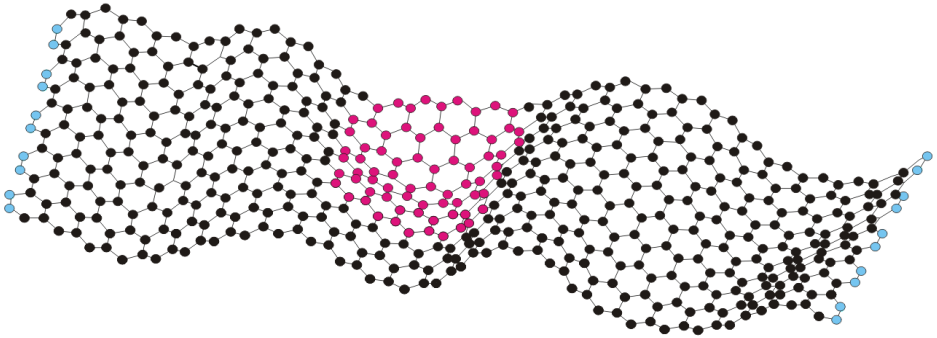

GPa
8-14
6-7
4-5
1-3
0

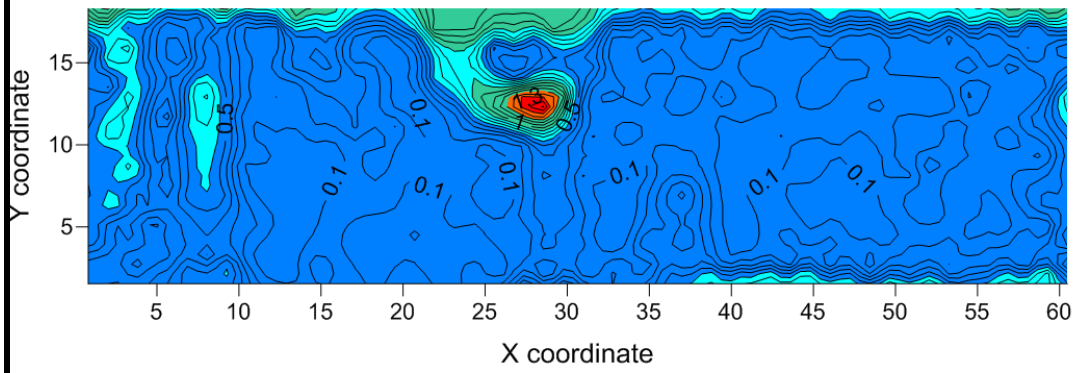

Energy gap, eV
0
0.2
0.4
20
22
24
26
28
30
Distance between the bridges, Å

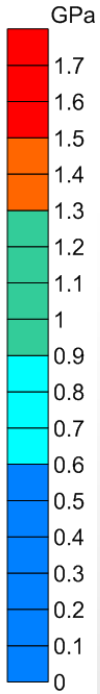

Ionization potential, eV
6.1
6.2
6.3
6.4
6.5
20
22
24
26
28
30
Distance between the bridges, Å

Prediction of the defects appearance







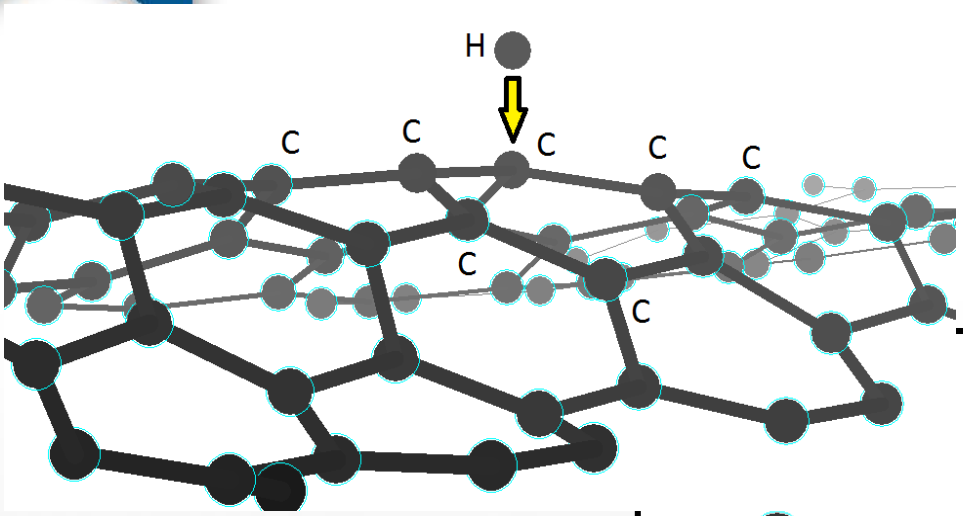


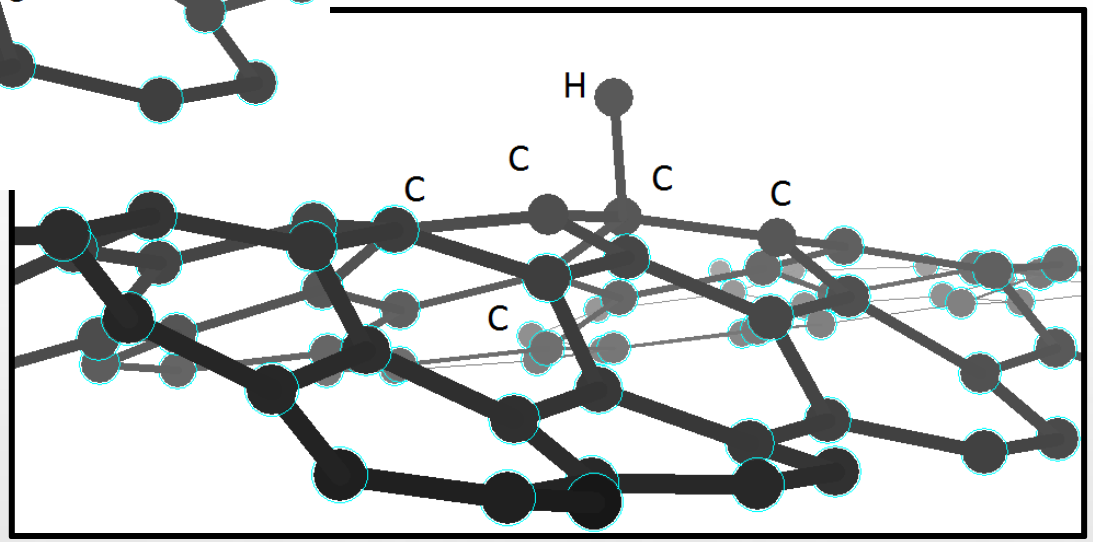
Defects of the C–C bond are observed only between atoms with a local stress value of about 1.8 GPa. One of the most stressed sections of the atomic grid containing a defect is presented in Fig. 4. From the Figure it is clearly seen that after C–C-bond breaking the atomic grid reconstructs and the stress 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

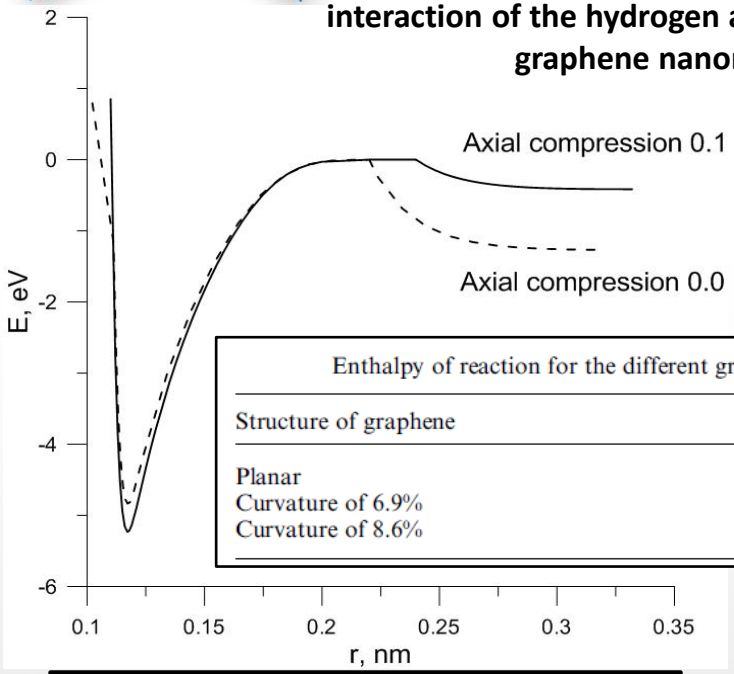
on the atomic network





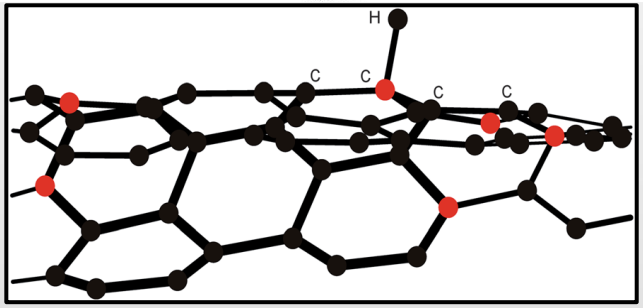
Olga E. Glukhova, Michael M. Slepchenkov Influence of the curvature of deformed graphene nanoribbons on their electronic and adsorptive properties: theoretical investigation based on the analysis of the local stress field for an atomic grid // Nanoscale 2012. Issue 11. Pages 3335-3344. DOI:10.1039/C2NR30477E.

