Carbon nanotubes — based the cold cathode for field emission electronic

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Directions of research

I. *In silico experiments*

- Saratov State University

II. Natural experiments

Samples were prepared in conjunction with "Technological Center» of The Institute of Nanotechnology of Microelectronics of RAS,
The Institute of Radioengineering and Electronics (IRE) of Russian Academy of Sciences (RAS)

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

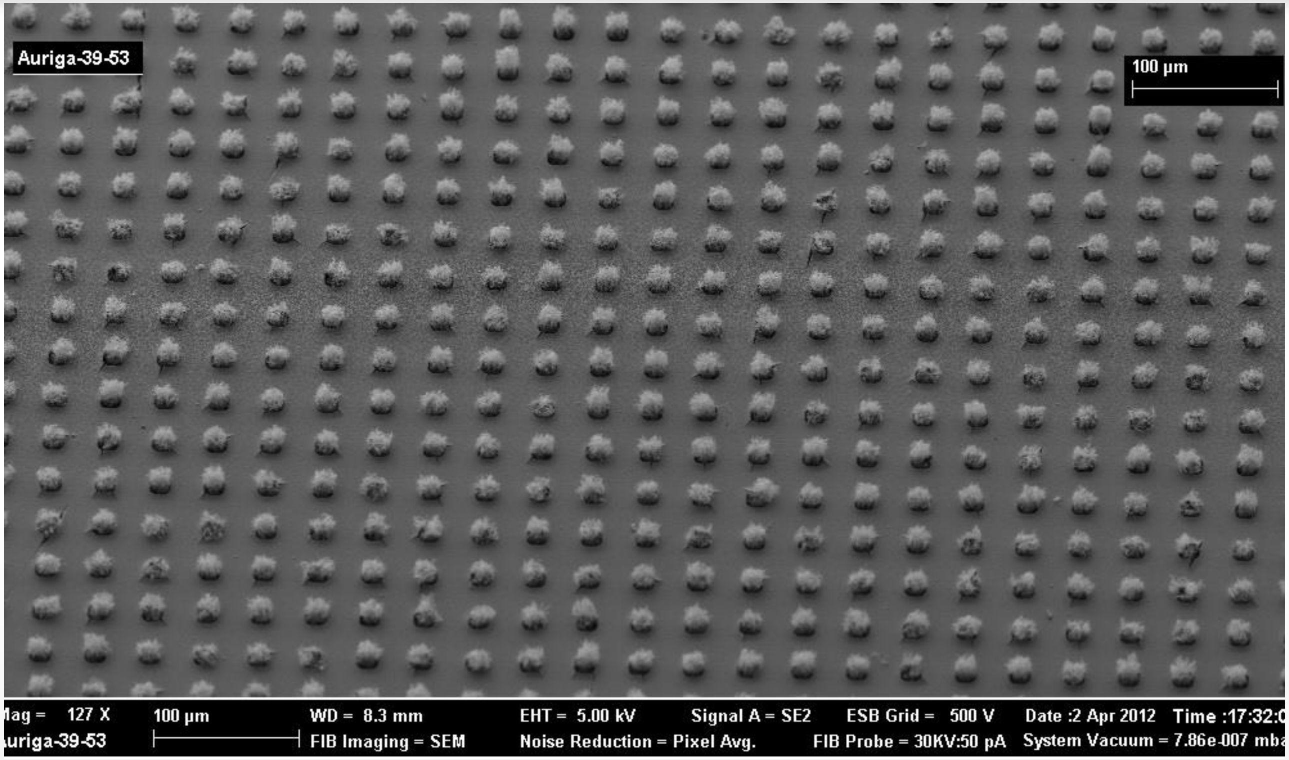
- **MPI programming interface** allows to organize computing clusters;
- **NVidia CUDA** technology allow to perform calculations calculations on display adapters**.**

Applications of the parallel program

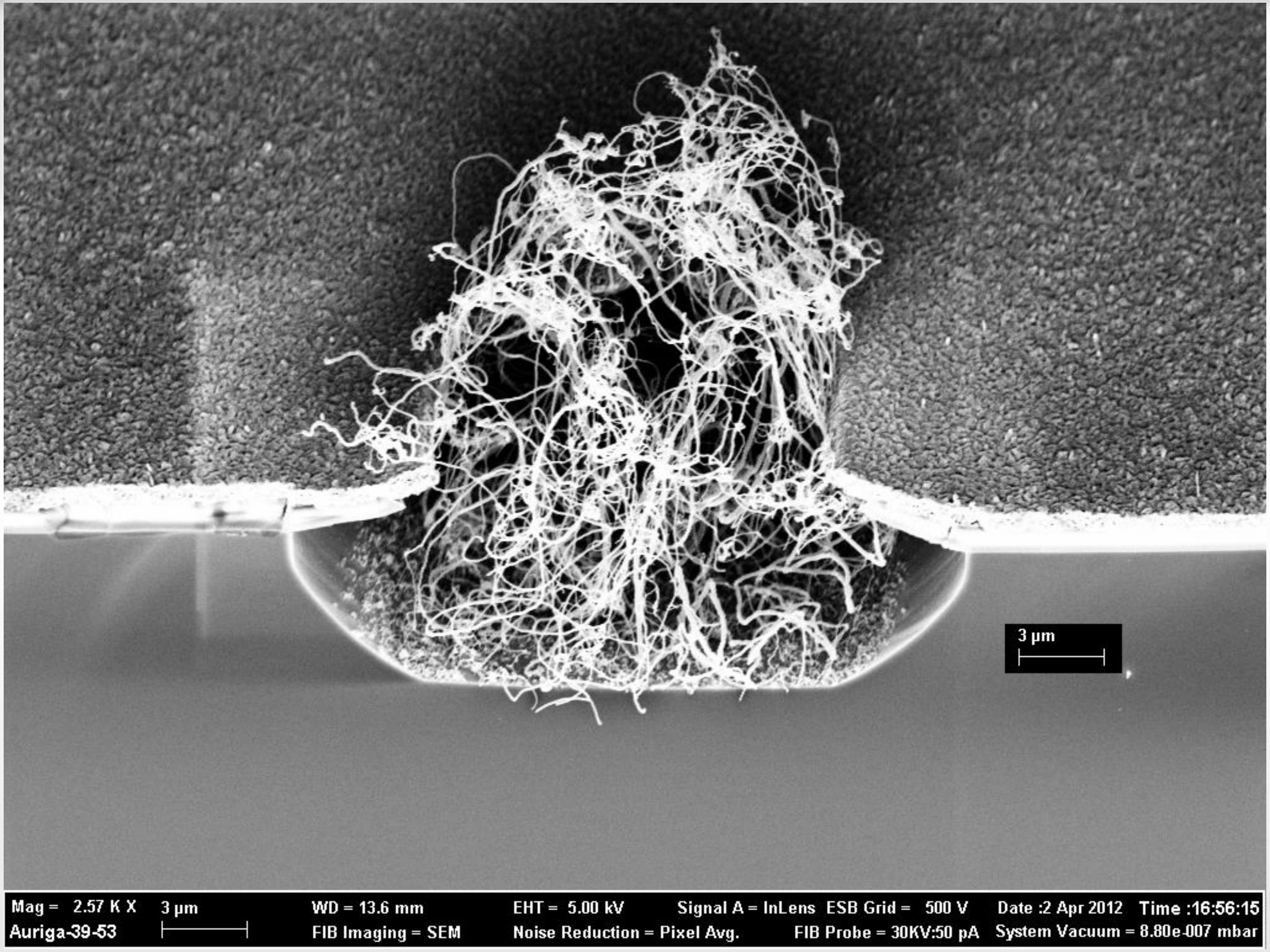
- **Simulation** of micro-and nano-devices;
- **Virtual testing** of nanodevices to determine their technical parameters;
- **Virtual testing** of technologies for new materials;
- Study of the **physical and mechanical properties of the element base** in devices of **micro-and nanoelectronics**.

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

1.

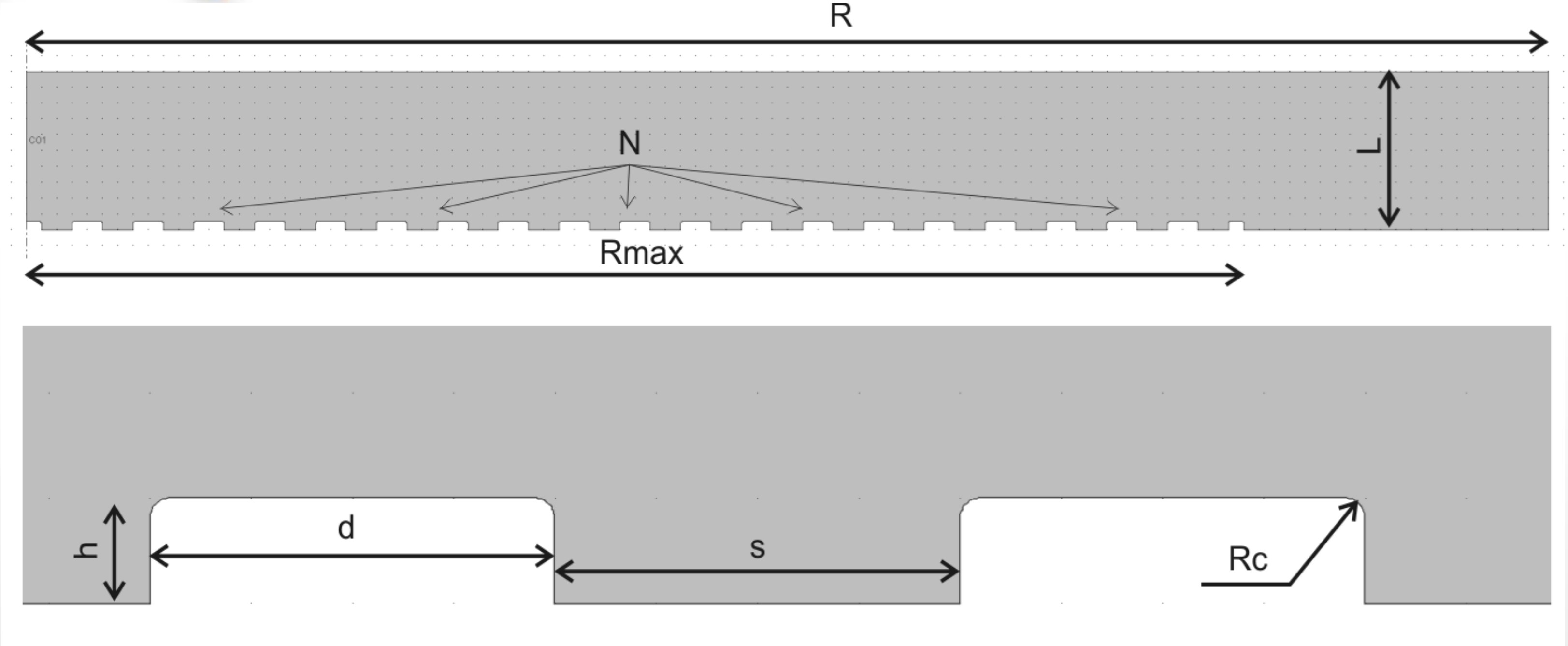


During experiments with the field emission cathodes on CNTs a significant decrease in threshold electric field and increase of current density of the field emission was observed in cases when the emitting film was deposited on the substrate as not continuous layer but in the form of a pattern. Due to this observation the influence of patterns on the cathode on the resulting field emission current from was calculated. In details we investigated one of a possible patterns of emitting material in the form of concentric rings of equal width.

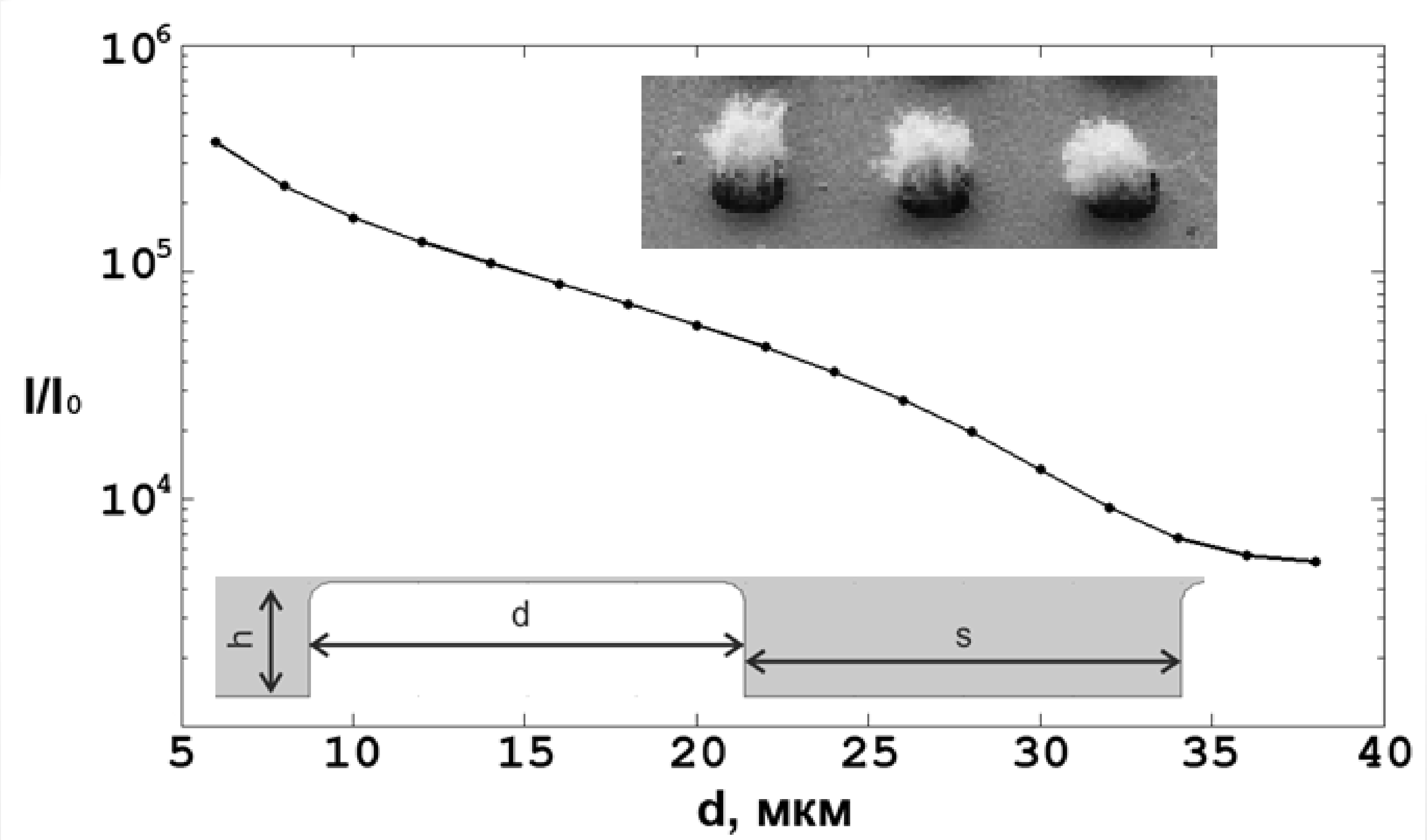


Concentric ring of pattern formed by array of CNT

Model of pattern



View of the computational domain for patterns as concentric rings and its variable parameters: thickness of the emitting film *h*, radius of inhomogeneities fillet *Rc*, width of ring *d*, the distance between the rings *s*, distance between anode and cathode *L*, number of rings *N*, radius of anode *R*.

