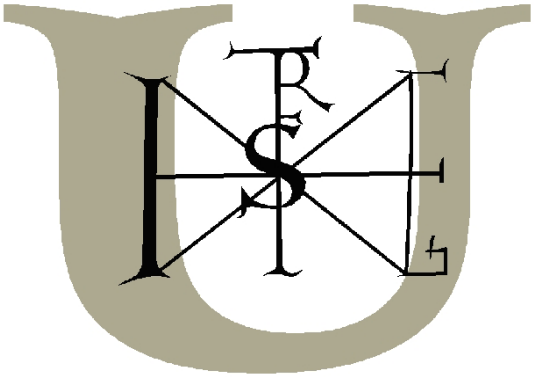

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TENSILE MODELLING OF MULTIDIMENSIONAL CARBON NANOTUBE STRUCTURES

Doctoral (Ph.D) dissertation thesis

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Affirmation of head of school Affirmation of supervisor

Content

1. Introduction, aims

1.1. Actuality of the theme

The execution of mechanical tests of different nano structures by experimental method is difficult and extremely expensive, entirely exact measuring could not be made till now. Concerning research works mechanical tests carried out with modelling and simulation means as well as nowadays by theoretical way have got significant importance.

In case of carbon nano structures the mechanical test are important in particular as the strongest chemical bonds to be in solids ensure the forces keeping together atoms in these structures, so the carbon nanostructures are the materials with the highest strength consequently.

The basis of theoretical, molecular mechanical tests, of carbon nanostructures is that the bonding forces among atoms are known. The atomic forces can be determined as gradient of potential function of bonding. Granting the atomic forces with formulas can be considered correct only order of magnitude at present. The calculated and estimated properties correspond to reality only order of magnitude, too.

The Y branches have got stressed importance between carbon nano structures. It can be solved with branches to derive the extremely high strength of carbon nanotubes to be in axis direction also into more directions of space generally. Because of electric behaviour also the Y branches are the most interesting. If industrial technology can exist to establish nano electronics based on carbon nano structures family then it is certain that some parts of fundamental building units get out of Y branches aggregation.

Different researchers found in technical literature got order of magnitude differences have got great importance during later application and manufacturing. The cause of calculations is the different use of the Brenner potential. It was mentioned that the researchers used the Brenner cutting function according to different standpoints. The aim was to avoid the breakpoint came into being on the force function or it to be to such lace where it did not fall into the calculation of maximum.

1.2 The aim

I set myself as an aim to realize with molecular mechanical simulations the mechanical tests of Y branches of carbon nanotube in this research work. I drew up the following tasks:

1. I develop a proper algorithm to the Y branches tensile simulation,
2. the formulas of atomic forces are only exact in order of magnitude till now because of this I plan analyse at first that the calculations made with such punctuality, hoe reliable the simulation results are, in which cases can they give real results,
3. I carry out runs to tensile- simulation on different Y branches,
4. I analyse the behaviour of Y branches exposed to tensile load, I examine the formation of bonding's, the failure process, I determine the weak points of structures,
5. I search connection, the topological characteristics how determine the failure process.

2. Material and method

2.1 Algorithm to the tensile- simulation of carbon nanostructures

I have developed a molecular mechanical algorithm to the tensile-simulation of carbon nanostructures. Setting out from the technical literature the basis of this algorithm is that I also calculate the atomic forces from the gradient of the potential function describing the chemical bondings. I choose the Brenner-potential function for this aim. As it was usual at energetic potential functions generally Brenner also gave the potential function (V_{ij}) (V_A) as the resultant of corresponding members of attractive and repulsing (V_R) effects to the **i** and **j** direct neighbour atom-pairs:

$$V_{ij}\left(r_{ij}\right) = V_R\left(r_{ij}\right) - \overline{B}_{ij} V_A\left(r_{ij}\right) \qquad (2.1.1.)$$

where $\mathbf{r_{ij}}$ – is the distance between **i** and **j** atoms. The attractive and the repulsing members are described with the following expressions:

$$V_R = \frac{D_e}{S-1} e^{-\sqrt{2S}\beta(r_{ij}-R)} f_{ij}\left(r_{ij}\right) \qquad (2.1.2.)$$

$$V_A = \frac{D_e S}{S-1} e^{-\sqrt{2/S}\beta(r_{ij}-R)} f_{ij}\left(r_{ij}\right) \qquad (2.1.3.)$$