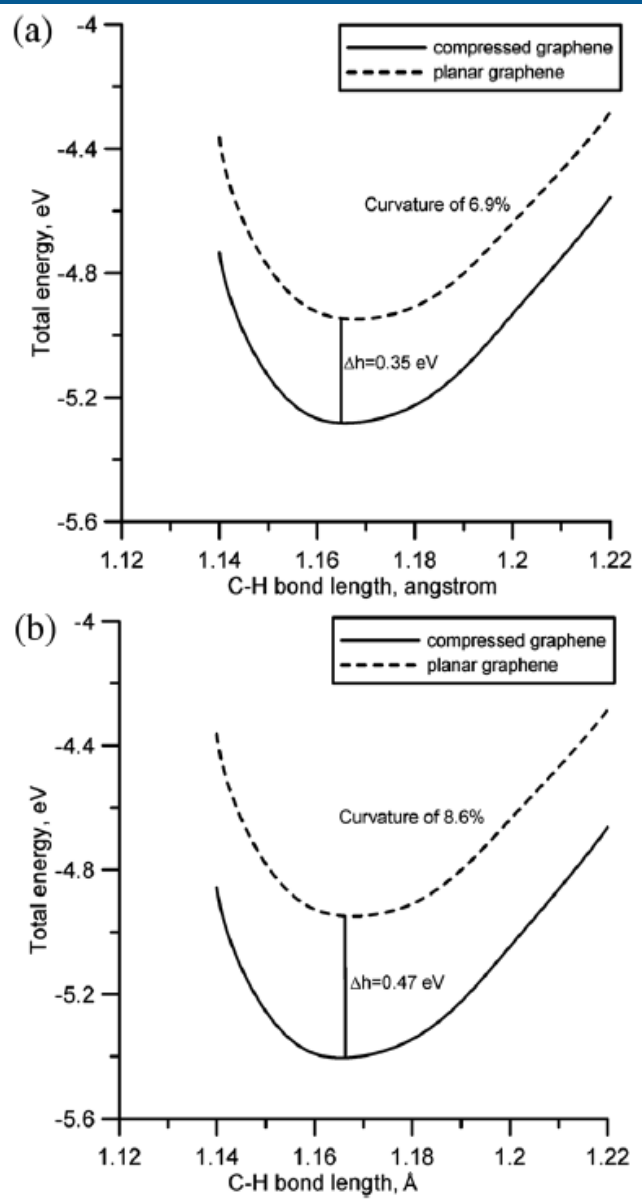
The total energy of the structure depends on the distance between the hydrogen atom and the carbon atom. (The dashed line is the interaction of the hydrogen atom with planer graphene nanoribbon; the solid line is the interaction of the hydrogen atom from wave-like graphene nanoribbon)



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}

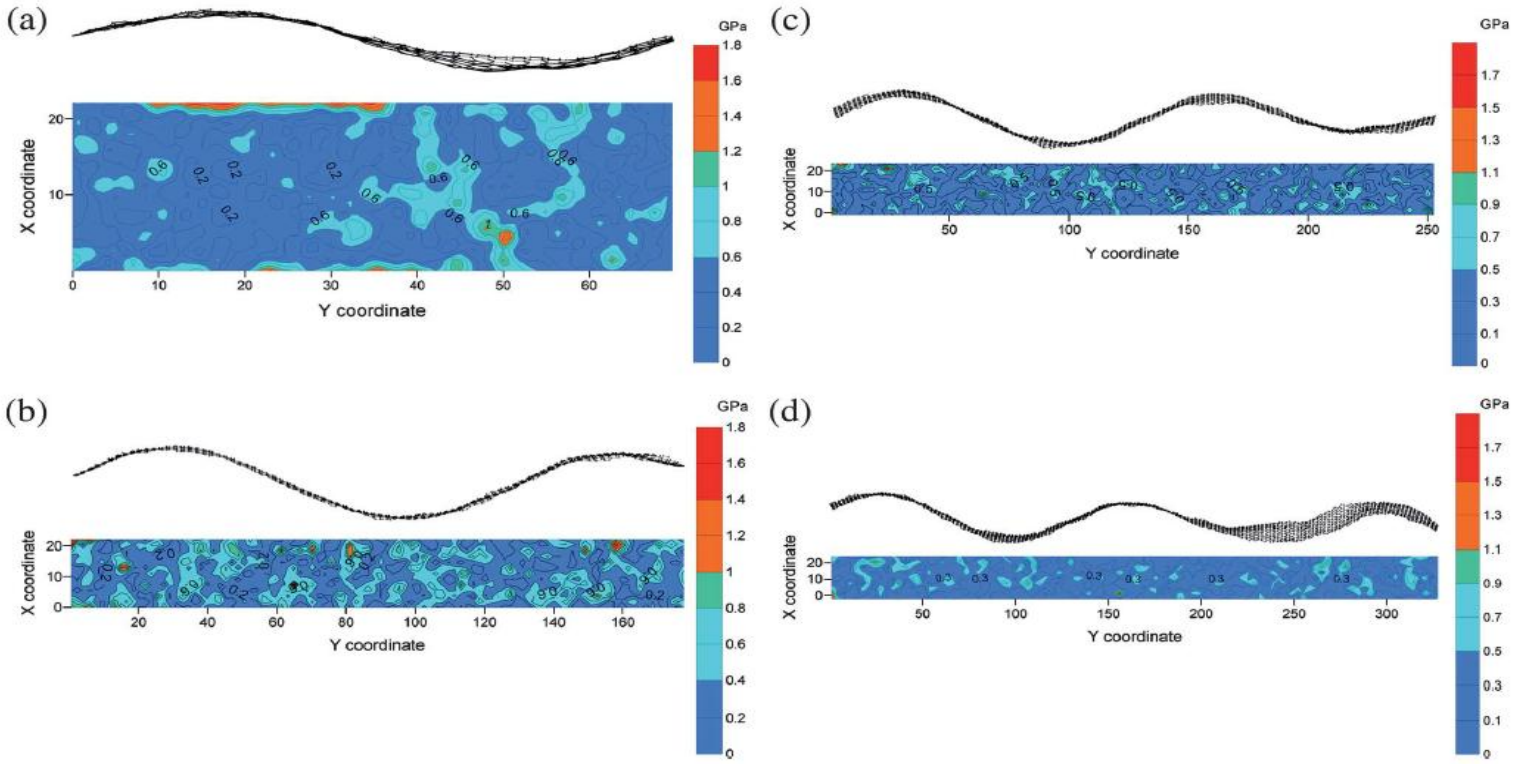




The dependence of the chemical C–H interaction energy on the length of the C–H bond for the planar and compressed graphene nanoribbon: (a) with curvature of 6.9%; (b) with curvature of 8.6%.