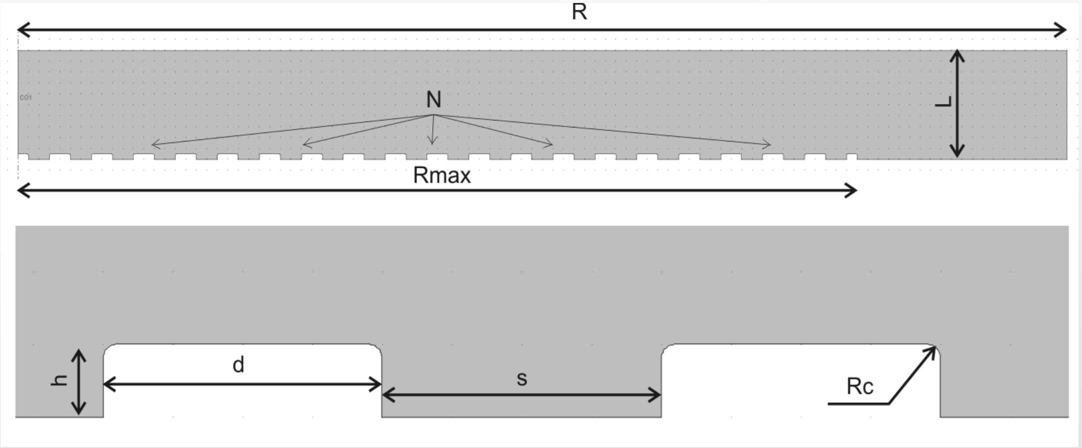


Increasing of the emission current of the cathode with an annular pattern in relation to the cathode without a pattern depending on the width of the ring d. Calculations were made for $d + s$ = 40 um, N = 20, R_c = 1 um, h = 5 um, L = 100 um.

Conclusions

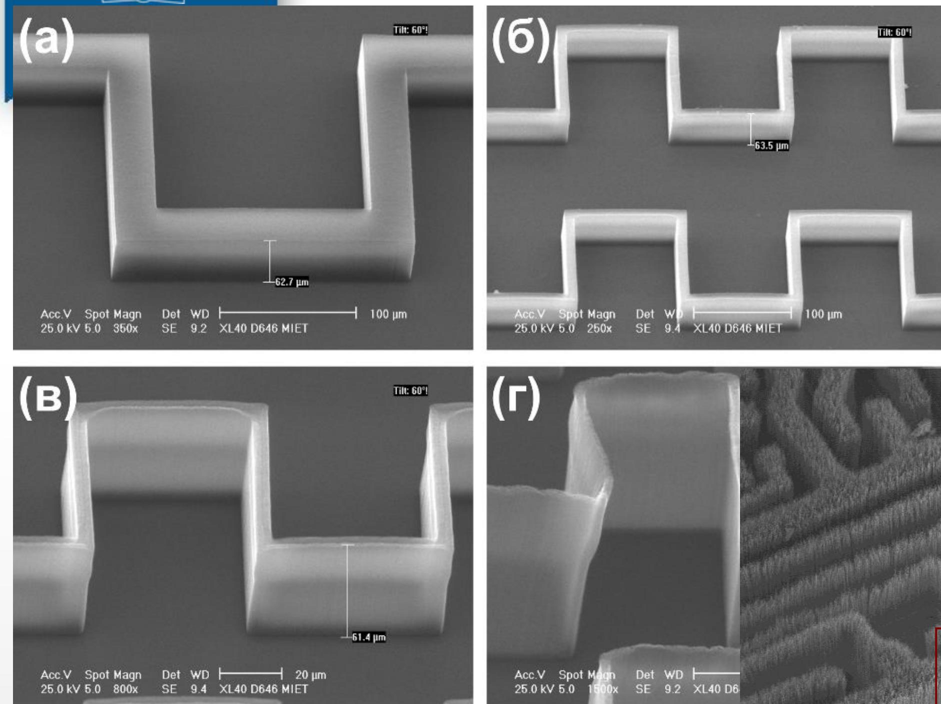
1. Calculation shows that the increase of emissions with decreasing of width of the emitting ring can reach several orders of magnitude, that will inevitably lead to the destruction of the pattern. Such increase of current indicates that the operating voltage of the system can be reduced by 2-4 times.

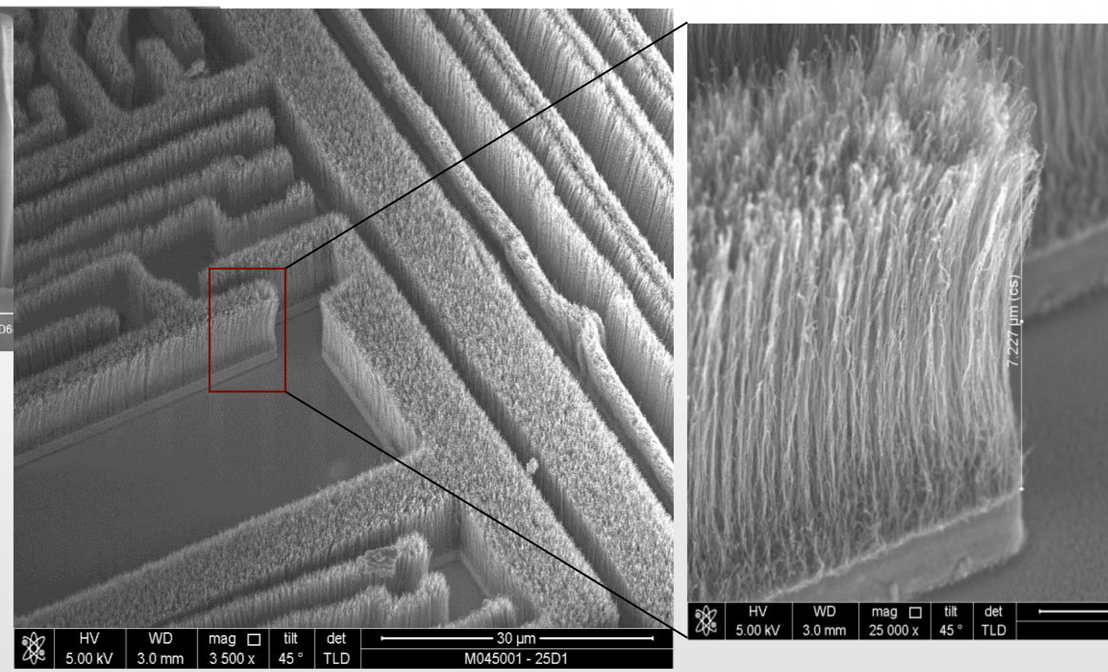
2. These results allow to conclude that the optimal width of the ring d with parameters listed above, lies in the range of d = 20-30 mkm, increasing of the current in this case is significant, but still does not exceed allowable limits, after which thermal decomposition of emitting film and degradation of the cathode occurs. Cathode with patterns can be recommended to application in pulsed modes with sufficiently high duty cycle.



Examples of different patterns / meanders

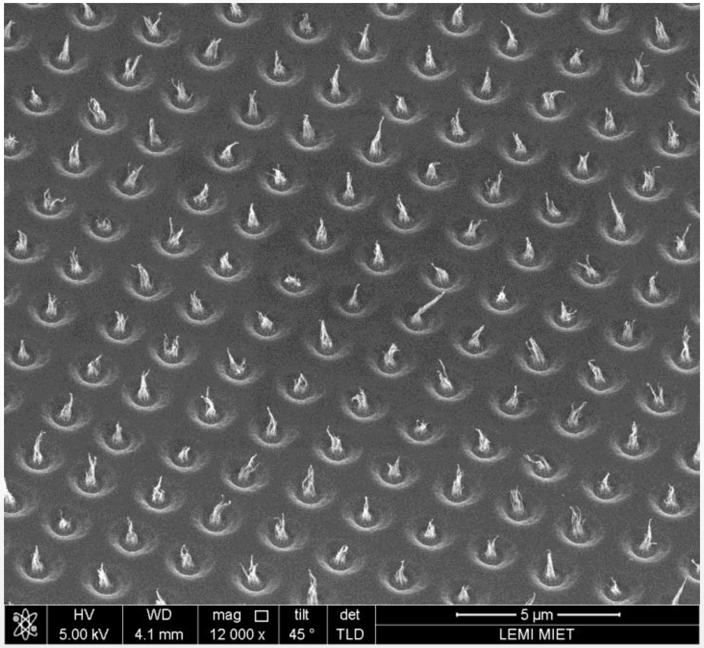
A. S. Basaev, E. V. Blagov, V. A. Galperin, A. A. Pavlov, U. P. Shaman, A. A. Shamanaev, S. V. Shamanaev and A.S. Prihodko. Specificities of Growth of Topological Arrays of Carbon Nanotubes // ISSN 1995_0780, Nanotechnologies in Russia, 2012, Vol. 7, Nos. 1–2, pp. 22–27.

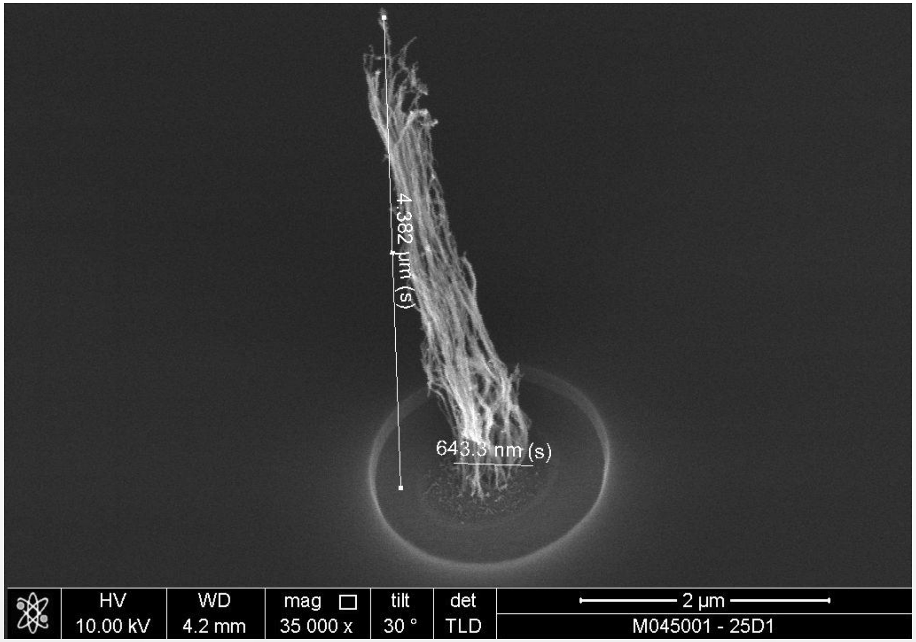




SEM images of CNT arrays as meanders with width: a) 30 um, б) 10 um, в) 5 um и г) 1,5 um, synthesized on the tool «CNT-3»

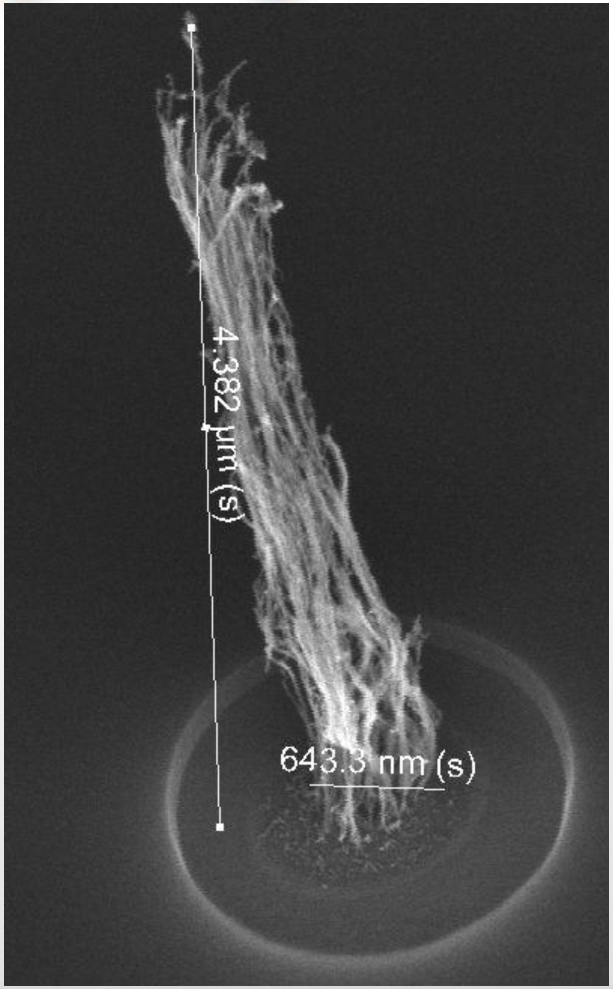
Development and optimization of cathode emission matrices on the base of CNTs obtained by setting Nanofab 800 Agile

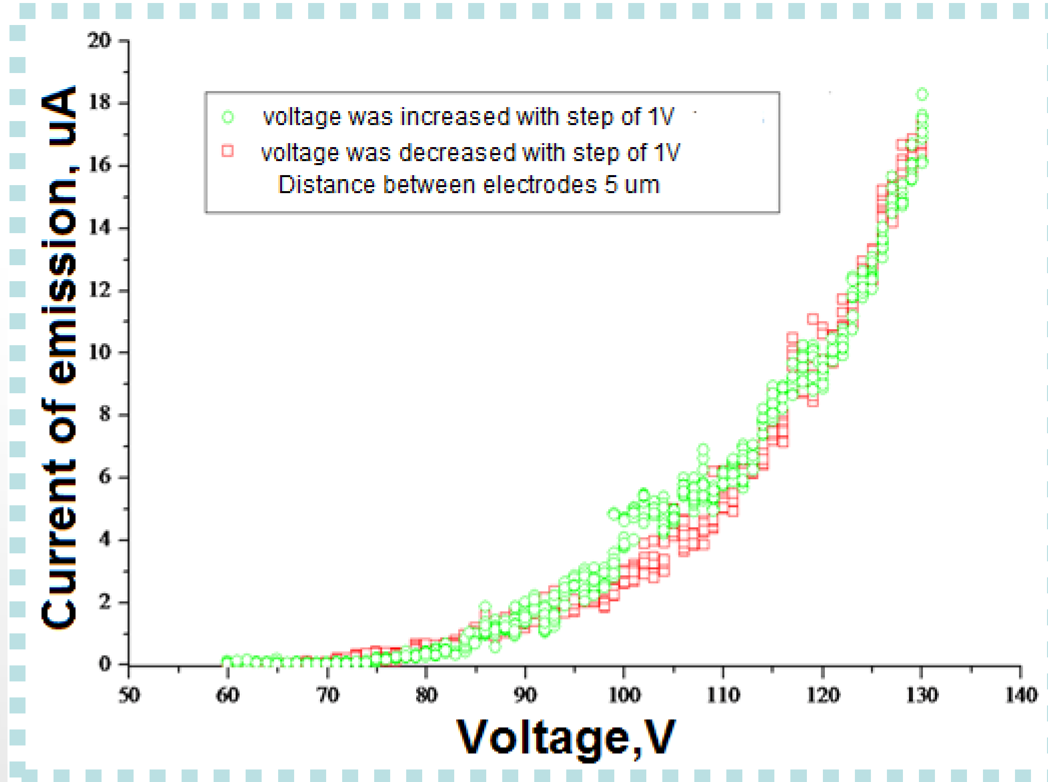




SEM images of structured array of CNT formed with application of electron beam lithography and a separate beam