The parameters: De, S, β and R are the constants concerning the material, or are physical constants in the formulas describing the attractive and repulsing members (2.1.2) and (2.1.3)

The fij (rij) so called cutting function role is to limit the interactions to within a given action radius:

$$f_{ij}(r_{ij}) = \begin{cases} 1, & r_{ij} < R_1 \\ \left[1 + \cos\left(\frac{r_{ij}-R_1}{R_2-R_1}\pi\right)\right] / 2, & R_1 \le r_{ij} \le R_2 \\ 0, & r_{ij} > R_2 \end{cases} \qquad (2.1.4.)$$

The cutting effect is effective between R_1 and R_2 from 1 to 0 reduces. Brenner suggests R_1=1,7 Å value as the starting point of the cutting effect, avoiding with this the surroundings of the standstill equilibrium position (r_{ij}=1,42 Å), and suggests the cutting to R_2=2 Å value.

The B_{ij} is that constant in the (2.1.1) formula with the help of which not only the **i** and j atomic pair is taken into account, but the direct neighbours of these, as well as the bonding angles:

$$B_{ij} = \left[1 + \sum_{k(\neq i,j)} G(\theta_{ijk}) f_{ik}(r_{ik})\right]^{-\delta} \qquad (2.1.5.)$$

where:

- the summation has to be made to the direct neighbours of **i** and **j** atoms,
- Θijk is the bonding between **i** and **j** atoms, as well as the bonding angle between the **i** and **k** atoms,
- the following connection concerns to taking into account the bonding angles:
-

$$G(\Theta_{ijk}) = a_0\left[1 + \frac{c_0^2}{d_0^2} - \frac{c_0^2}{d_0^2 + (1+\cos\Theta_{ijk})^2}\right] \qquad (2.1.6.)$$

The (2.1.5) and (2.1.6) connections also have got constants: δ, a_0, c_0 and d_0, choosing of which can be from Brenner tables (Brenner 1990).

Finally, as the local surroundings of **i** and **j** atoms can be different, Brenner suggests a calculated correction constant as average of these to the (2.1.1) formula:

$$\overline{B}_{ij} = (B_{ij} + B_{ji})/2 \qquad (2.1.7.)$$

Several authors observed that cutting function of Brenner formulas have got extremely strong effect to the calculation of atomic forces: there is a break point on the potential function at $r_{ij}=R_1$ atomic distance. At R_1 place on the gradient of the potential function, thus on the function determining the atomic force there is also a break point which attend here also with sudden incline change, **Figure 1/a**.

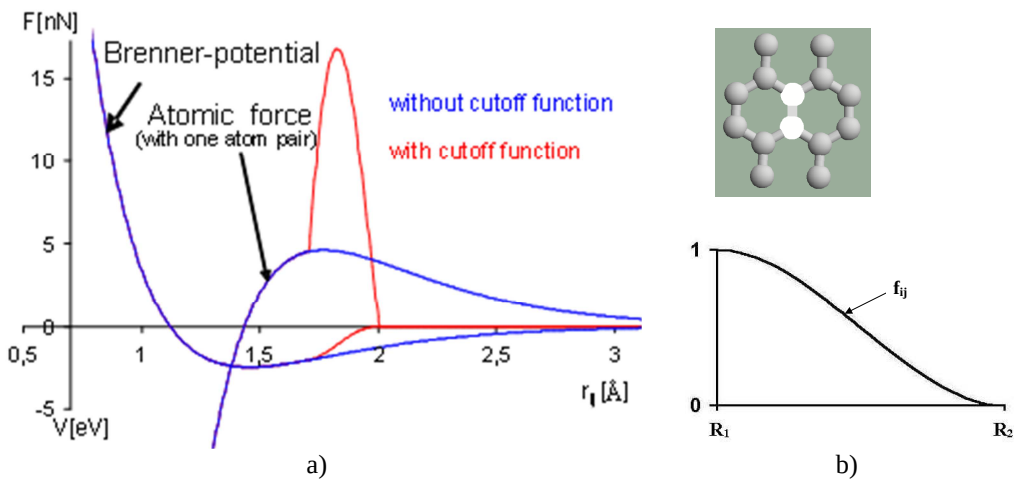


Figure 1/a: The effect of the cutting function to the Brenner potential and its derivative, to the function determining the atomic force. Both diagrams concern to one direct neighbouring atom-pair.
b: The course of the cutting function $f_{ij}(r_{ij})$ between R_1 and R_2