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

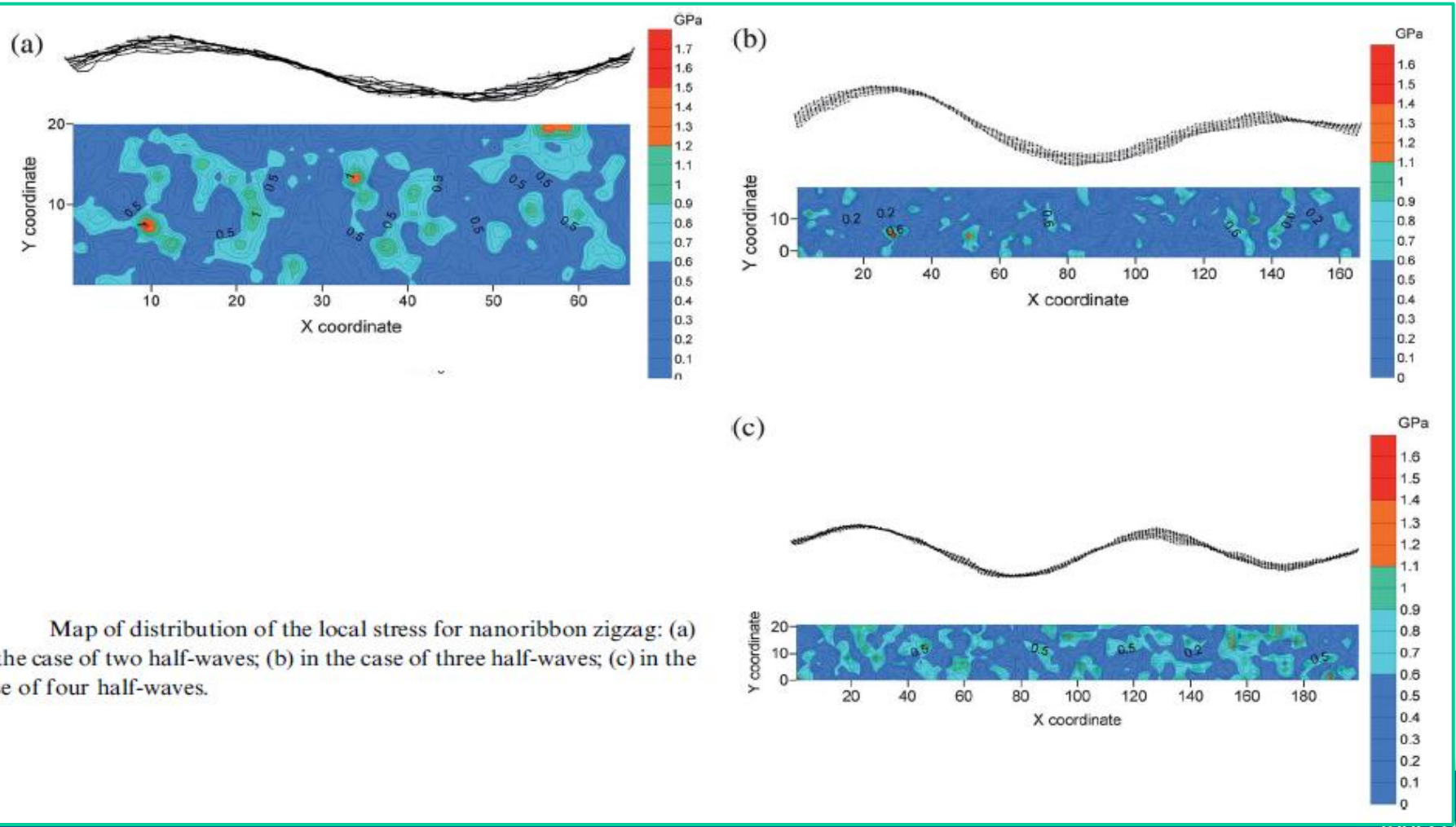
Number of half-waves	Number of atoms in structure	Length of nanoribbon/Å	Length of half-wave/Å	Amplitude of half-wave/Å	Number of hexagons in half-wave	Width of nanoribbon/Å
2	646	71.0	35.5	2.2	9	22.4
3	1634	181.7	60.5	5.3	14	
4	2318	258.4	64.6	5.65	15	
5	3002	335.12	66.2	5.4	15	



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

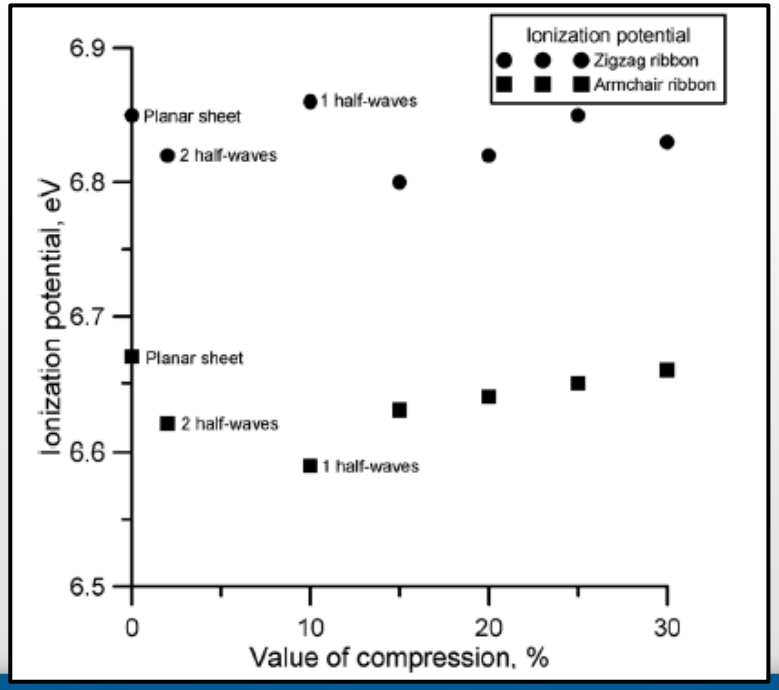
Number of half-waves	Number of atoms in structure	Length of nanoribbon/Å	Length of half-wave/Å	Amplitude of half-wave/Å	Number of hexagons in half-wave	Width of nanoribbon/Å
2	550	65	32.5	2.8	12	19.88
3	1390	165.18	55.06	5.4	20	
4	1670	198.7	49.6	5.6	20	

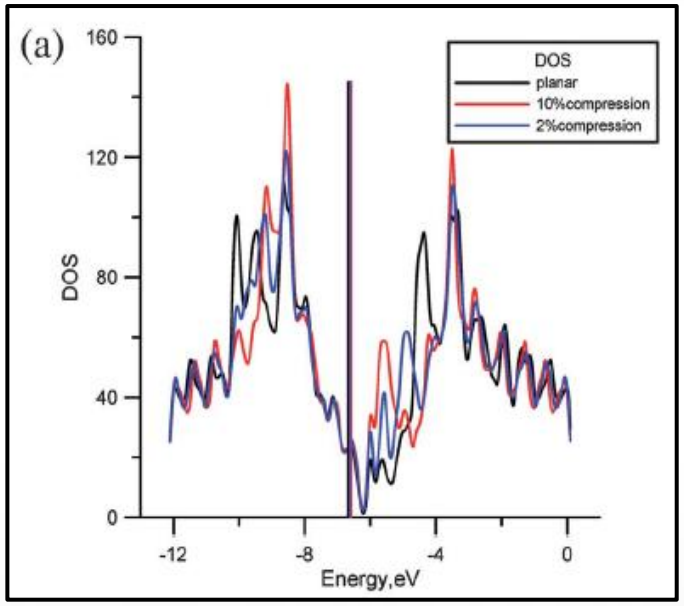


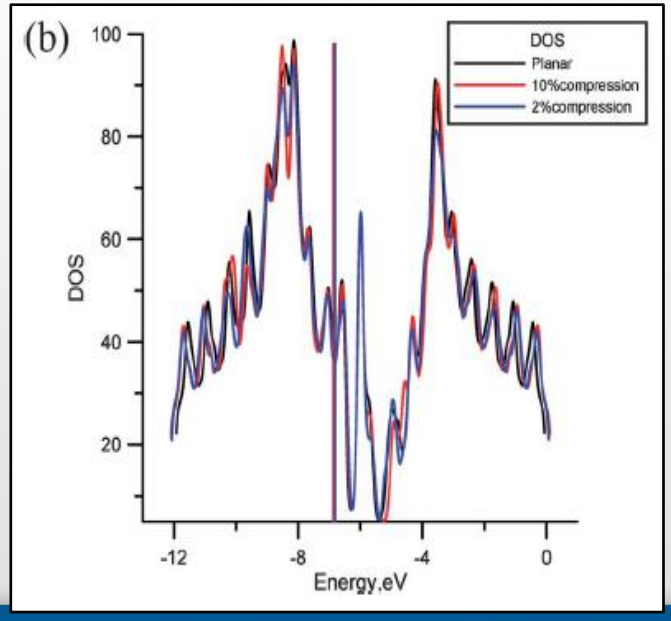
Map of distribution of the local stress for nanoribbon zigzag: (a) in the case of two half-waves; (b) in the case of three half-waves; (c) in the case of four half-waves.

Some parameters of the electronic structure of nanoribbons

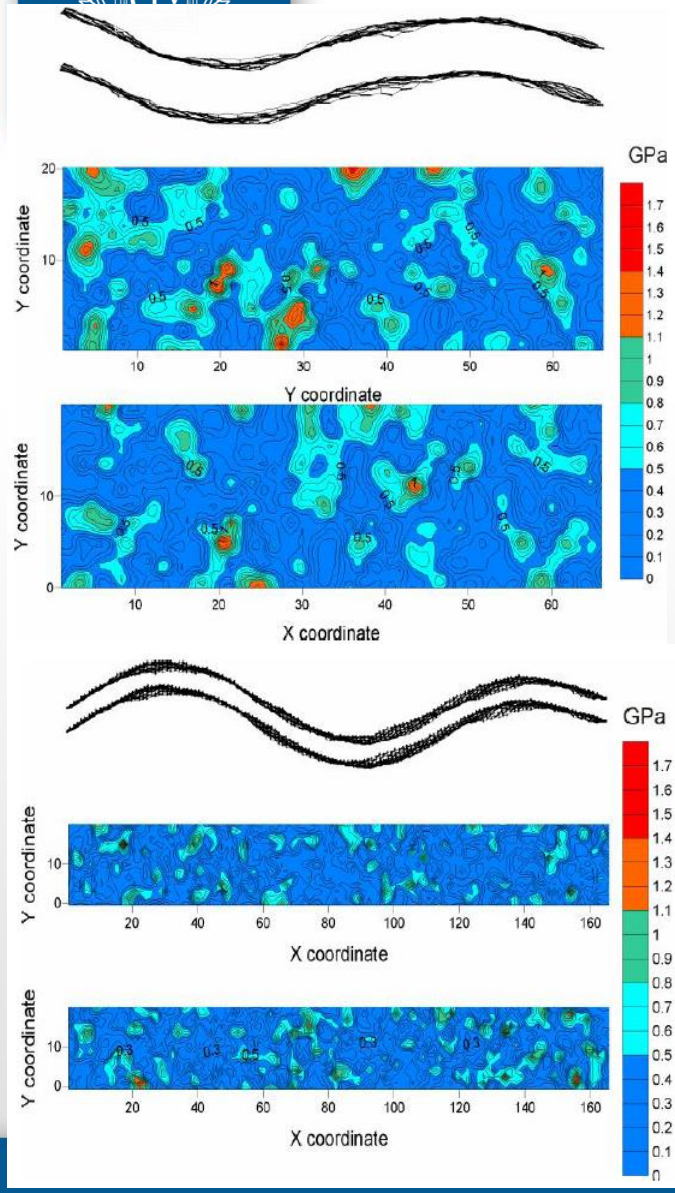
Number of half-waves	Length of half-wave/Å	IP/eV	E_{gap}/eV
Armchair ribbon of width 22.4 Å			
2	71.0	6.63 (6.65)	0.04 (0.03)
3	181.7	6.50 (6.53)	0.04 (0.03)
4	258.4	6.44 (6.47)	0.02 (0.01)
5	335.12	6.41 (6.44)	0.04 (0.02)
Zigzag ribbon of width 19.88 Å			
2	65	6.82 (6.84)	0.04 (0.02)
3	165.18	6.79 (6.81)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