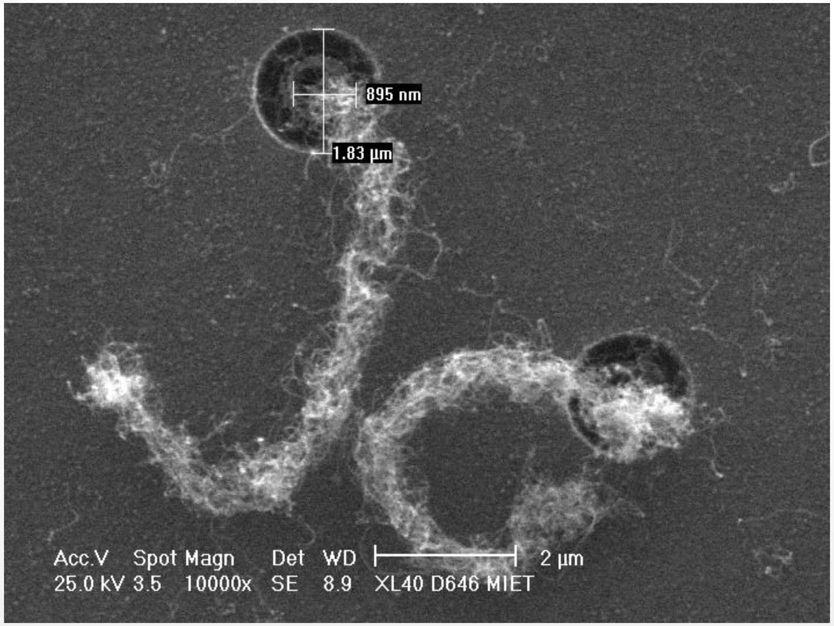
Pressure: $1 \cdot 10^{-5}$ Pa.
The distance between the electrode and the beam : 5 um.



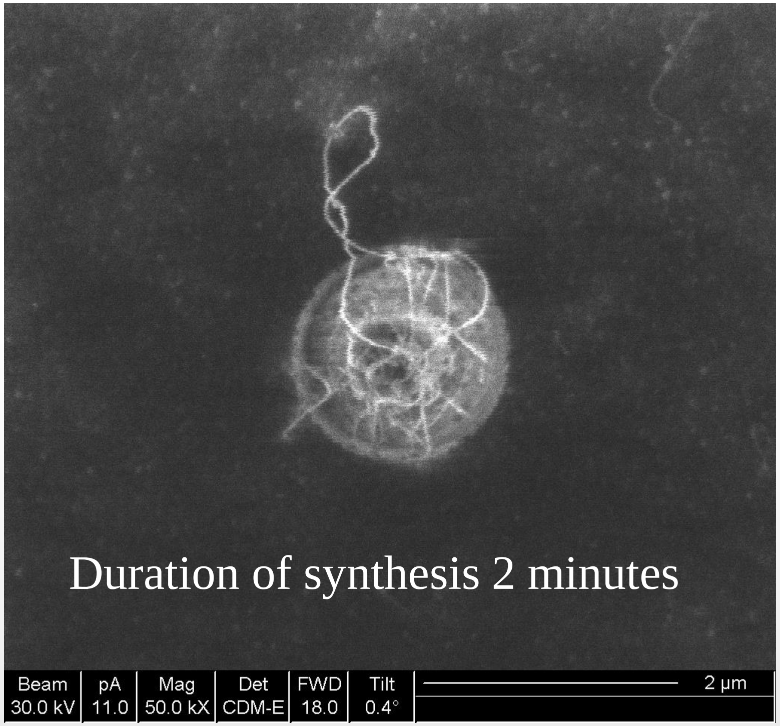


Samples were prepared in conjunction with "Technological Center»

Possibility of CNTs application for solving 3D assemblies and interconnections



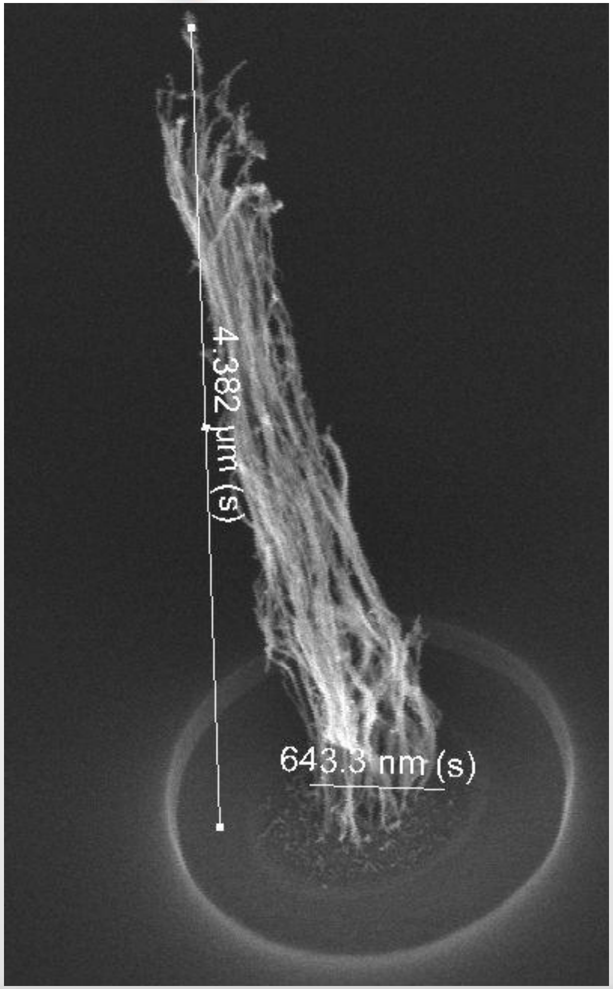
Duration of synthesis 10 minutes

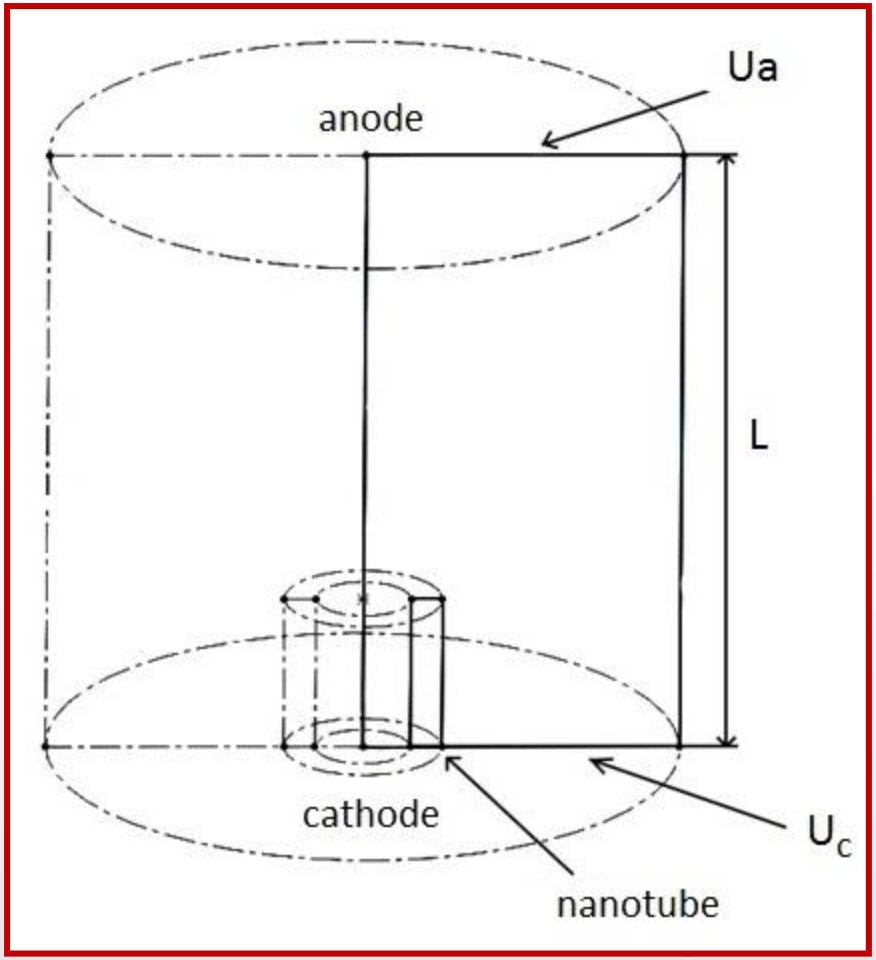


SEN images of CNT grown in contact window on the tool CNT-3: (a) duration of synthesis 10 minutes, (б) duration of synthesis 2 minutes

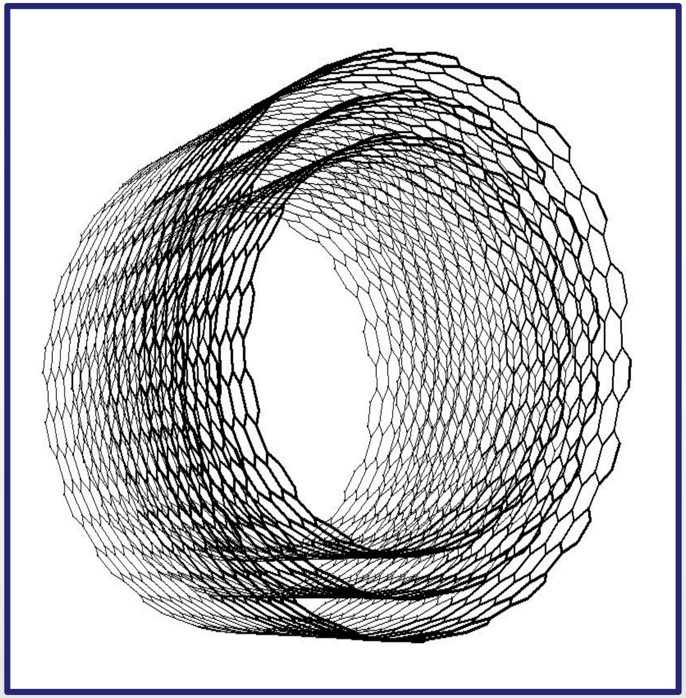
Samples were prepared in conjunction with "Technological Center»