2.2 The algorithm

I present the steps of algorithm in the **Figure 2**:

- The input of the algorithm is the table of the carbon atoms' (x, y, z) coordinates from the model of the carbon nano-structure examined.
- Before starting there is a need to define the extreme position, fixed places in the structure.
- One step of the tensile- simulation, the distance between fixation starts increasing run with 0,01 Angstrom)
- The calculation of the equilibrium place between atoms of the fixed places to be increased distance belongs to the given step. This calculation is an iteration which tends to search the minimum of a multivariate function (the Brenner potential-function) according to mathematics. I used for a gradient method to minimum – searching.
- During suitable steps the behaviour of the structure can be followed in the tensile process. I solved the demonstration on the graphic surface on molecular modelling system the DTMM (Desktop Molecular Modeller).

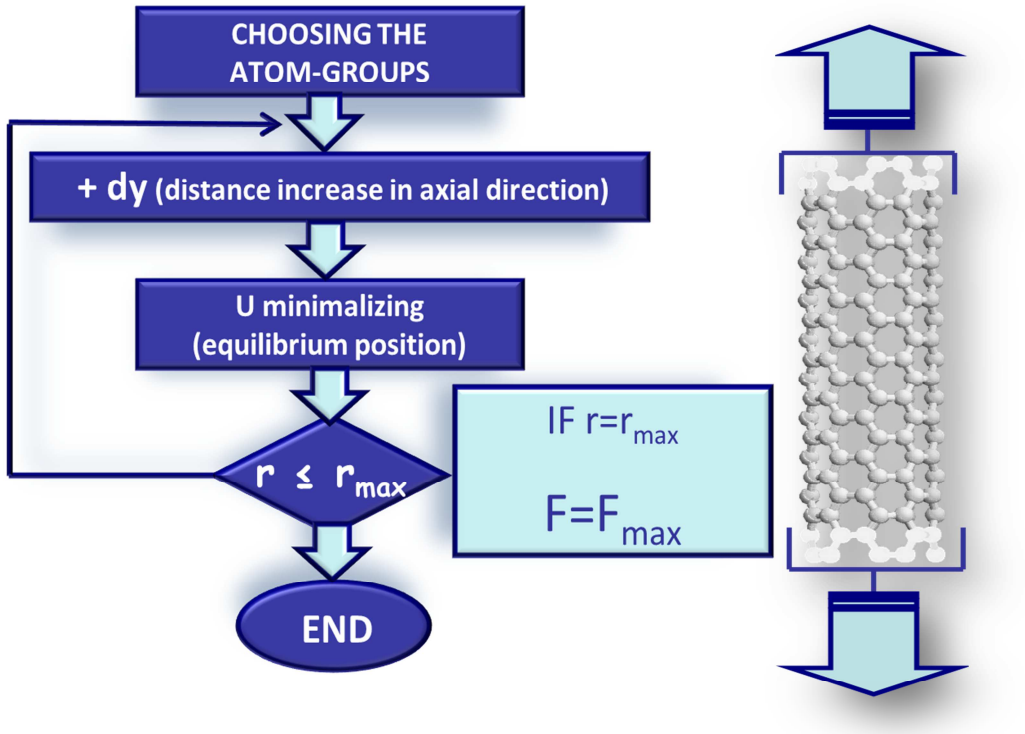
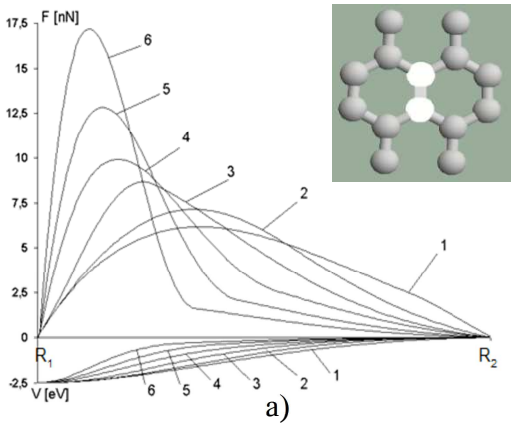