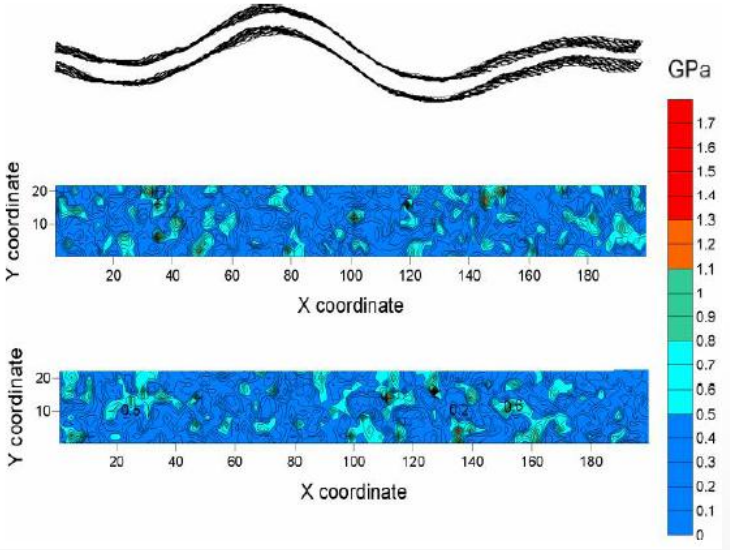






The compression process of bi-layer graphene



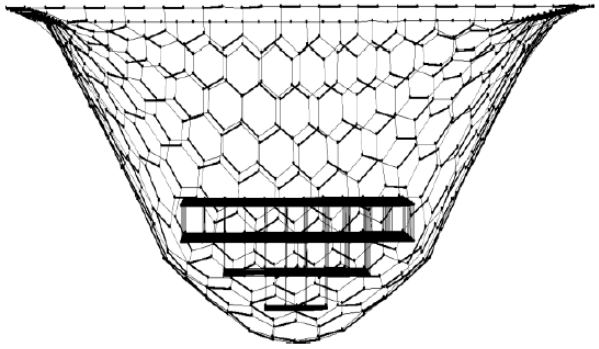


Geometrical characteristics of the curved zigzag bi-layer graphene nanoribbons compressed up to 98% of the initial length

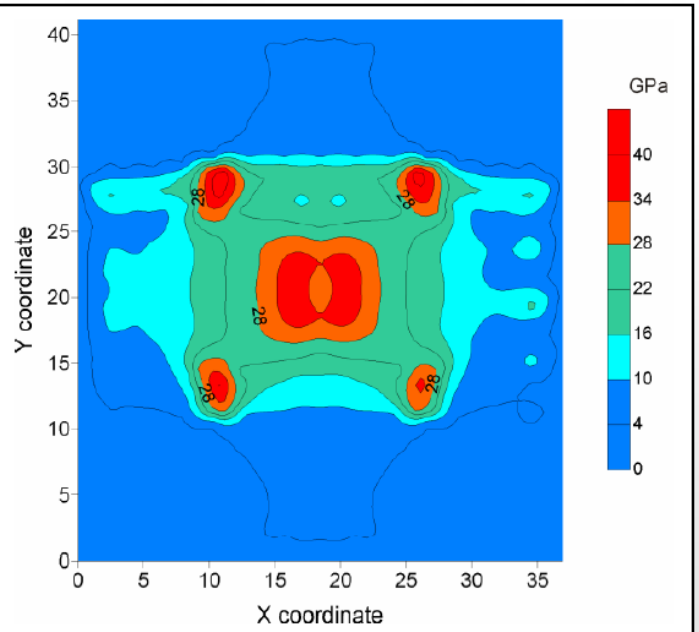
Number of half-waves	Number of atoms in structure	Length of nanoribbon, Å	Length of half-wave, Å	Amplitude of half-wave, Å	Number of hexagons in half-wave	Width of nanoribbon, Å
2	1100	65	32.3	3.1	13	
3	2780	165.18	55.4	5.48	20	19.88
4	3340	198.7	49.8	5.55	20	

Investigation of the one-layer graphene plate

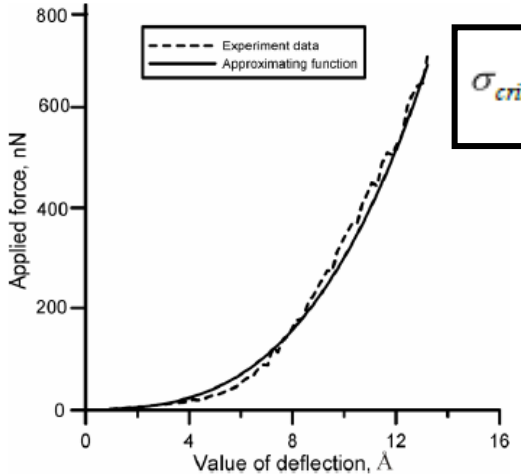
The deflection of the graphene sheet (620 atoms) by means of the platinum pyramid (376 atoms).



The image of the platinum pyramid and graphene sheet through 13.2 ps after the start of the experiment.



Map of the local stress, calculated thought 13ps after the start of the experiment.

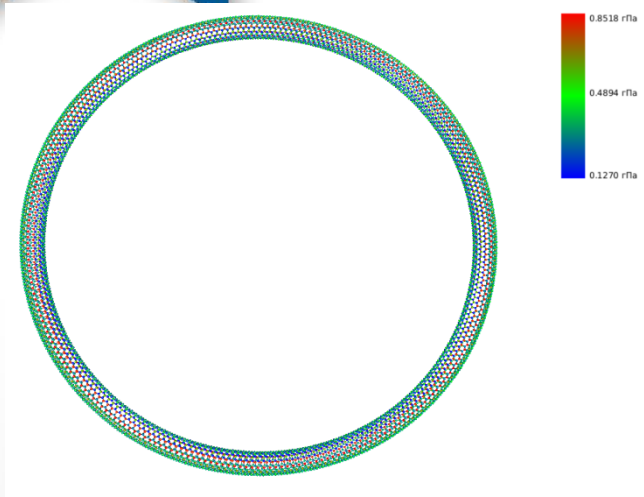


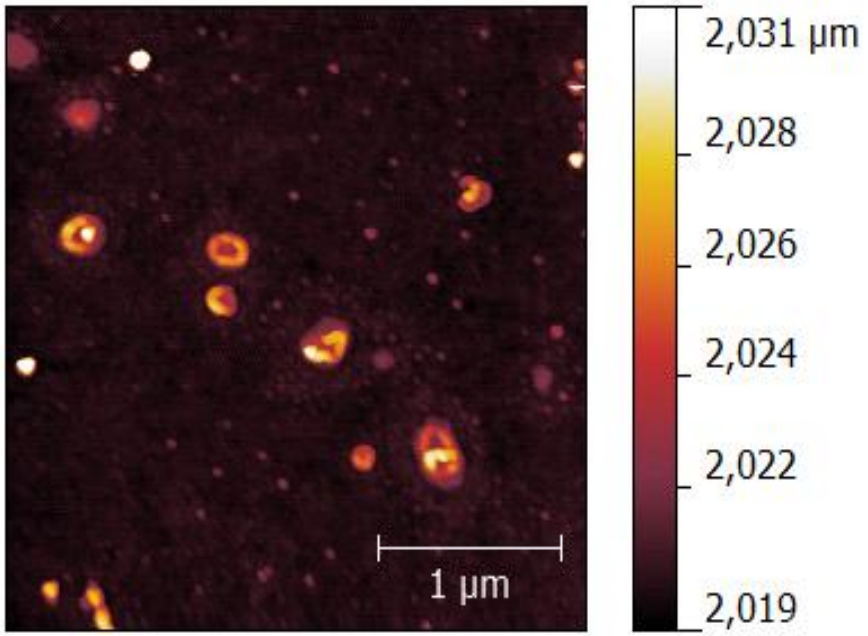
The dependence of the applied force on the bending deflection in the center of the upper plate bi-layer graphene plate. The dashed line corresponds to data obtained in the experiment, the solid - approximated function.