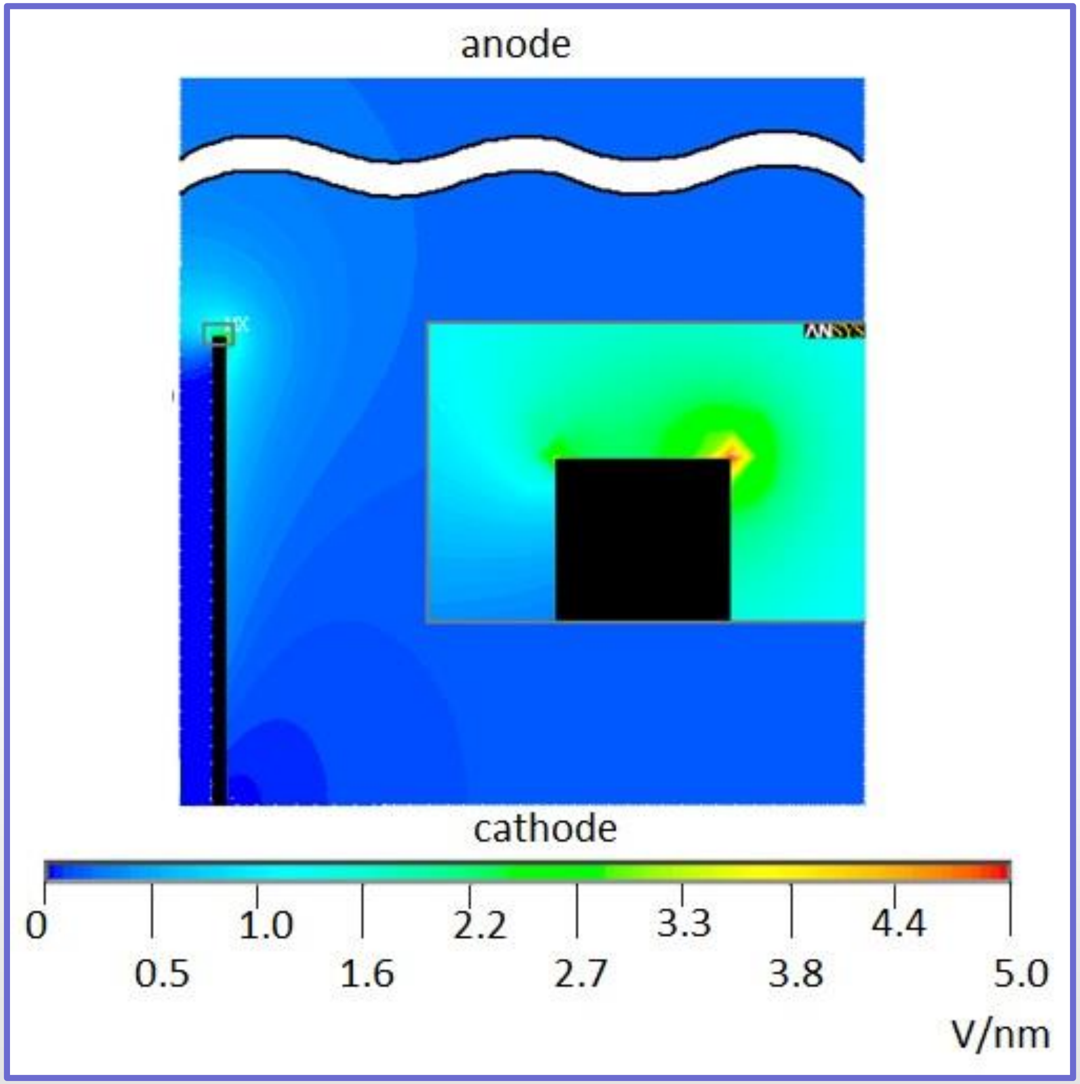
2. Study of the CNT as a solid cylinder



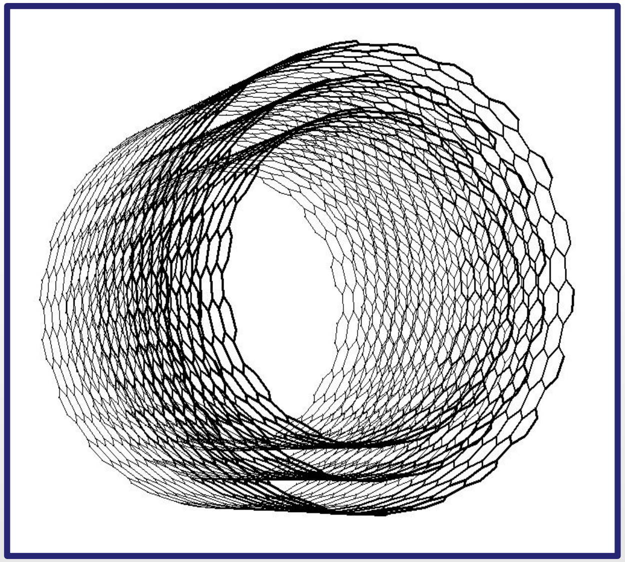


Model for the calculation of the field strength

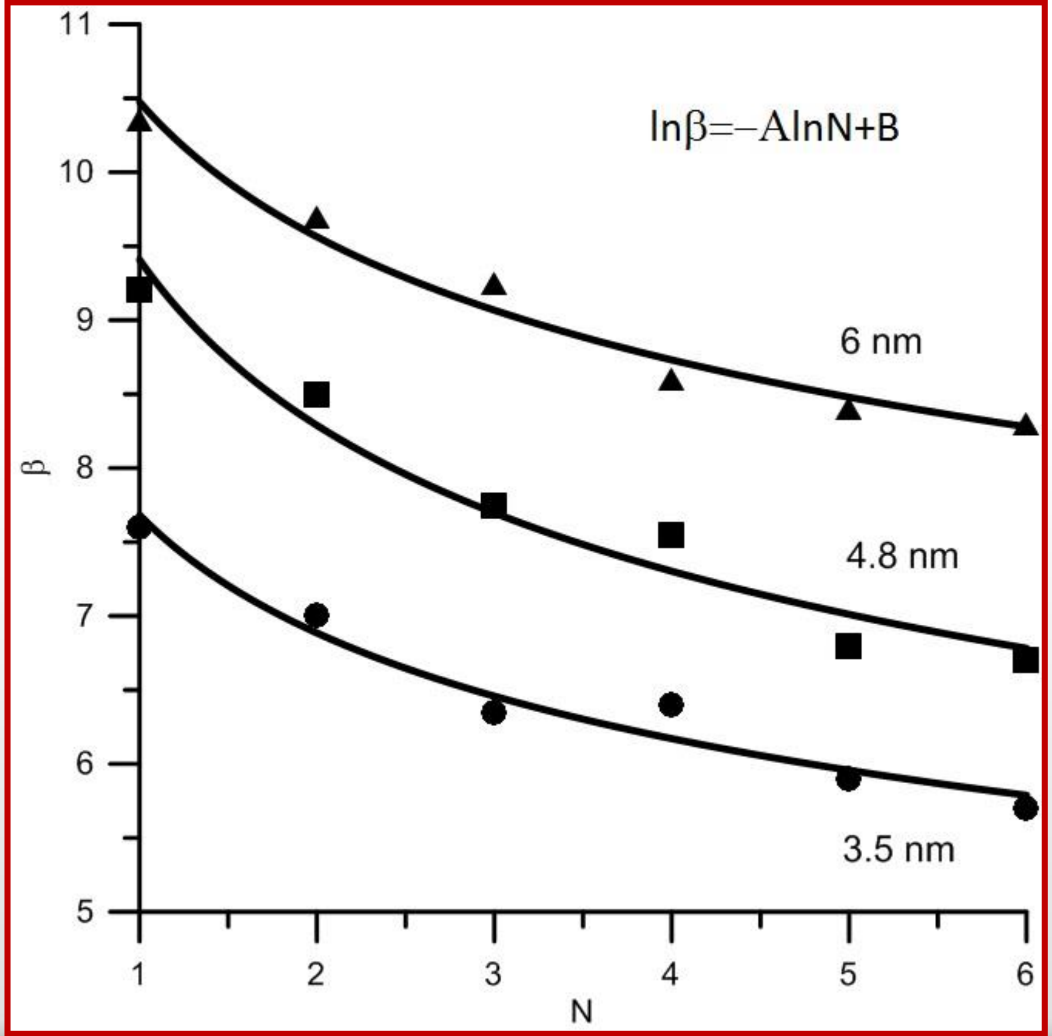



anode
cathode
0
1.0
2.2
3.3
4.4
0.5
1.6
2.7
3.8
5.0
V/nm

Dependence of the field-amplification factor β on number of the CNT-layers N



ANSYS 13.0

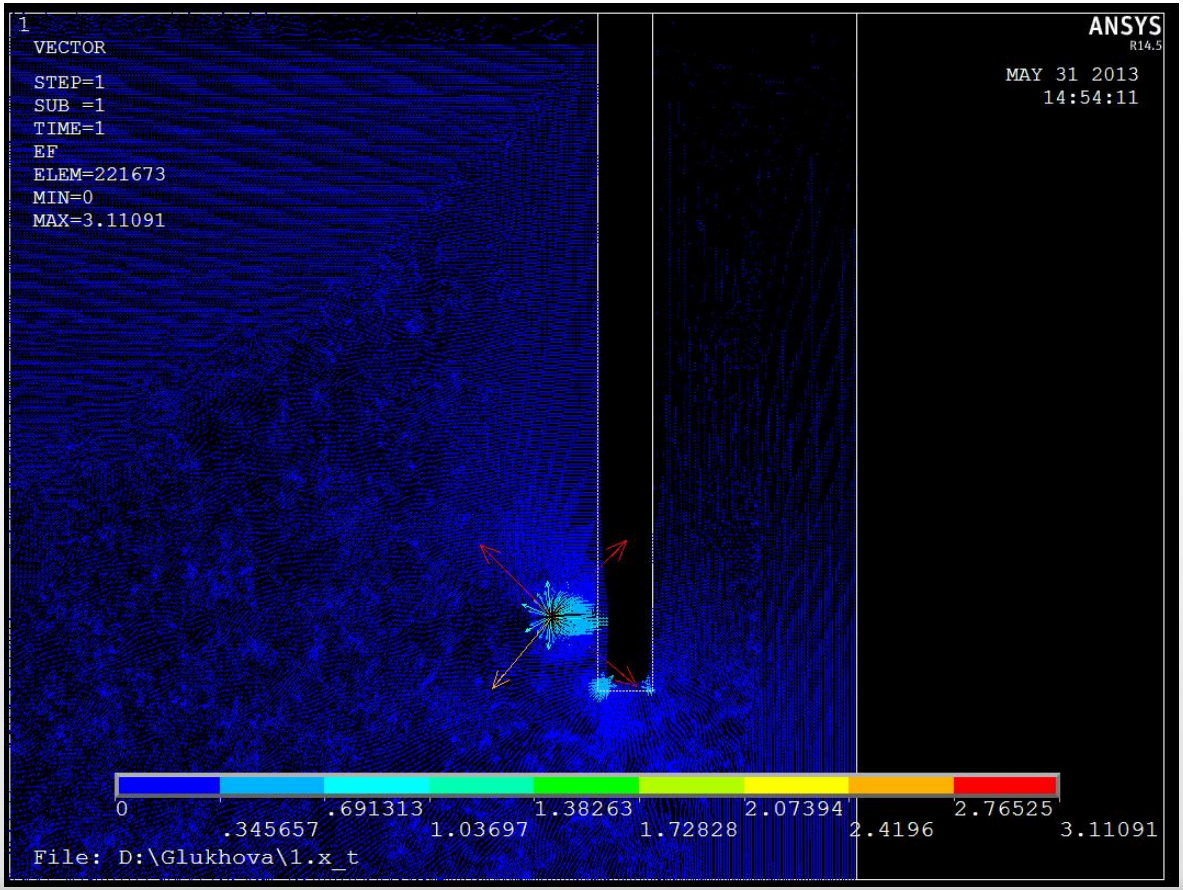


2. Inhomogeneous electric field.

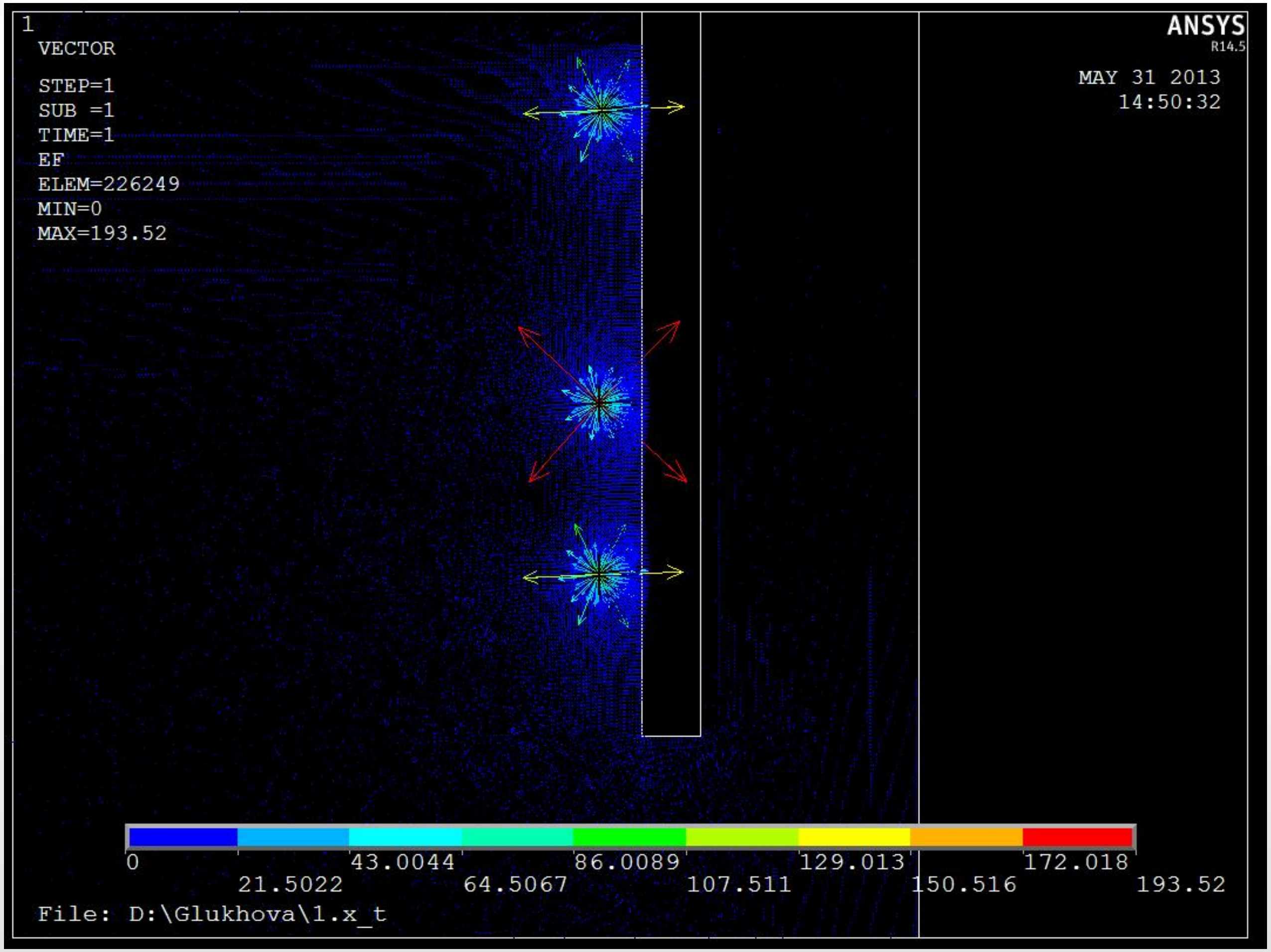
CNT as the solid cylinder in the field (FEM-calculations)

Influence of number of the plasma atoms on the electric field strength of CNT

1 plasma atom



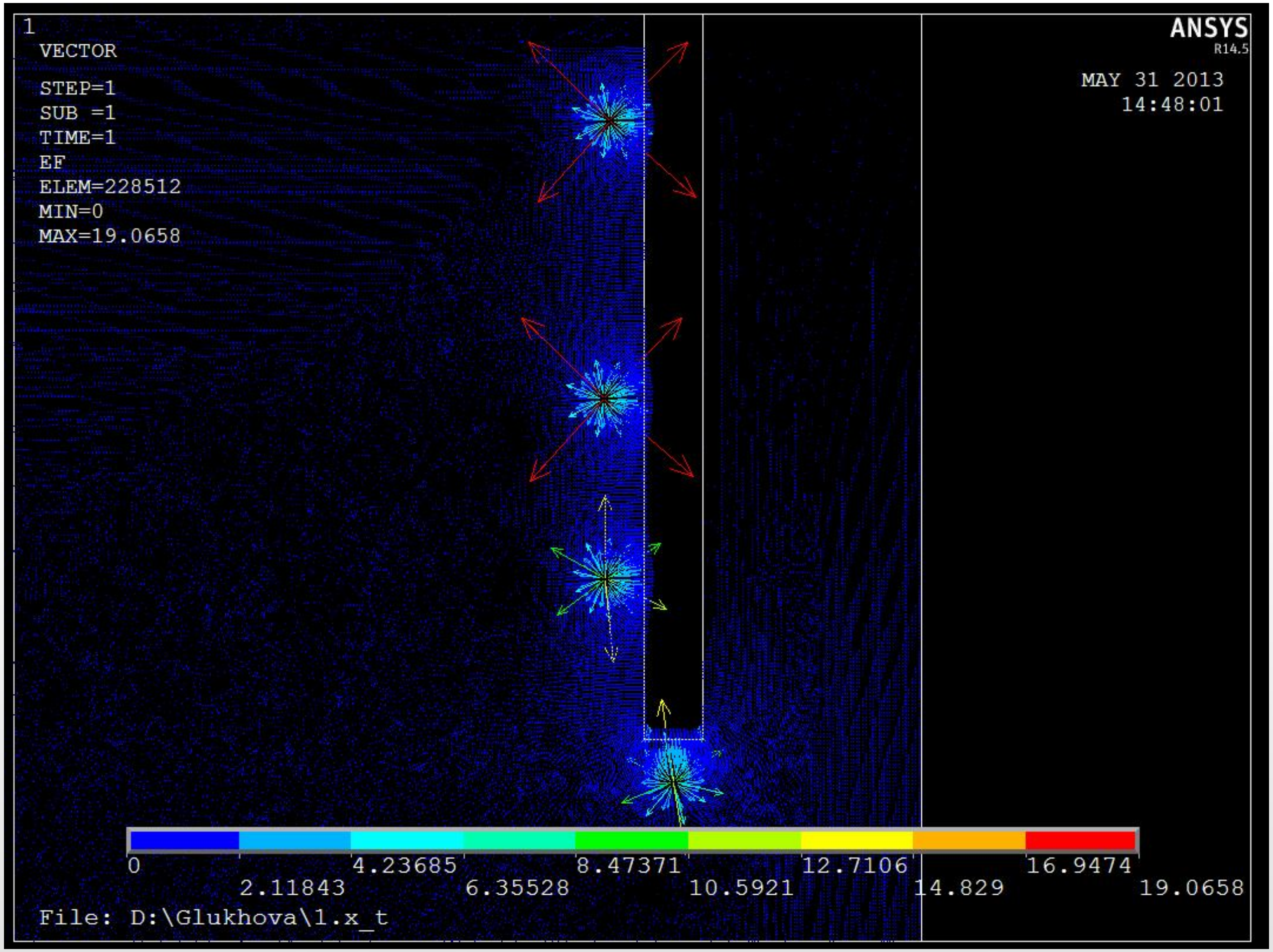
Influence of number of the plasma atoms on the electric field strength of CNT