Figure 2: The process-figure, where the process of tensile-simulation can be seen, the demonstration on a model respectively

2.3 The applicability of tensile-simulation algorithm.

I examined seven different cases to the change of the energetic potential-function and the atomic force-curve running off. I discarded the f_{ij} (r_{ij}) function from the Brenner formulas namely I interpreted to "1" value identically in the first case.

I chose six different R_T, f_r value-pairs to the f_{ij} (r_{ij}) correction function in the six following cases and I developed six different atomic force-functions whit this. I present these six different cases in **Figure 3**. The potential-function running off can be seen on the diagram in the part under the horizontal axis in the six different cases. The derivative of the potential-function that is the atomic force-function is presented on the part over the horizontal axis in six different cases. The differences are smaller on the potential-functions however the variation of the free parameters causes more drastical changes on the atomic force-functions in the correction-function. Thus the question is: the change of the atomic force-function what changes will cause in the behaviour of carbon nano-structure?



a)

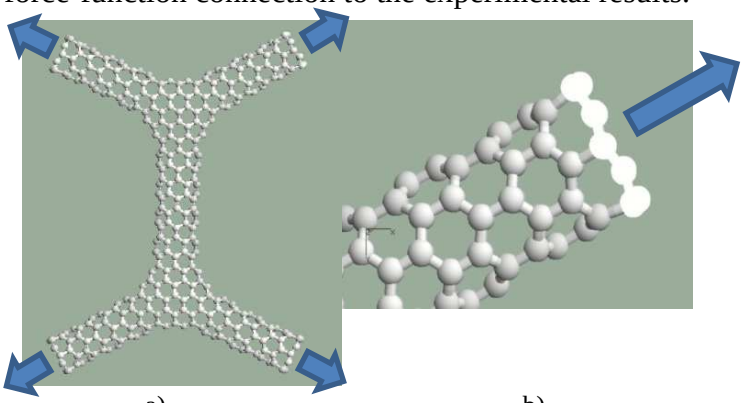
Number	R_T	f_T
1	1.7	0.8
2	1.9	0.2
3	1.8	0.15
4	2.0	0.25
5	2.0	0.54
6	2.3	0.23

b)

Figure3.a/ The energetic potential-function is shown below the horizontal axis, above the horizontal axis the atomic force-function is shown, calculated between two neighbouring (marhed white) atoms.
b./ The free parameters of the correction function

I carried out seven tensile simulations using seven different atomic force-functions with algorithm mentioned previously. I made the runnings off to the appearance of failure. I always used the loads the axis direction on the structures (**Figure 4**)

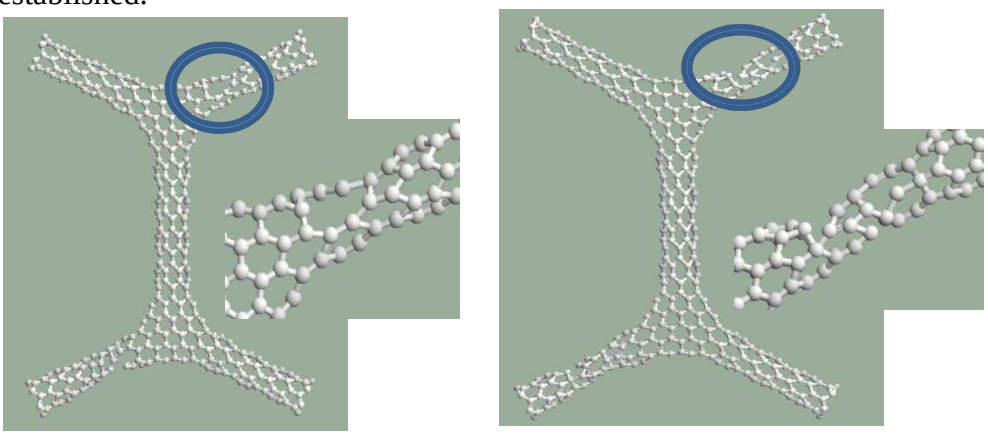
I calculated with the original Brenner-potential in the first case, where I didn't take into account the cutting function or the effect of the correction function, that is its value was identical "1". I searched that failed place, where the structure destructed failed during the tensile-simulation process. After that I determined the effect of the correction function by using the six different value-pairs of the free parameters. I wanted to examine that determining the weak point how exact is needed with this simulation series of the atomic force-function connection to the experimental results.