$$\sigma_{critical} = \frac{F_{lim}}{S_{surface}} = 126GPa$$

$$F = 0.35\zeta^3 + 1.7\zeta$$

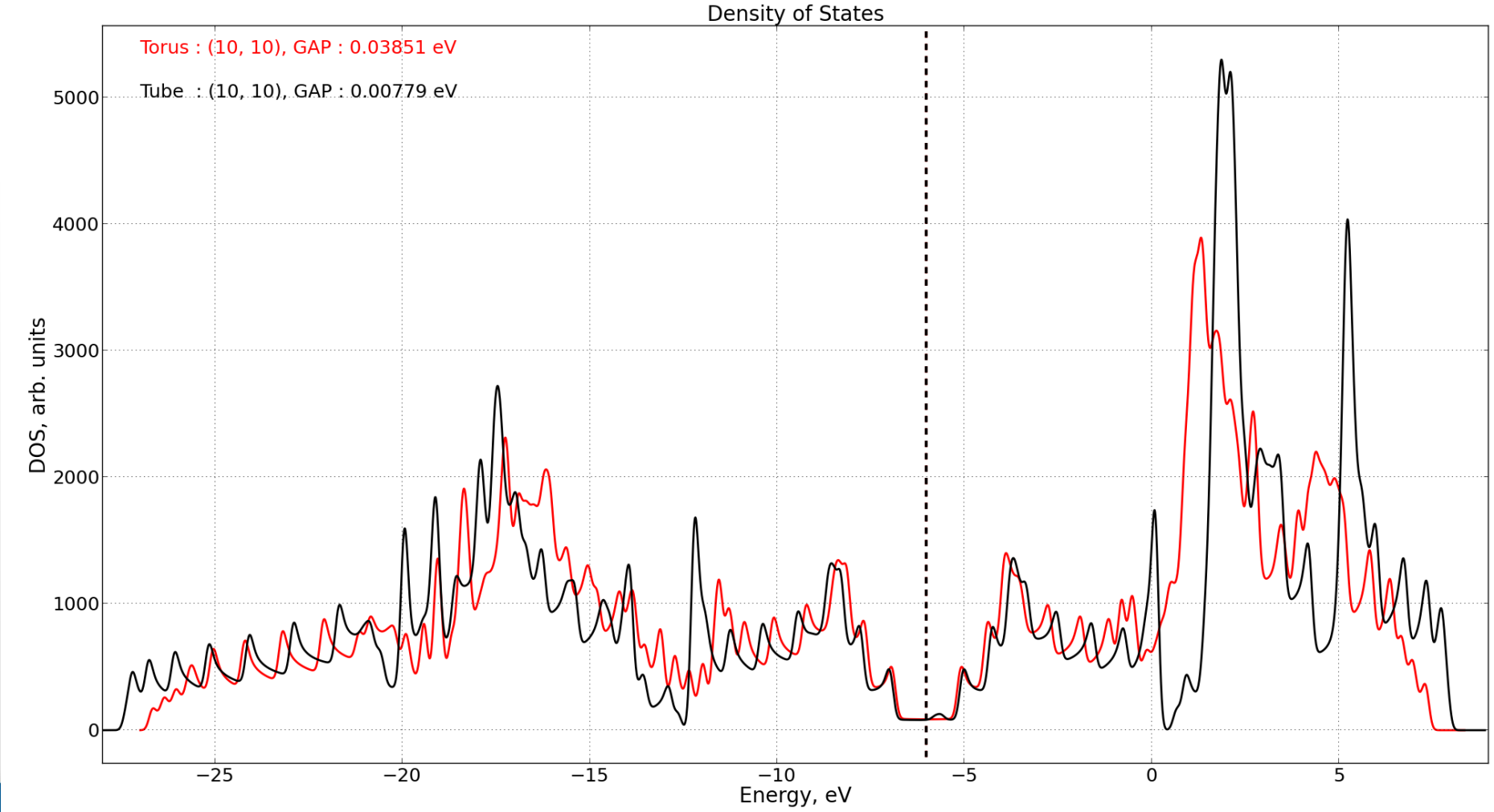
Nanotorus

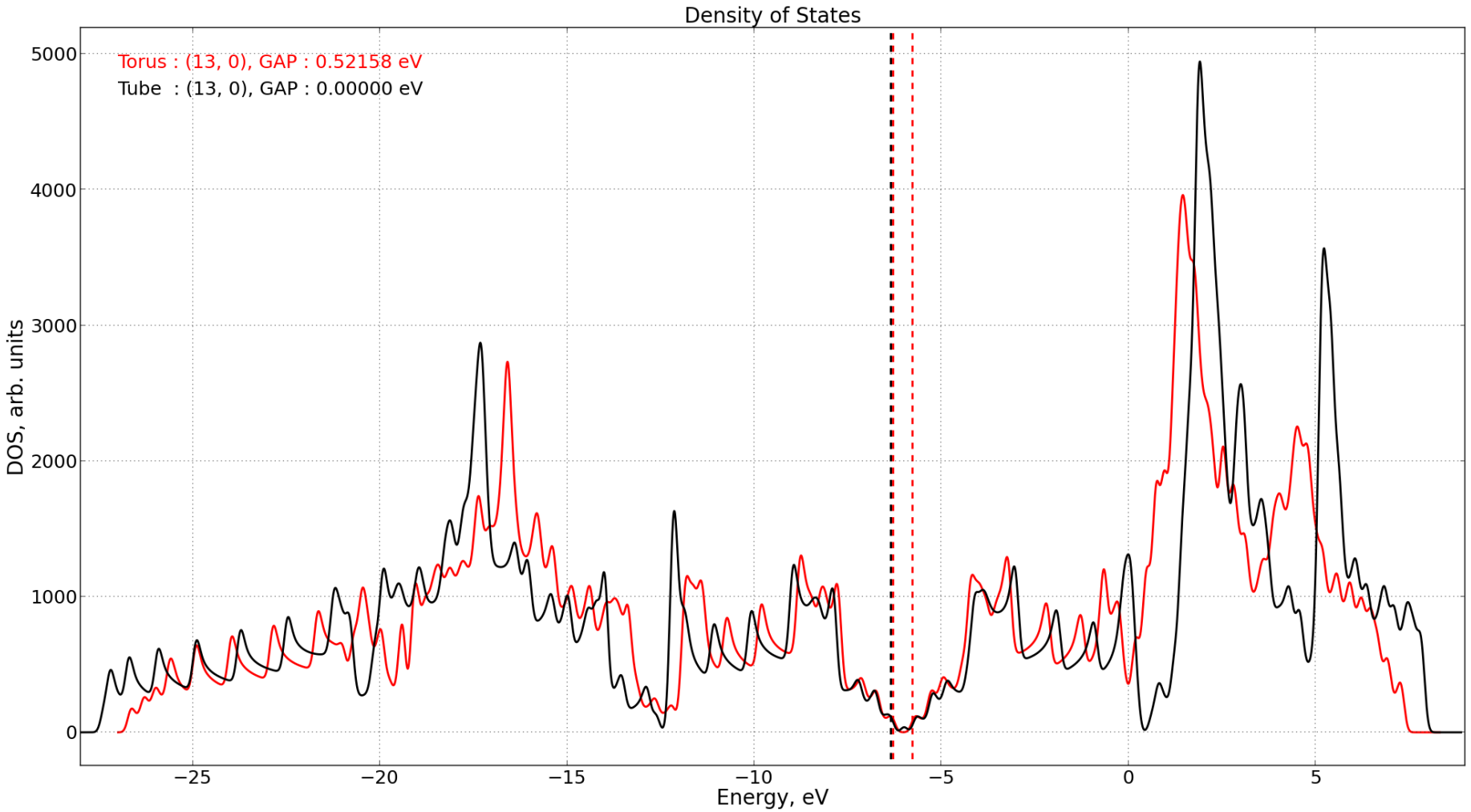


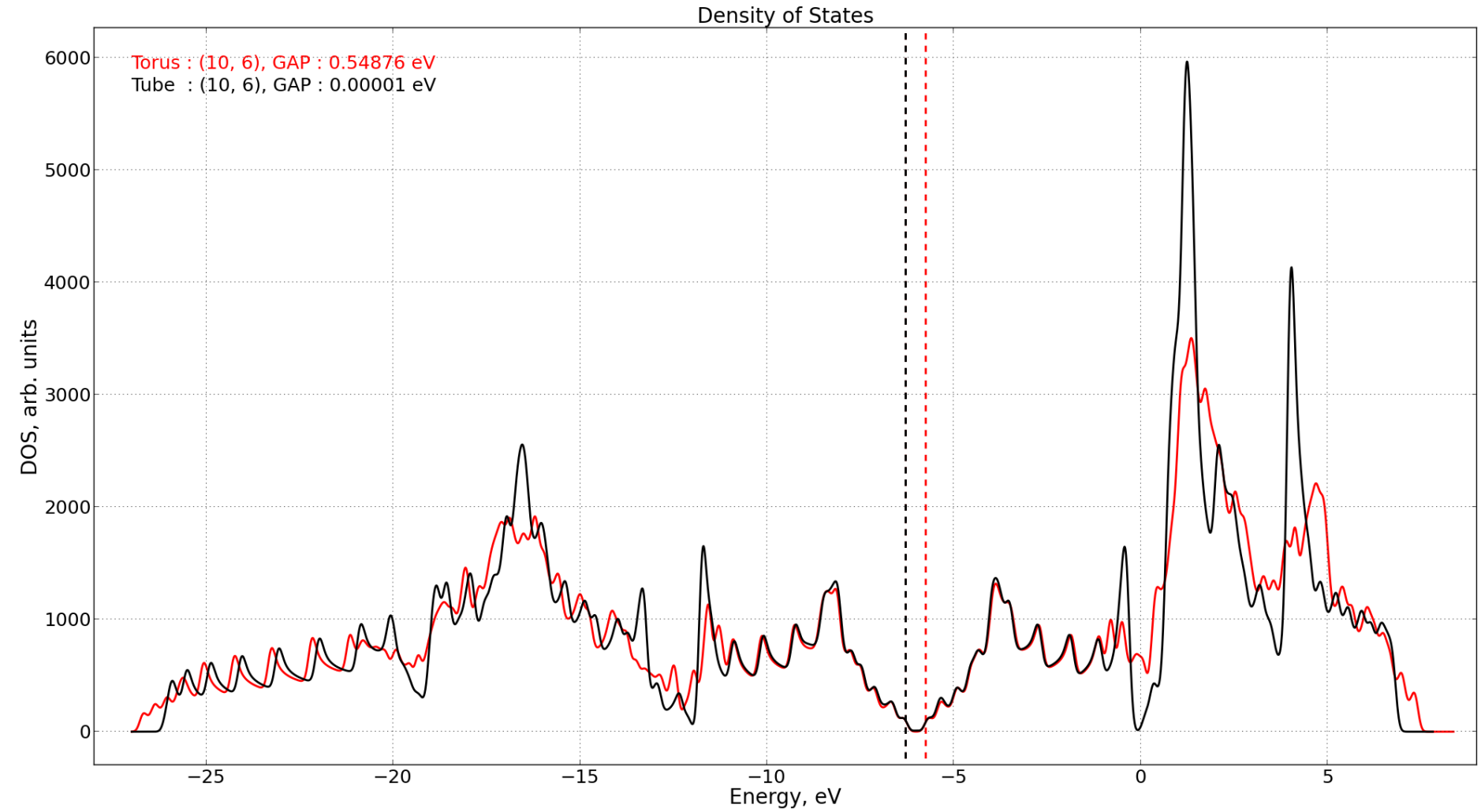


(m,n)	D, nm	Rtube, nm	atoms
(10, 10)	20	1	8192
(13, 0)	20	1	7800
(10, 6)	20	1	7872

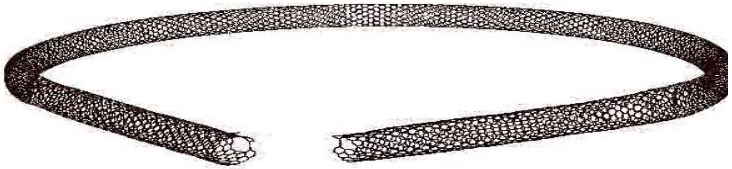
(m,n)	Etotal, eV	GPa
(10, 10)	-61004.19	0.85
(13, 0)	-58073.51	0.51
(10, 6)	-58601.96	0.93

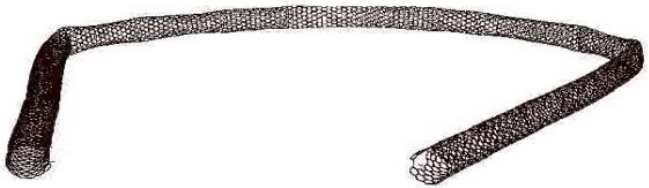

Density of States