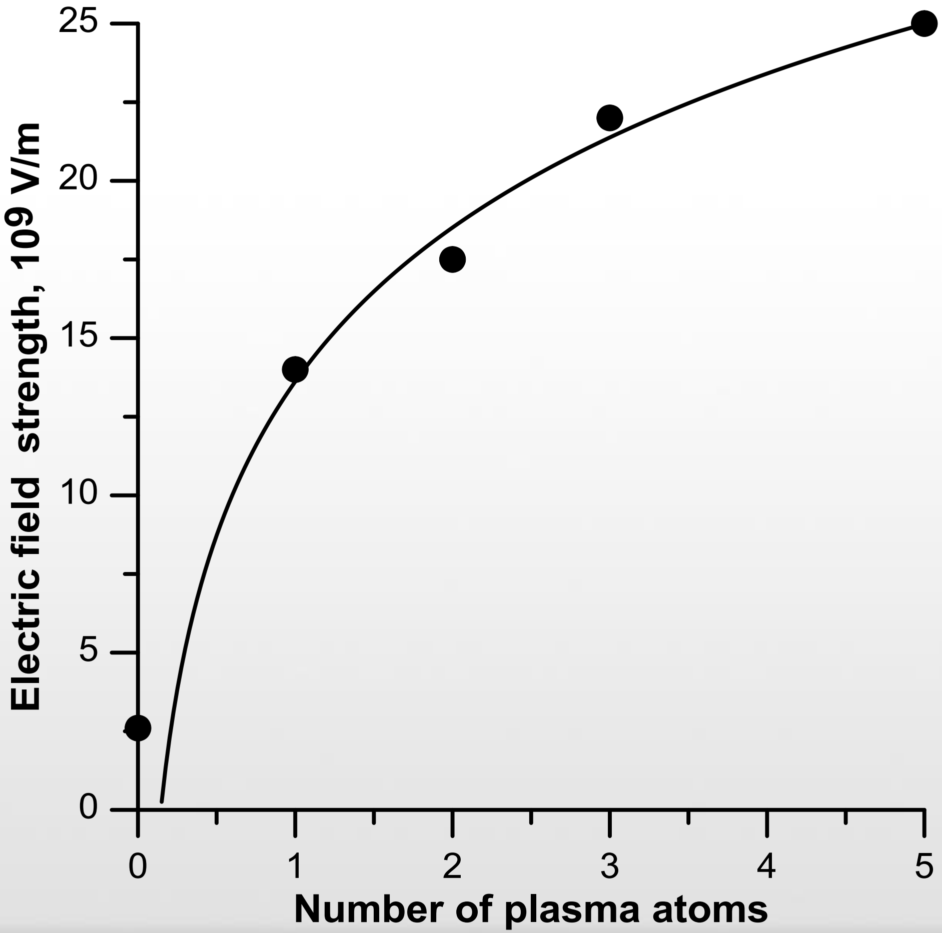
3 plasma atom

Influence of number of the plasma atoms on the electric field strength of CNT

4 plasma atom

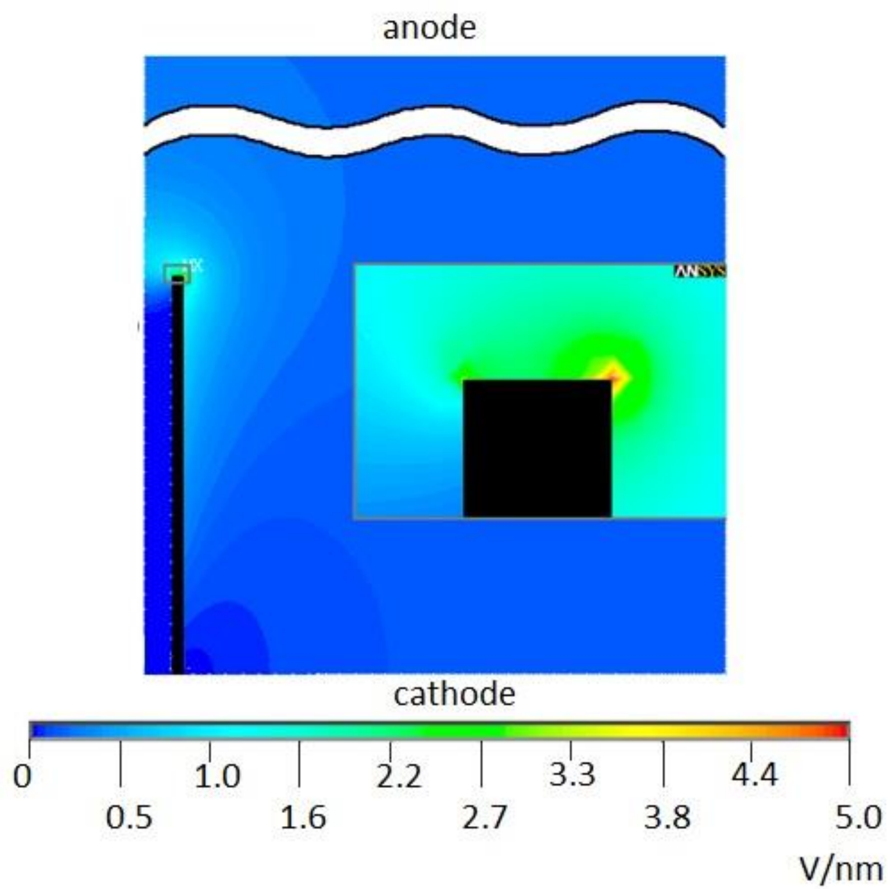


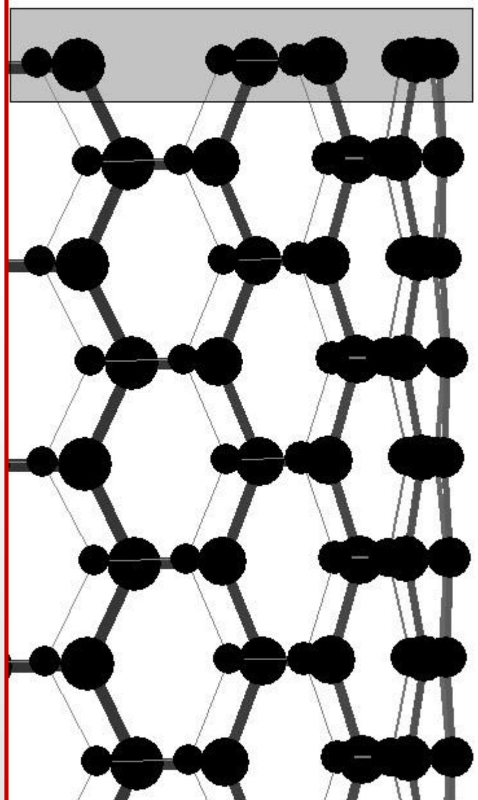
Rising strength on the surface of the nanotube in length of 100 nm and and diameter of 2 nm depending on the number of atoms of the plasma



3. The atomic structure of CNT in field

Distribution of the field strength along the length of CNT (h=300 nm, d=2 nm)

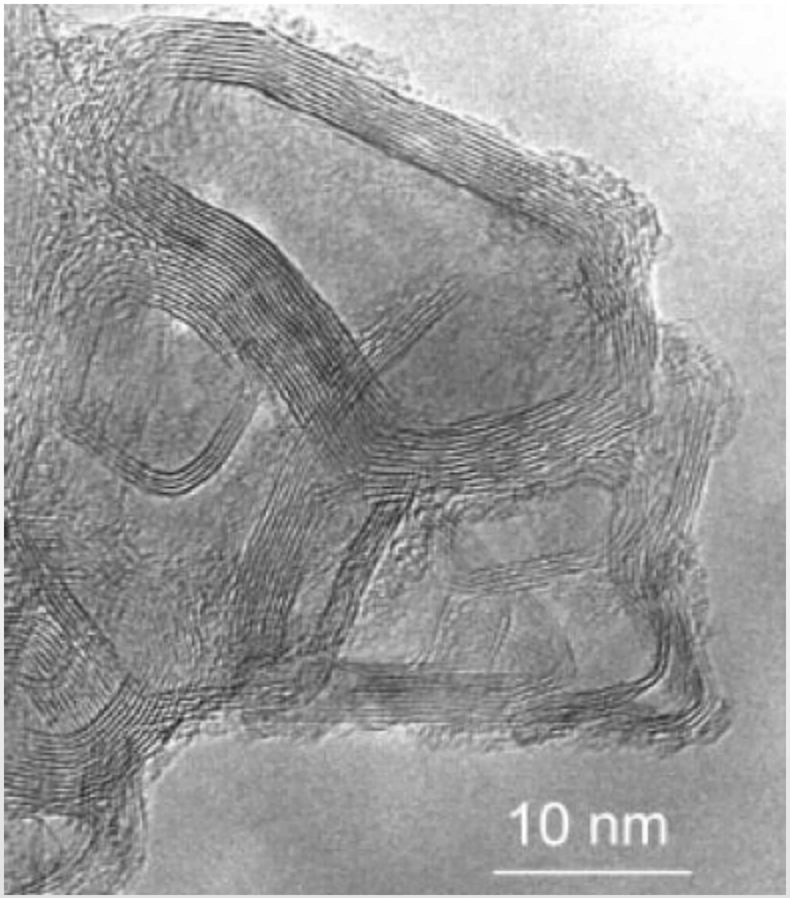




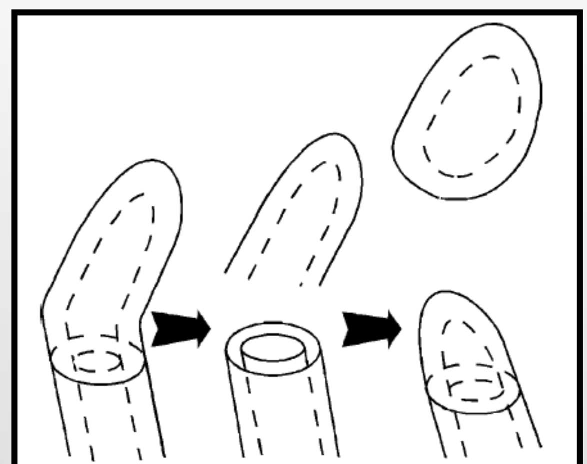
E,V/nm	j,A/cm^2	I,nA
6.22	6.64E+6	51.02
3.4	5.10E+2	3.94E-2
2.7	2.85	2.20E-5
1.9	8.95E-5	6.91E-10
1.5	0	0
0.9	0	0
0.7	0	0

Evaporation of atoms from CNT

Field evaporation of a carbon nanotube anode at extremely high electric fields of 1–2 V/Å was reported (*K. Hata, M. Ariff, K. Tohji, Y. Saito: Chem. Phys. Lett.* ***308****, 343, 1999*)



In the paper (*Appl. Phys. A 73, 301–304,2001*) was established that field evaporation of nanotubes accompanies field emission from a cold cathode at electric fields higher than 2 V/Å. Electron microscopy of the evaporation products reveals irregularly shaped carbon nanoparticles with a hollow core. The diameter of the particles is ~ 20 nm.



Zhong L. Wang and Rui Ping Gao, Walt A. de Heer and P. Poncharal // Appl. Phys. Lett., Vol. 80, No. 5, 4 February 2002

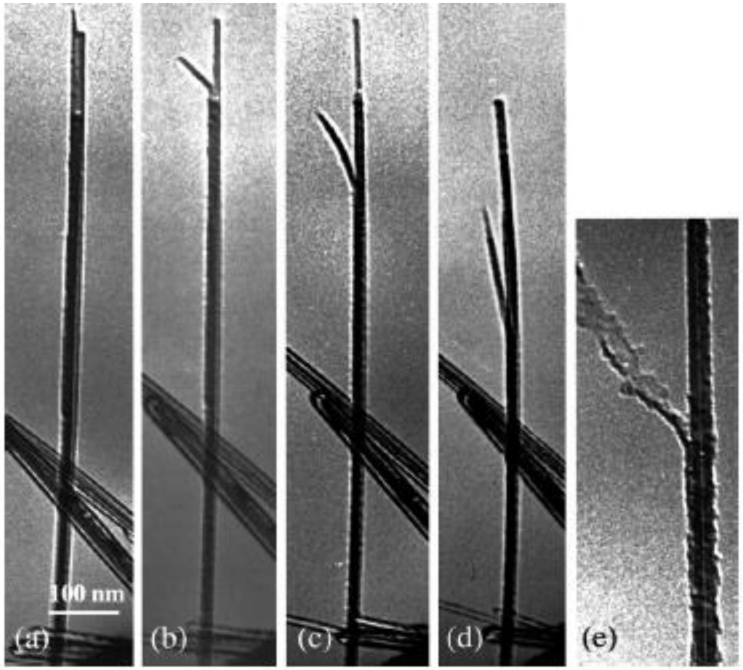


FIG. 3. "Splitting" process in structural damage. (a)–(d) Series of TEM images showing the structural damage of a carbon nanotube during field emission, in which the applied voltage and the emission current are: (a) $V=80$ V, $I=10$ μA, (b) $V=90$ V, $I=40$ μA, (c) $V=110$ V, $I=100$ μA, and (d) $V=130$ V, $I=250$ μA. The distance from the tip of the nanotube to the counter electrode was ~ 2 μm. (e) Nanotube that is experiencing the splitting of its outer layers during the damage.