a) b)

Figure 4. a./ The starting structure consists of 580 atoms
4. b./ The tensile is axial at all branches

I present the result of the running off with Brenner–potential examined as well as the result of the running off with modifyed correction function. I finished the running off when the destruction (failure) place could be established.



a) b)

Figure 5. a./ The structure examined with original Brenner–potential and destructed
b./ Example to the simulation result carried out with the modifyed correction function.

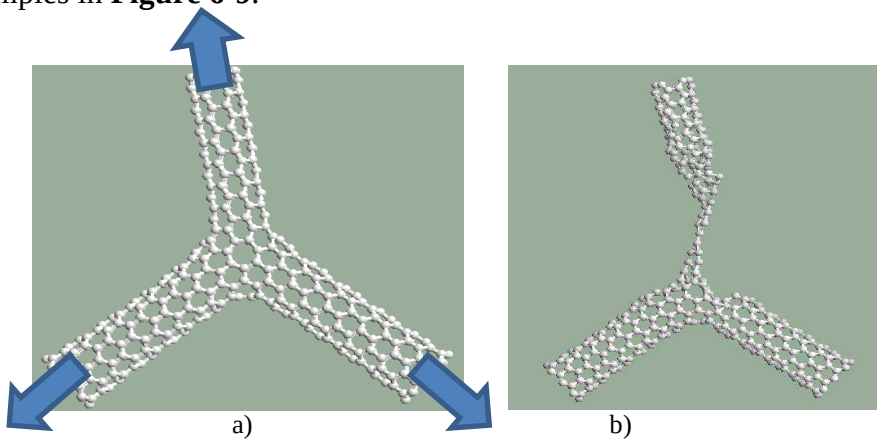
Finishing the running off I have established that the different correction functions resulted force – functions with different intensities, but these didn't effect the final result. My aim proved true that I can estimate the behaviour of structures with my algorithm. Looking for the weak cross-section doesn't depend on the intensity of load.

Desprite that the running off of the atomic force-function originated from the gradient of potential-function is not yet defined exatly outside the surroundings of equlibrium situation, the atomic force-function is still suitable to examine the behaviour of a given carbon nano-structure against tensile load, to search the weak point of the structure, to examine the failure process.

3. Results

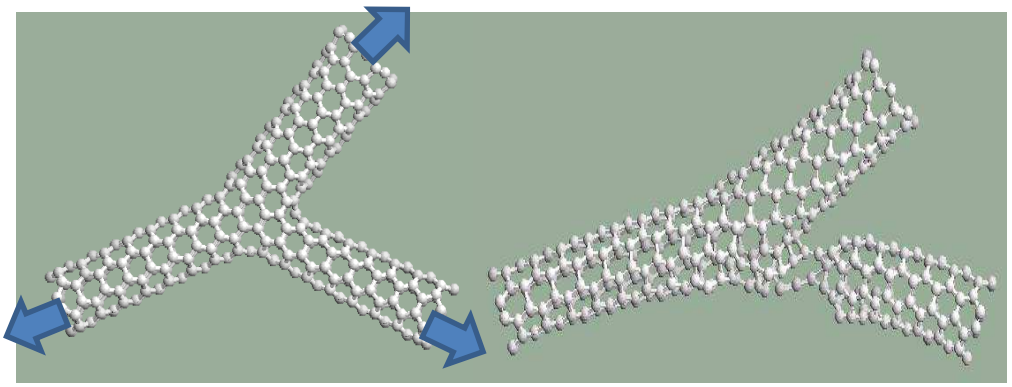
3.1. Investigations of carbon nanotube branch

I investigated the behaviour of different nanotube structures against tensile load in my dissertation. The basic elements form which different structures can be made are Y branches. These branches are built from nanotubes. Not only hexagonal rings can be found in the modal points of branches as in the nanotubes but heptagon rings too. Depending on that how are set these heptagon rings the topology of Y branch its structure will be different, they behave differently against of mechanical load. I show examples in **Figure 6-9**.