Torus : (10, 10), GAP : 0.03851 eV
Tube : (10, 10), GAP : 0.00779 eV
DOS, arb. units
Energy, eV
0
1000
2000
3000
4000
5000
−25
−20
−15
−10
−5
0
5

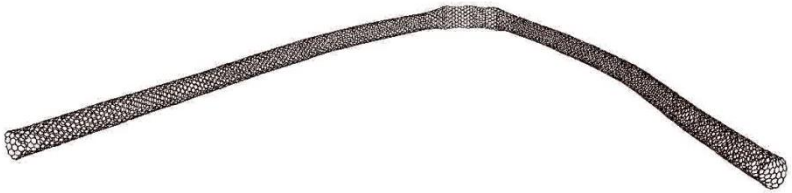

Density of States
Torus : (13, 0), GAP : 0.52158 eV
Tube : (13, 0), GAP : 0.00000 eV
DOS, arb. units
Energy, eV
5000
4000
3000
2000
1000
0
−25
−20
−15
−10
−5
0
5


Density of States
Torus : (10, 6), GAP : 0.54876 eV
Tube : (10, 6), GAP : 0.00001 eV
DOS, arb. units
Energy, eV
6000
5000
4000
3000
2000
1000
0
−25
−20
−15
−10
−5
0
5