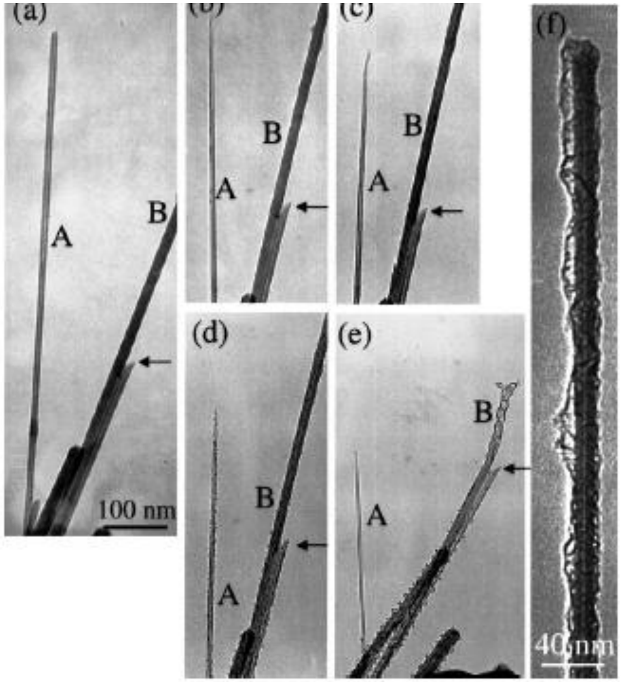
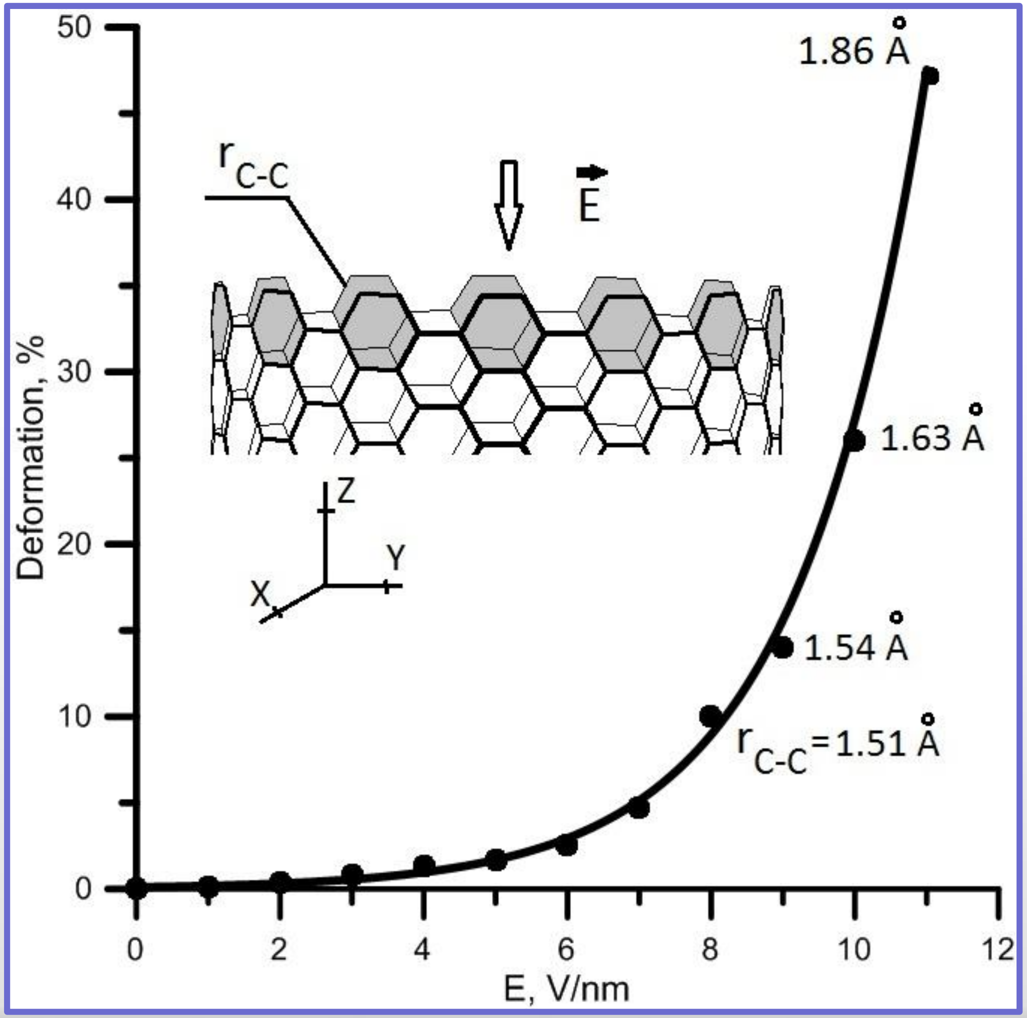
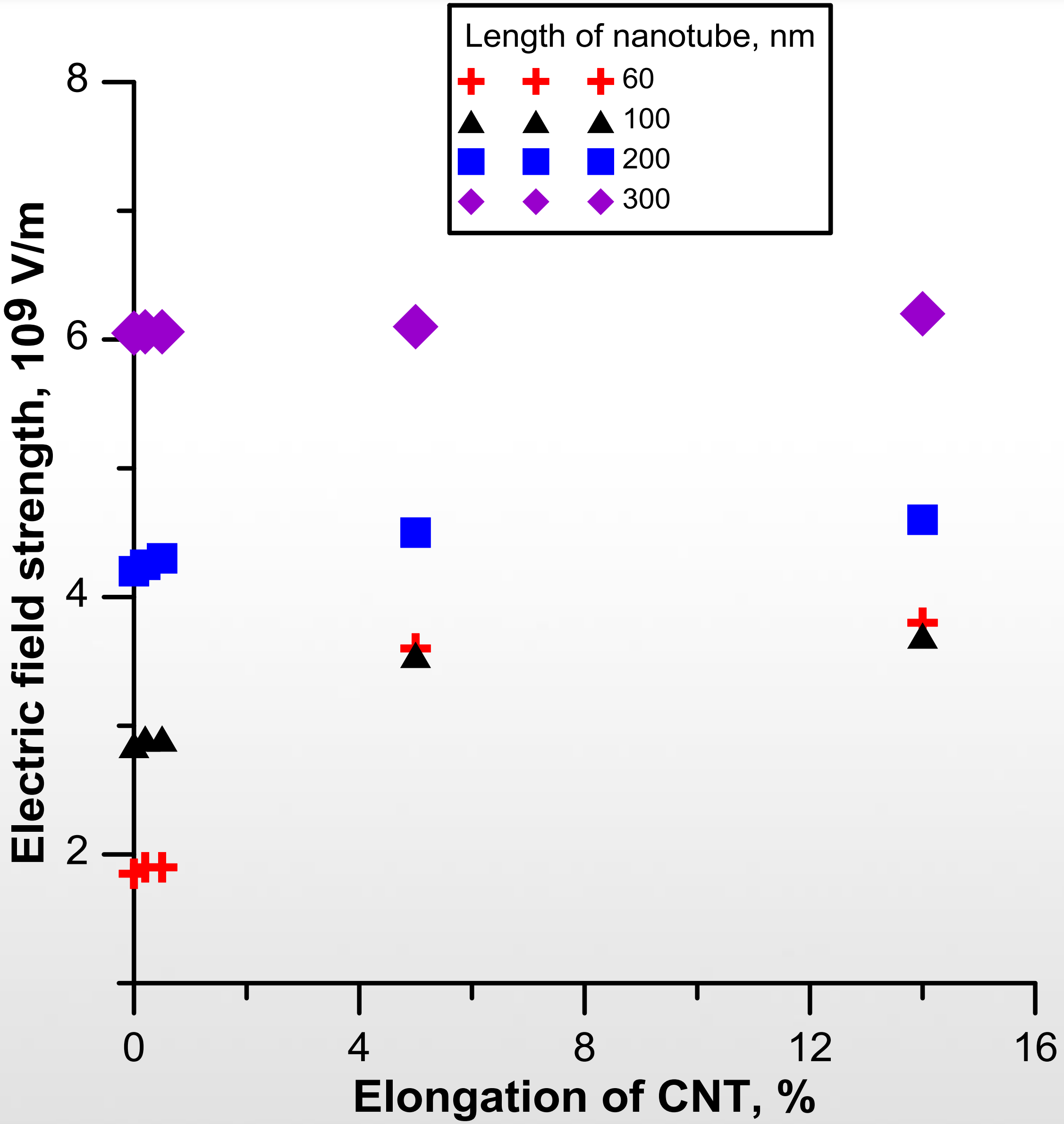


FIG. 4. "Stripping" effect in structural damage. (a)–(e) Series of TEM images showing the structural damage of a carbon nanotube during field emission. The applied voltages were (a) $V=100$ V, (b) $V=120$ V, (c) $V=140$ V, (d) $V=160$ V, and (e) $V=200$ V. The distance from the tip of the nanotube to the counterelectrode was ~ 4 μm. (f) A carbon nanotube after passing through a large current, showing the structural damage at the outer graphitic layers, while the internal layers are intact.

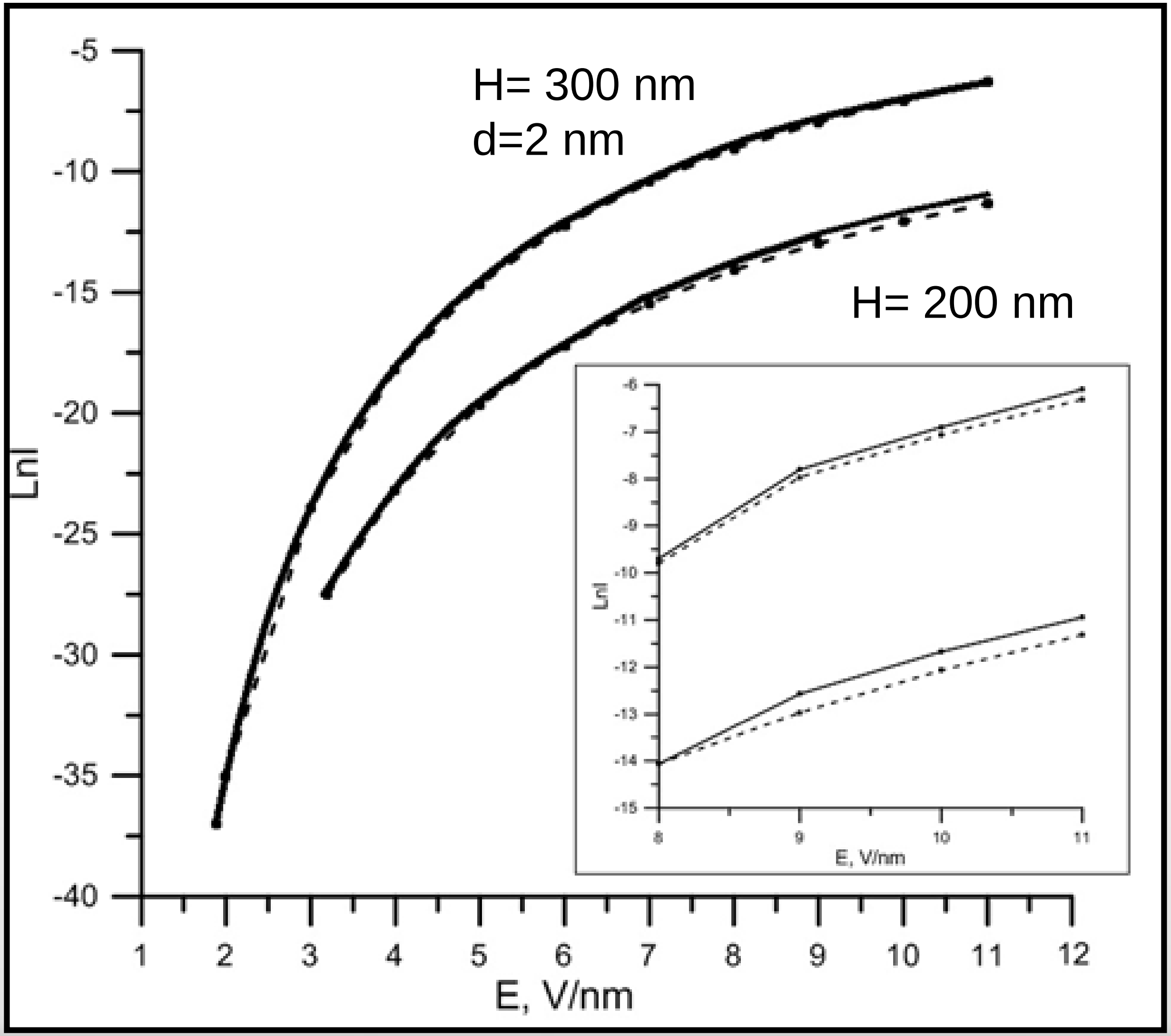
Influence of the electric field on the atomic cage of CNT



Effect of the ponderomotive force (extension of tubes) on the field at the end of CNT in length of 100 nm and diameter of 2 nm



Dependence of the emission current on the elongation of CNT in the electric field



4. New composite materials for cold cathodes

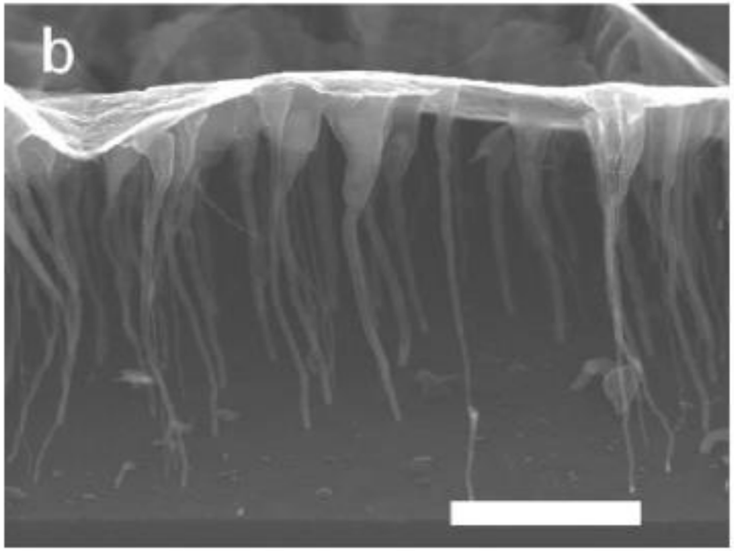
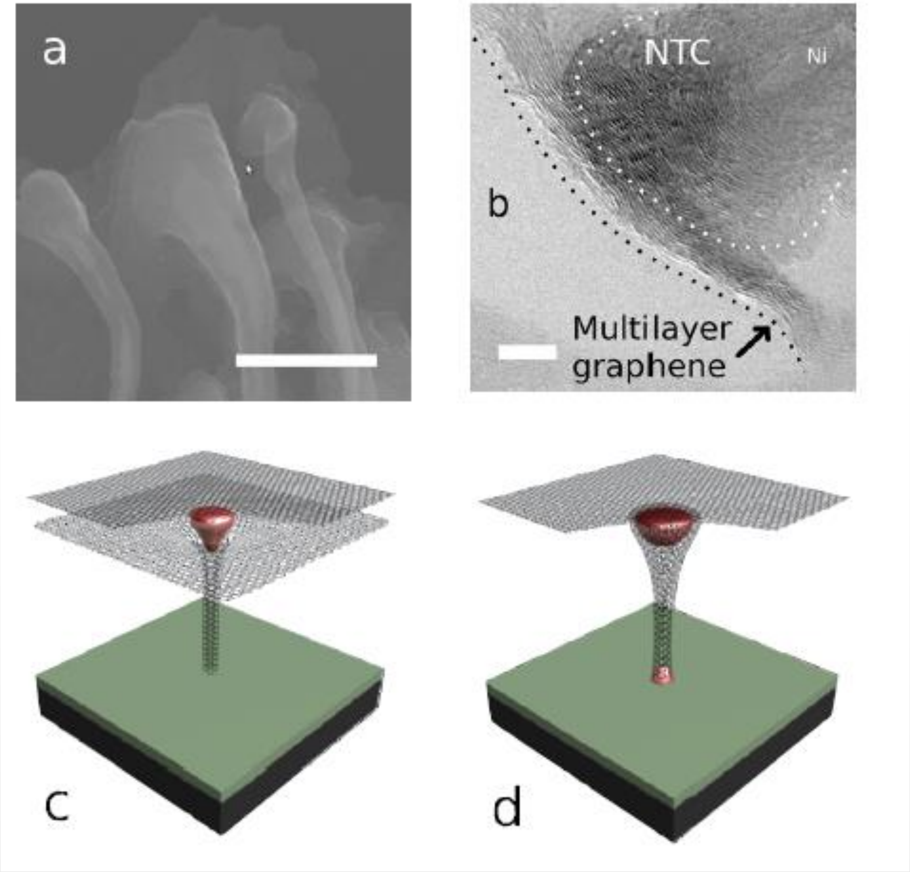


FIG. 1. Result of the CVD growth at 550 °C during 30 min. (a) Prior to growth, argon was flown at 30 Torr during 30 min. Propylene was then introduced at 30 Torr. (b) Propylene was introduced in the chamber without argon pretreatment. The scale bar is 1 μm in both images.