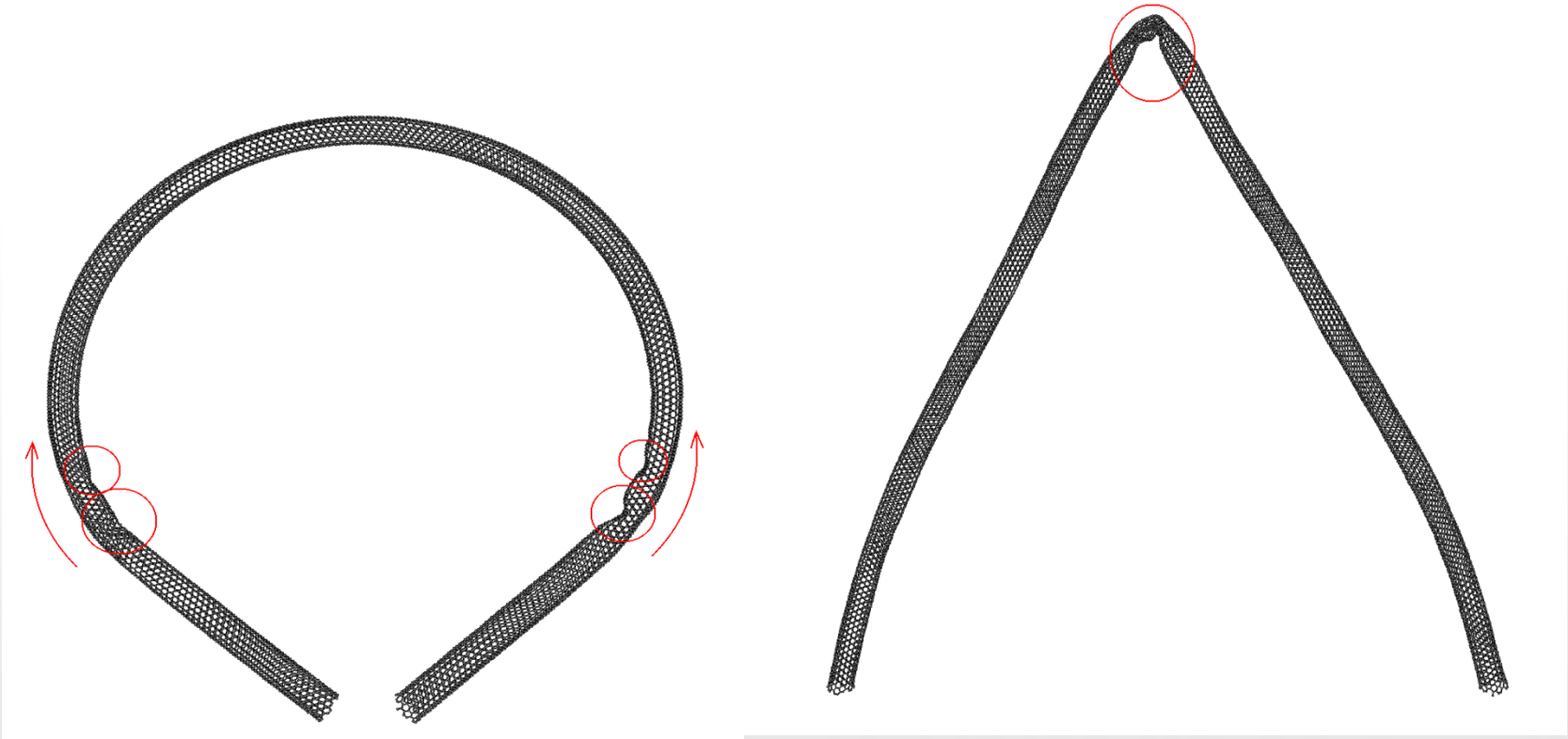
Destruction of the torus



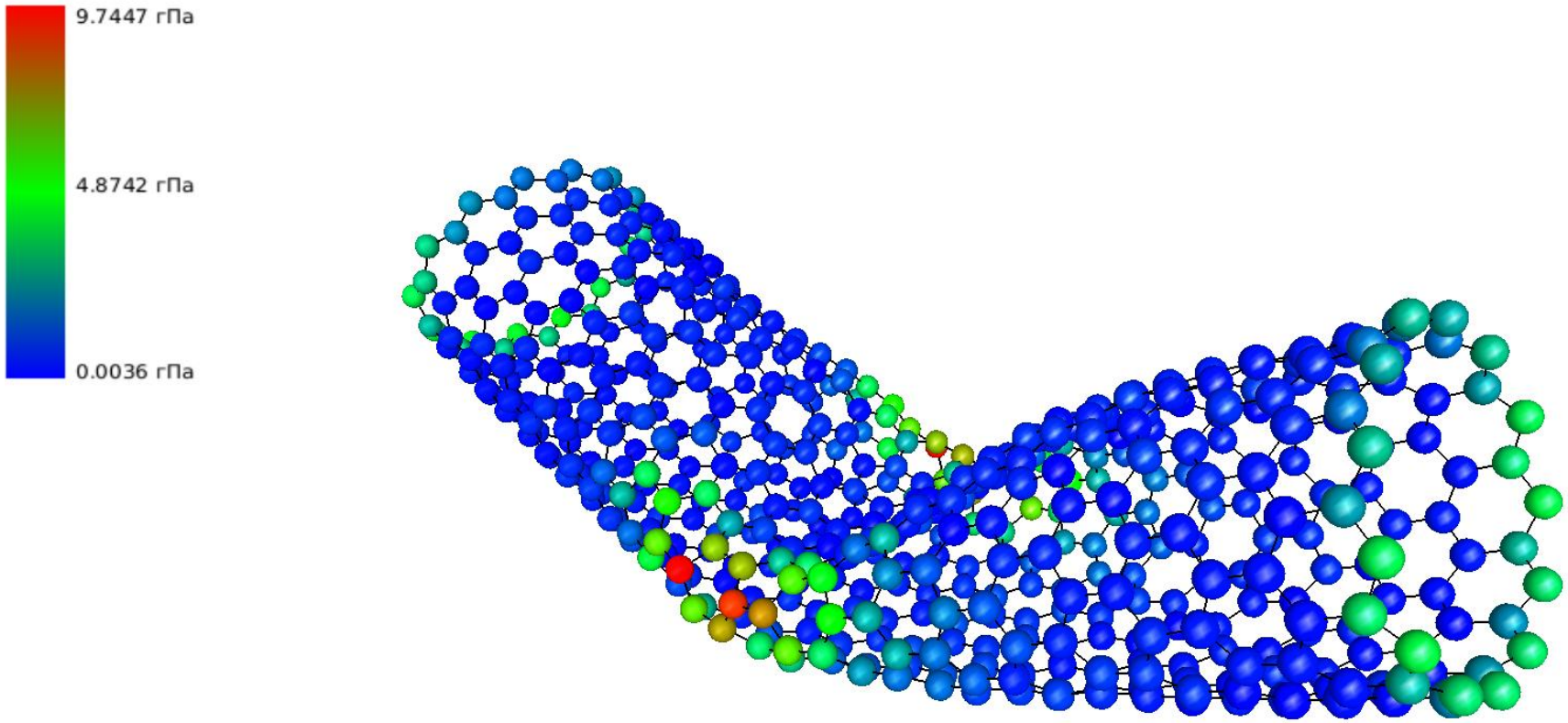


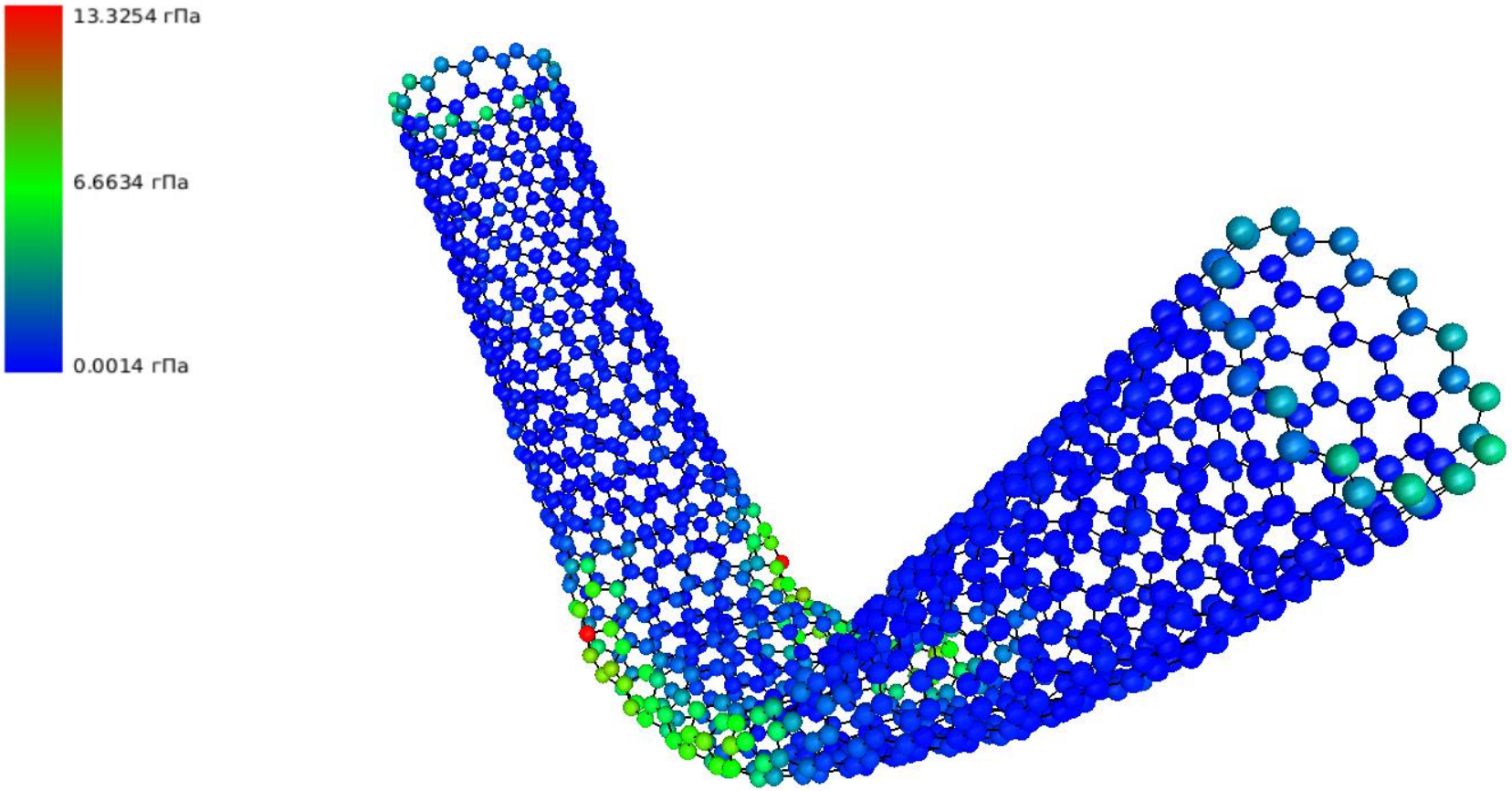


Deformation of the tube during the extension



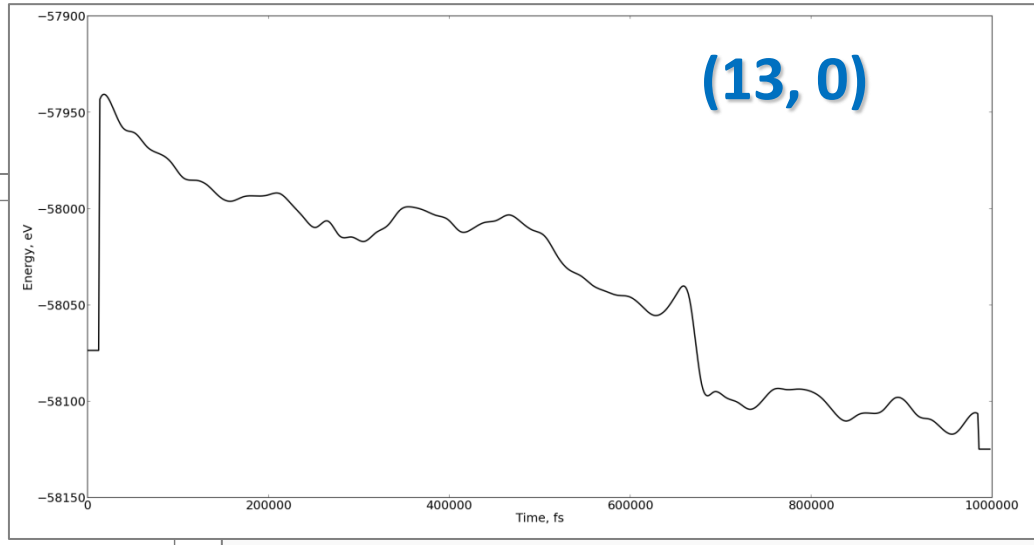
The area of the tube with the maximum of the deformation



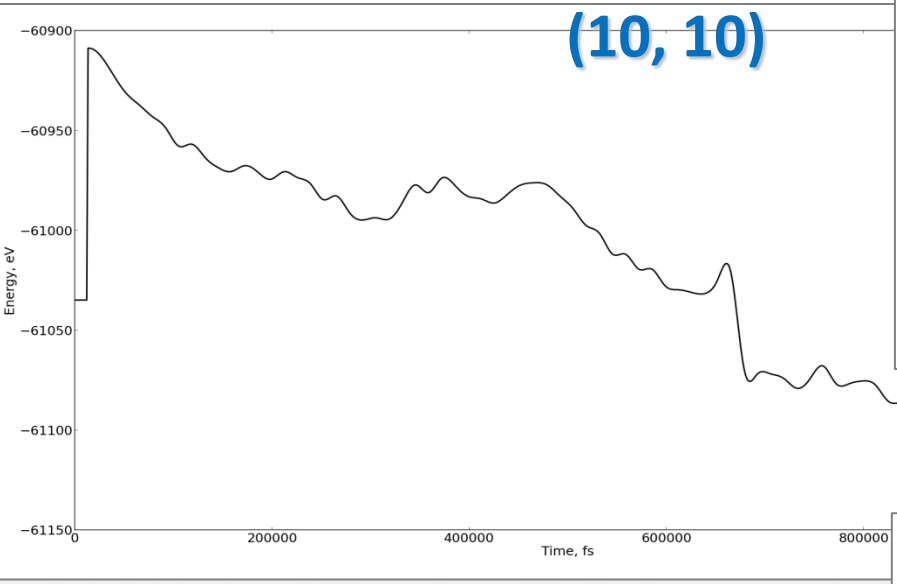


Change in the energy of the torus in extension

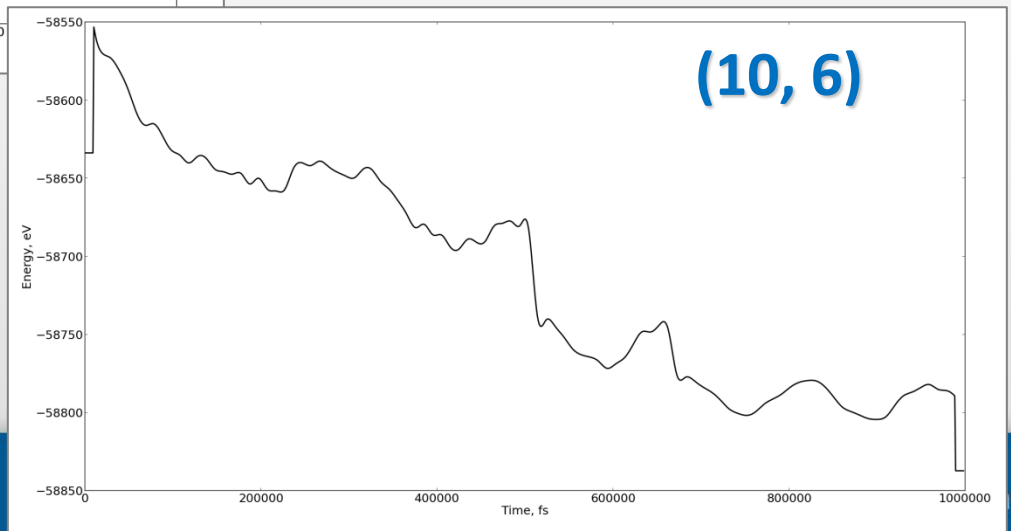
(13, 0)



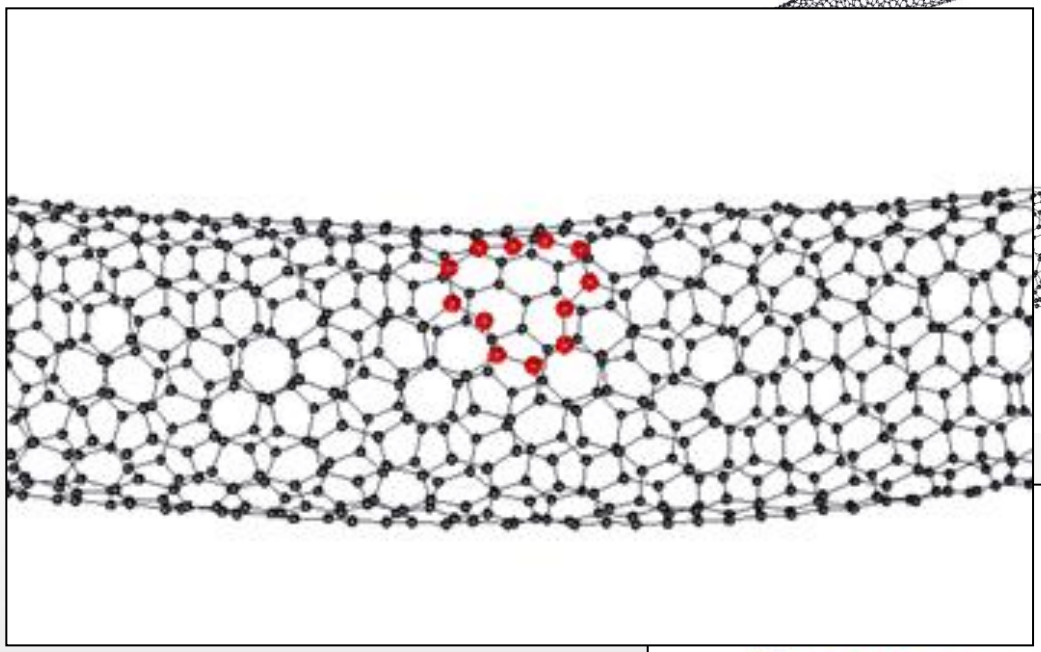
(10, 10)

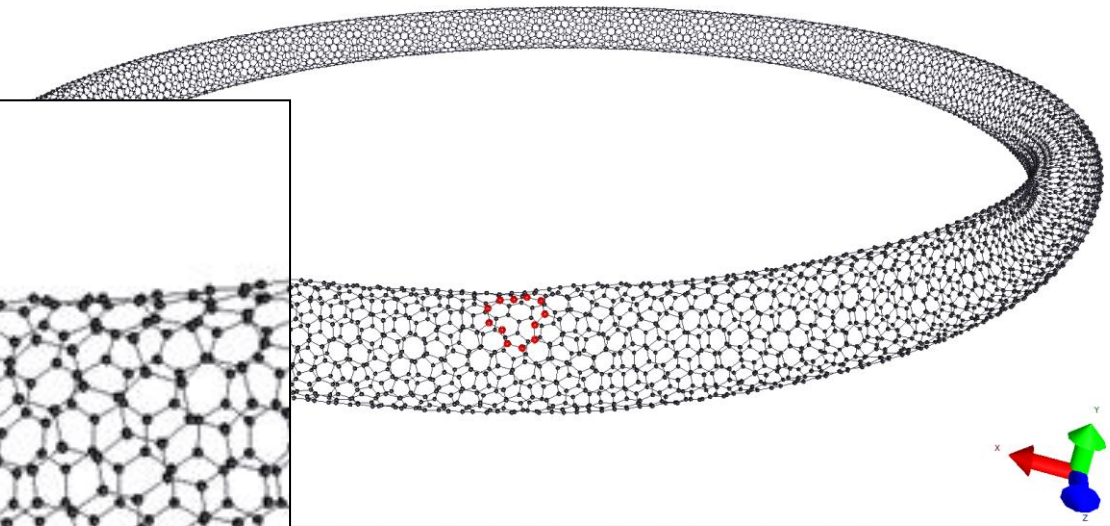


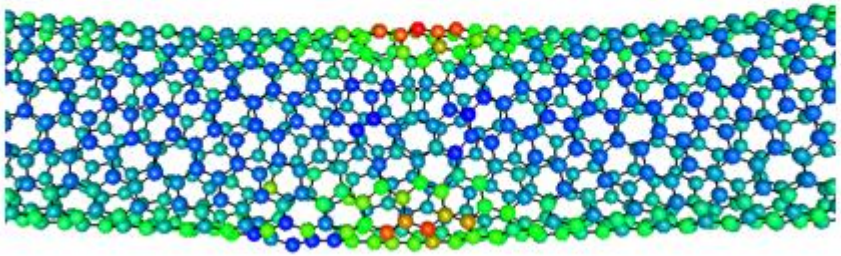
(10, 6)

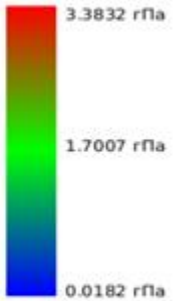


One defect in the atomic cage of the nanotorus (10, 6)









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