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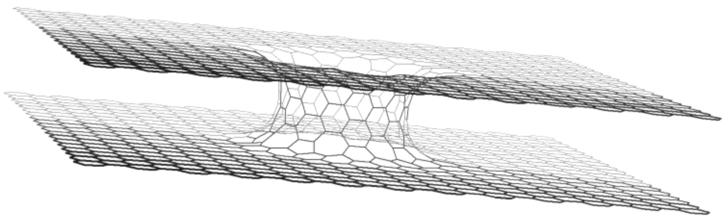
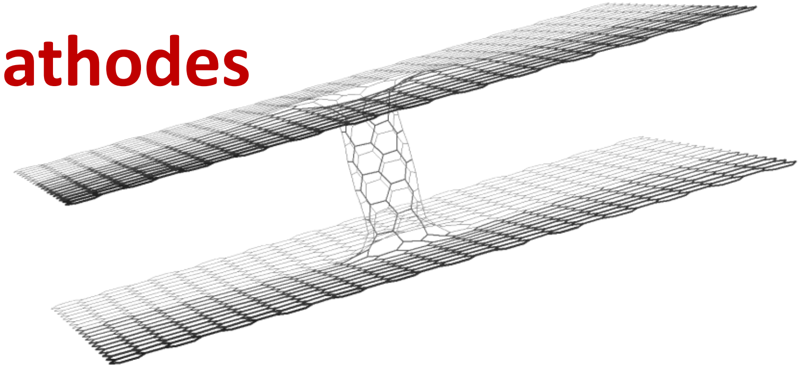
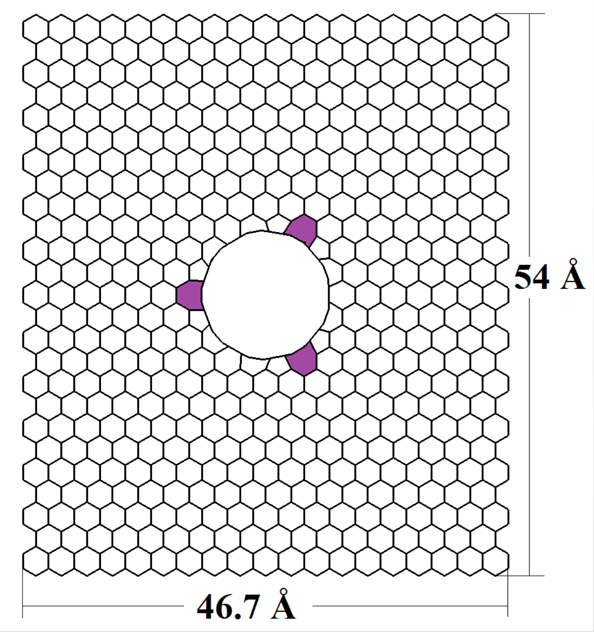
New composite materials for cold cathodes

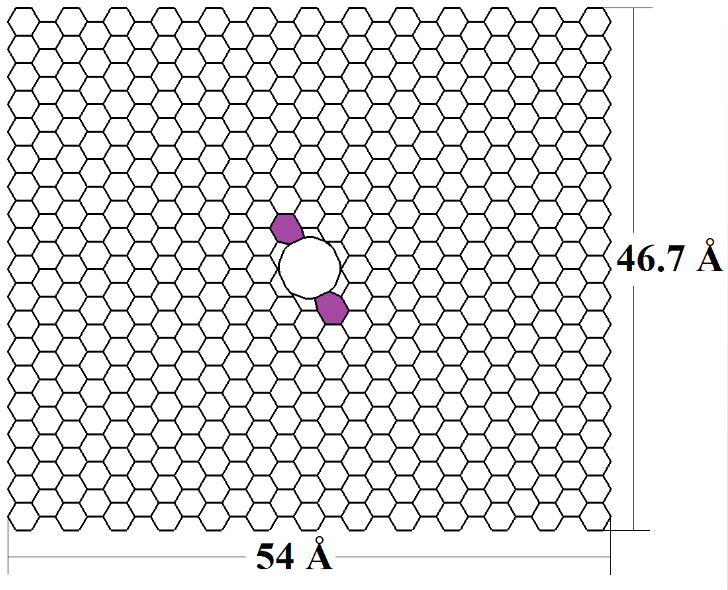


CNT -graphene composite . Tube in the composite has the diameter of 1.2 nm

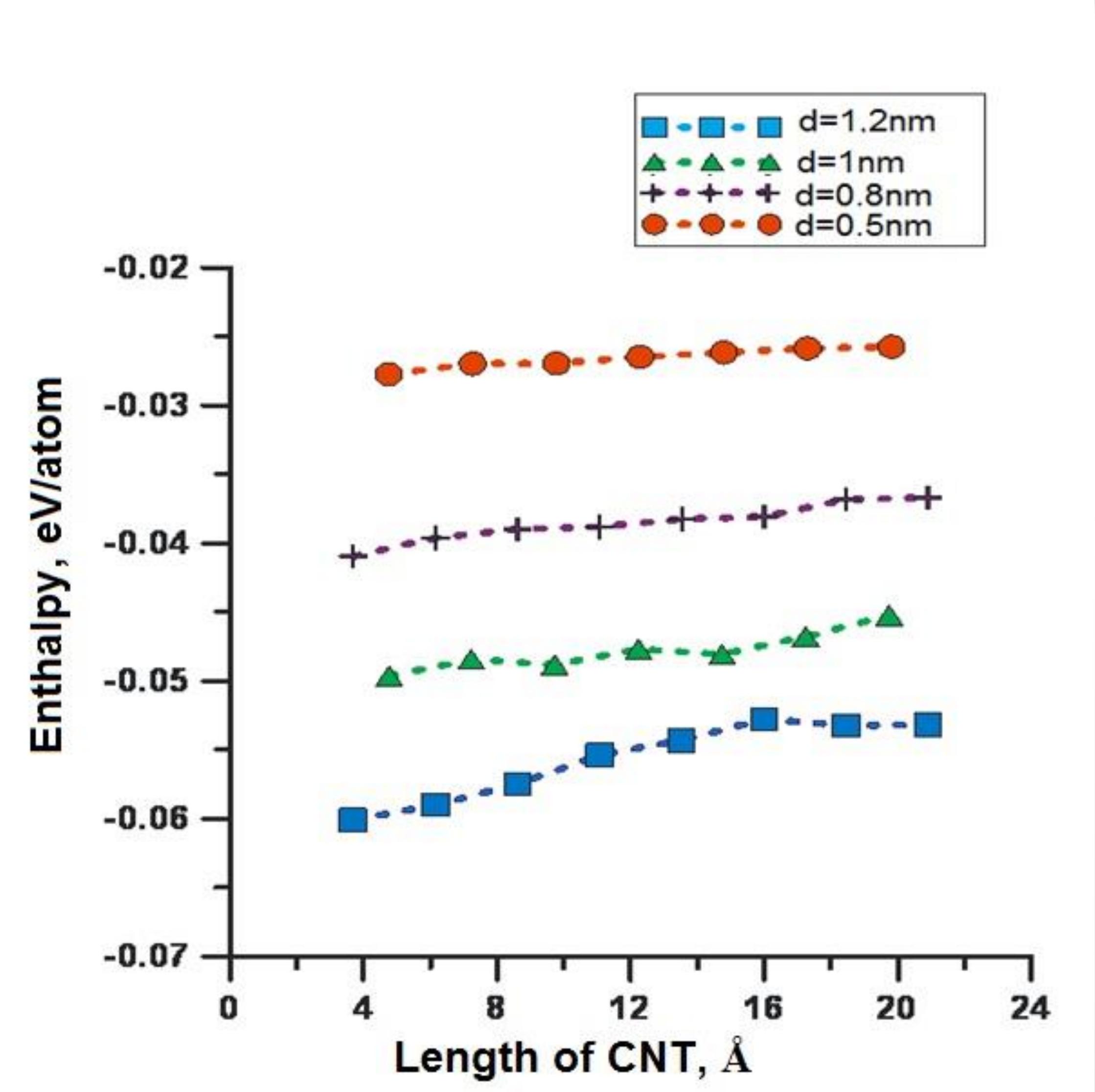


CNT-graphene composite. Tube in the composite has a diameter of 0.3 nm



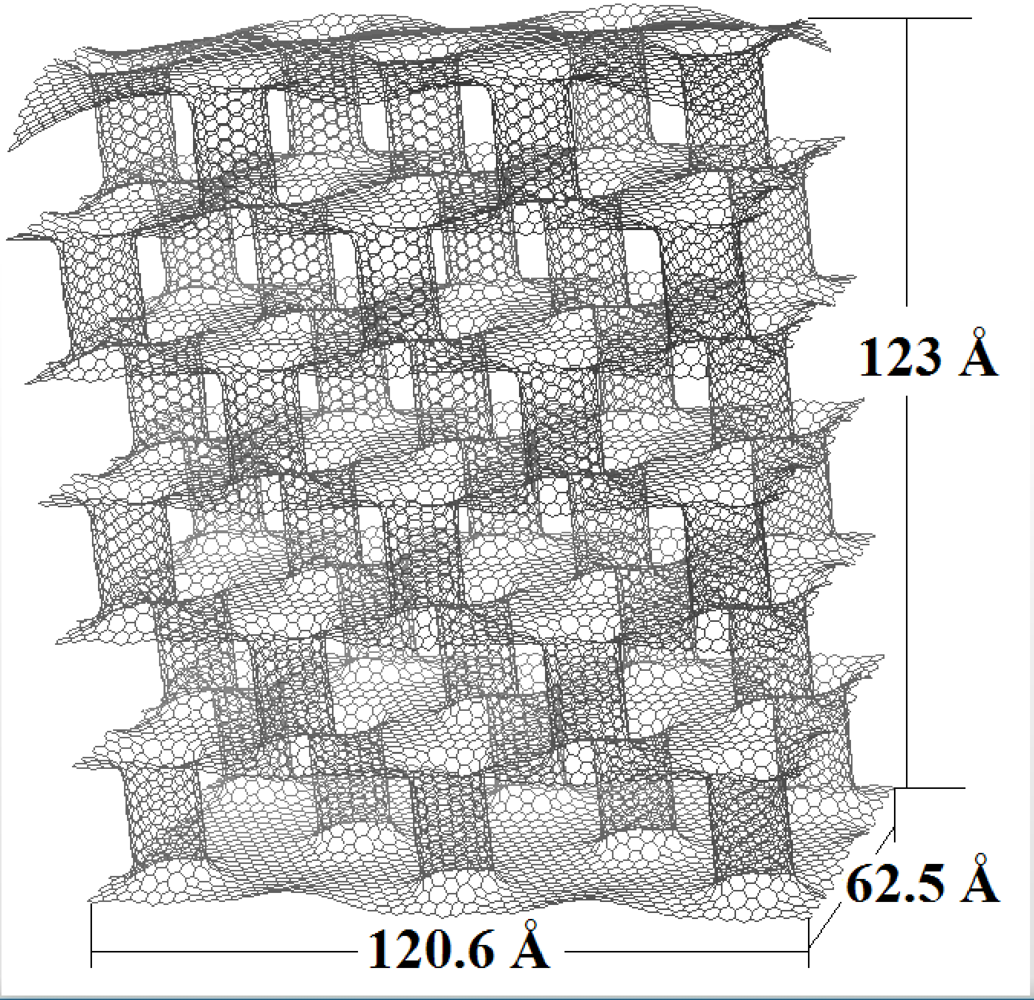


Region of defects in nanocomposites with the diameter of CNT 1.2 nm and 0.3 nm.

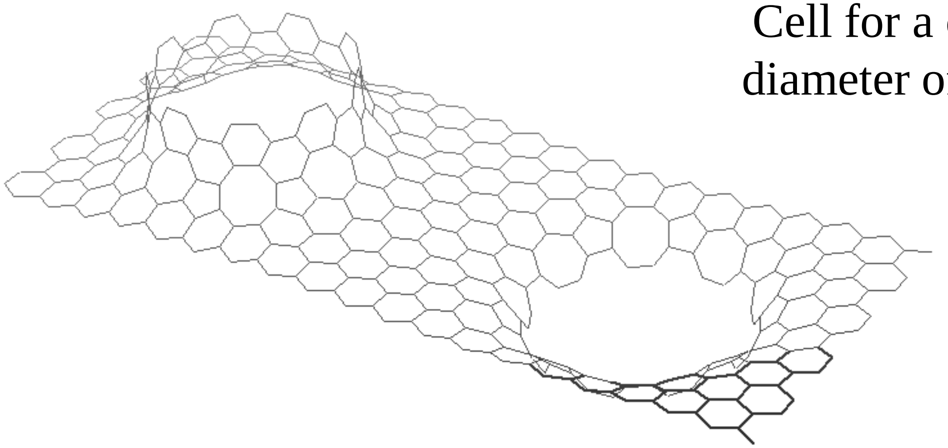


Dependence of the enthalpy on the length of the tubes

CNT/graphene composite. Diameter of tube in composite is equal to 1.21 nm, length of tube in composite is equal to 1.84 nm

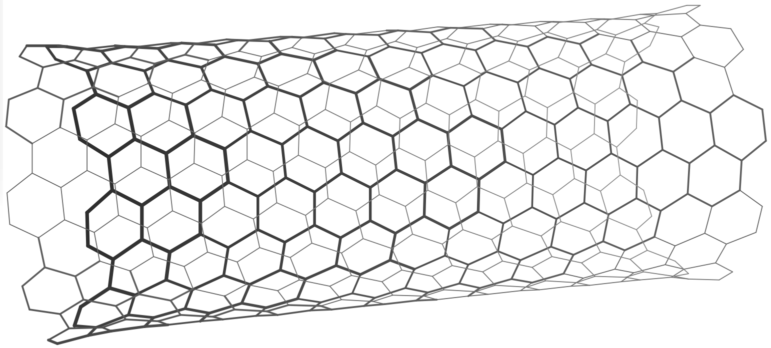


The total energy of the individual parts that make up the composite, eV	-201159.4
Energy of system, eV	-214036.1
Enthalpy, eV / atom	-0.45

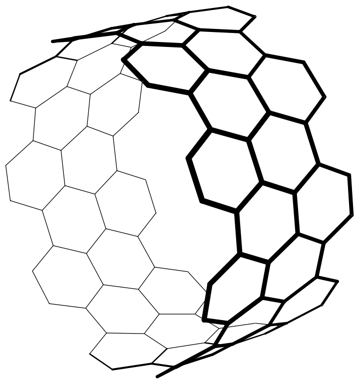


Cell for a composite with a tube diameter of 1,212 nm and length tube of 0,615 nm

The length of the nanotubes in the composite, nm	The diameter of nanotubes in the composite, nm
1,21	0,61
	0,86
	1,35
	1,84
	2,09



Tube with a diameter of 1.21 nm and a length of 3.07 nm



Elementary cell to create extended nanotubes

Extended CNT diameter 1.21 nm have:

Ionization potential: 6.6 eV

Energy gap: 0.69 eV

Table 1. Dependence of the ionization potential and the energy gap on the length of the tube. The diameter of the all tubes is equal to 1.21 nm

Length of the tubes in the composites, nm	Ionization potential, eV	Energy gap, eV
0.615	6.33	0.06
0.861	6.53	0.28
1.353	6.26	0.09
1.845	6.19	0.01
2.091	6.23	0.09

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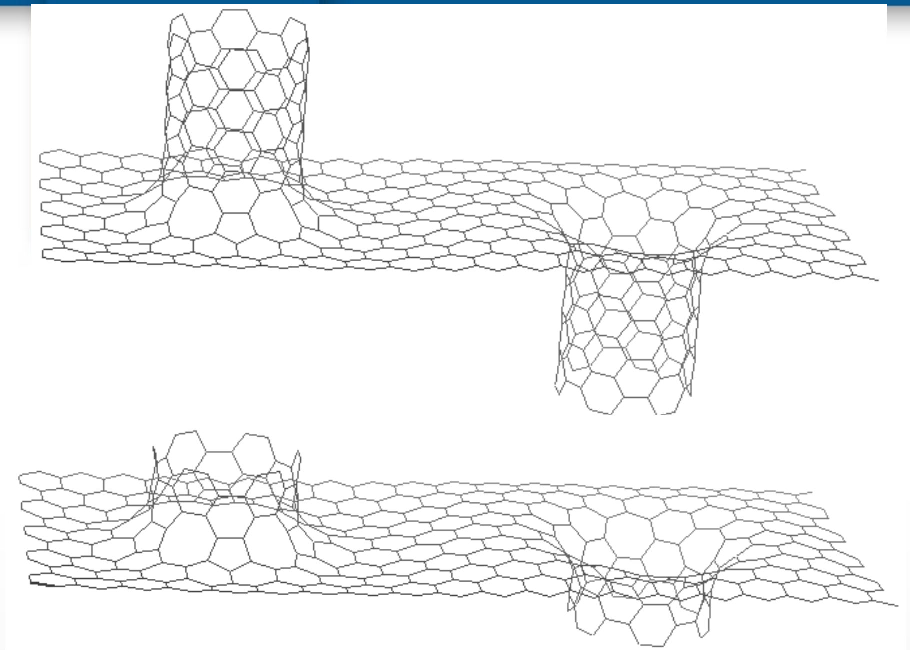
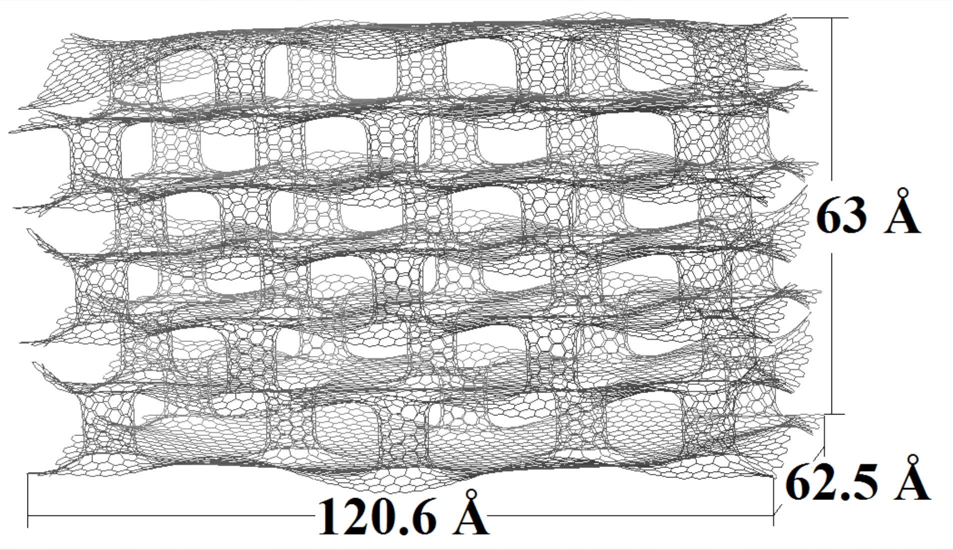
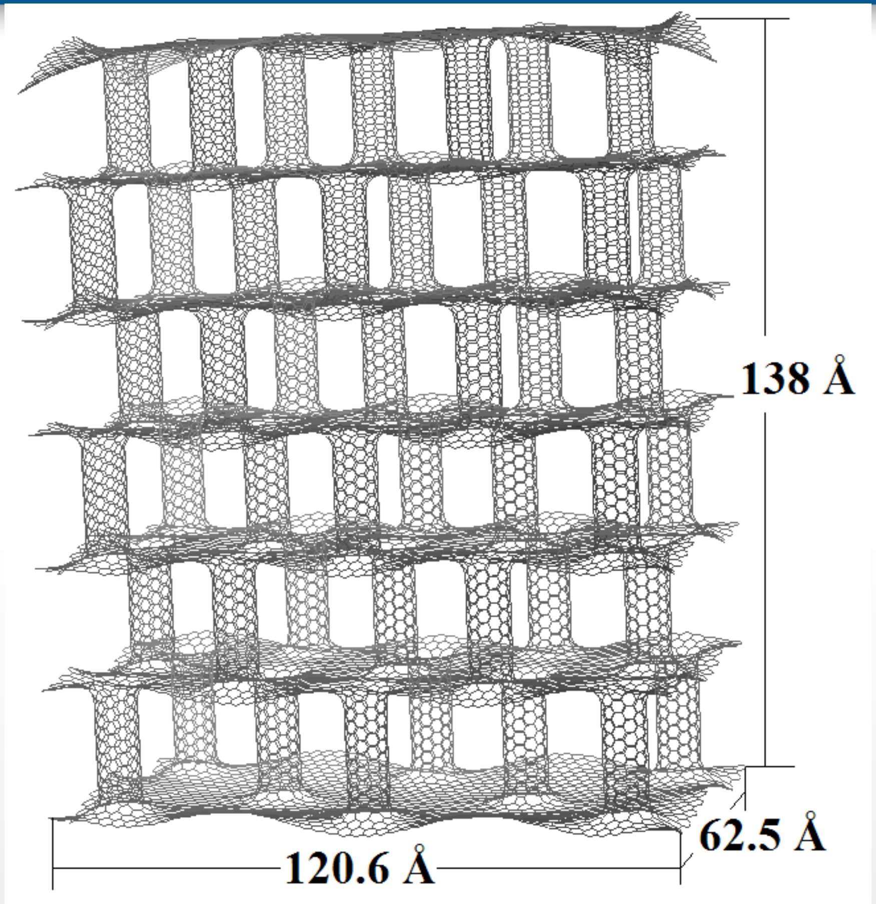






Examples of cells and composites for different lengths of tubes with the same diameter equal to 8.01 Å

Table 2. Dependence of the ionization potential and the energy gap on the length of the nanotubes in the composite, with its diameter of 0.801 nm.

The length of the tubes in the composites, nm	Ionization potential, eV	Energy gap, eV
0.369	6.73	0.06
0.861	6.2	0.02
1.353	6.21	0.05
1.845	6.16	0.08
2.091	6.19	0.02

Extended CNT diameter 0.801 nm have:
Ionization potential: 6.09 eV
Energy gap: 0.13 eV

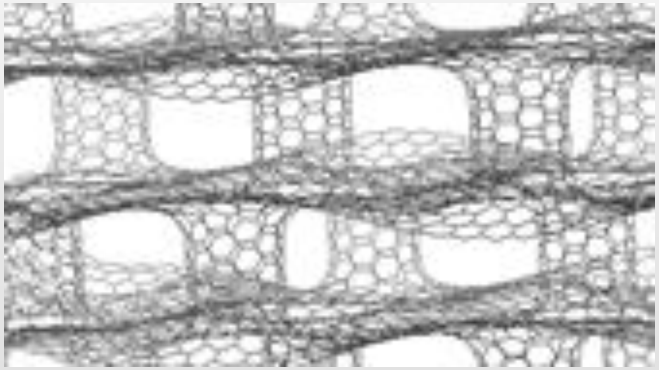


Table 3. Dependence of the ionization potential and the energy gap on the length of the nanotubes in the composite, with its diameter of 0.524 nm.

The length of the tubes in the composites, nm	Ionization potential, eV	Energy gap, eV
0.492	6.2	0.09
0.738	6.05	0.09
0.123	6.12	0.09
0.172	6.11	0.09
0.196	6.11	0.09

Extended CNT diameter 0.524 nm have:
Ionization potential: 6.71 eV
Energy gap: 0.71 eV

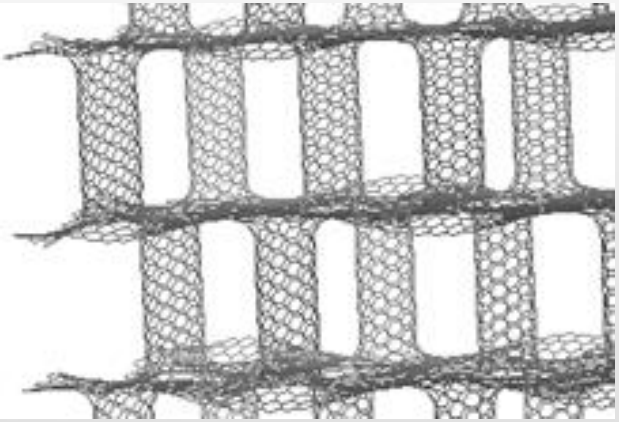
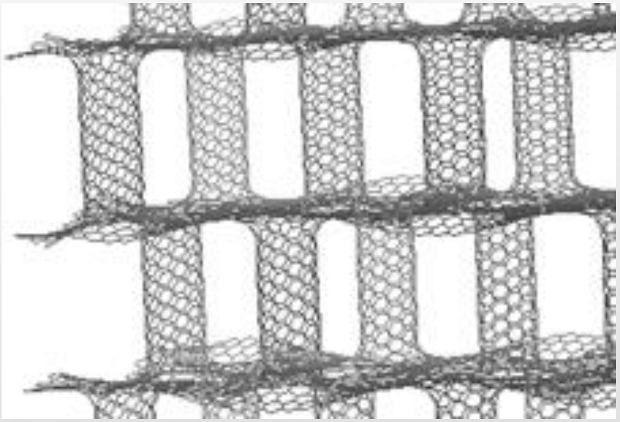
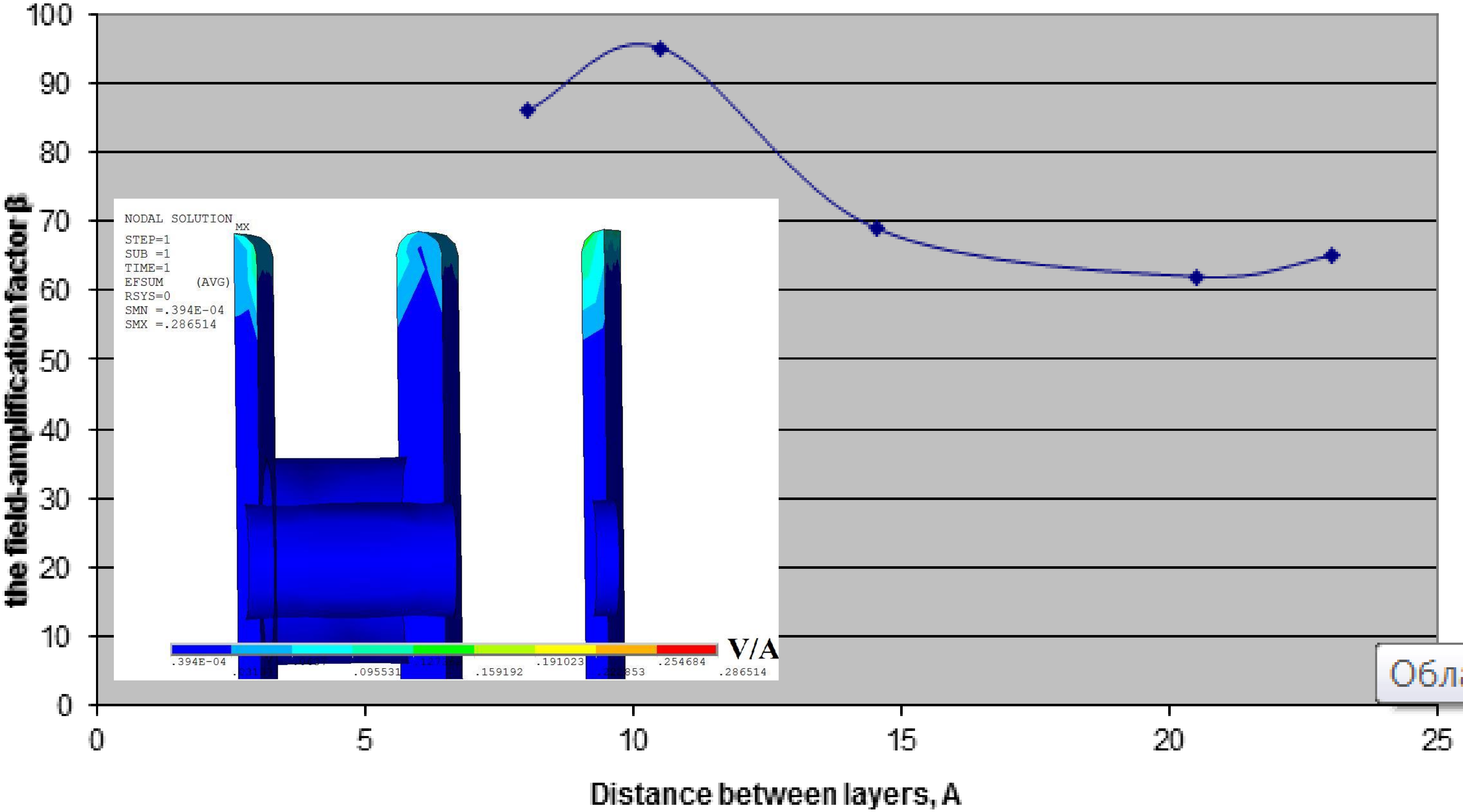


Table 4. Dependence of ionization potential and the energy gap on the distance between the carbon nanotubes in the composite.

The distance between the tubes, nm	Ionization potential, eV	Energy gap, eV
3.709	6.19	0.02
4.201	6.17	0.05
4.693	6.27	0.004
5.185	6.19	0.02
5.677	6.19	0.09



Dependence of amplification factor on the distance between the graphene sheets in the composite.



Thanks for attention!