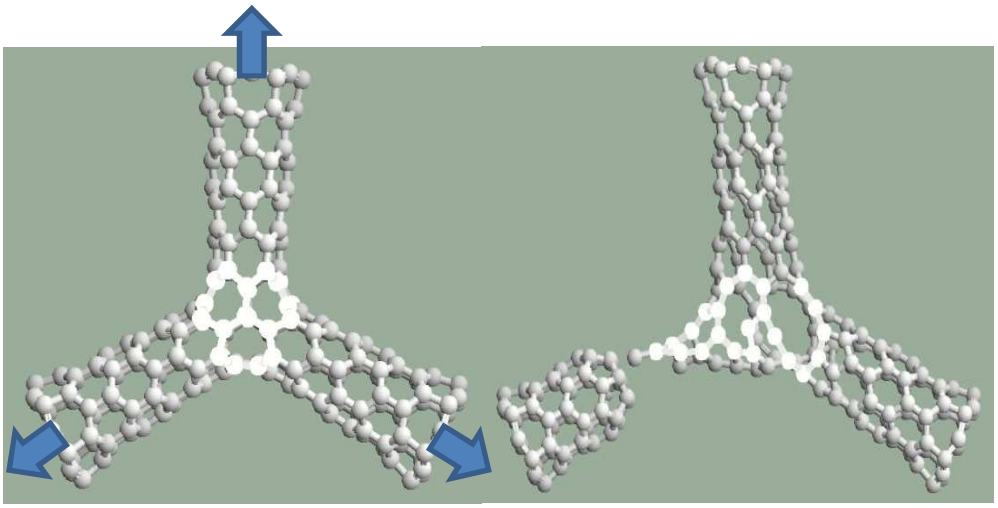
a) b)

Figure 6. a./ Asymmetric branch (lower two branches: 8,0 nanotube, upper branch: 4,4) marking the tensile directions.
b./ The failed structure



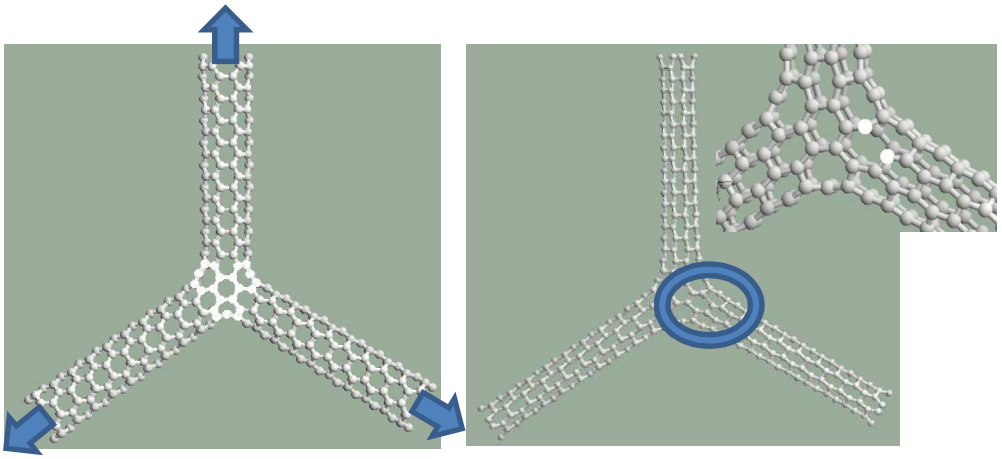
a) b)

Figure 7. a./ Asymmetric branch (lower two branches: 4,4 nanotube, upper branch: 8.0 marking the tensile directions.
b./ The failed structure



a) b)

Figure 8. a./ Symmetric Y branch (6,0) from nanotubes, marking the tensile directions.
b./ The broken structure



a) b)

Figure 9. a./ Y branch made from armchair type nanotube with loads
b./ The primary failure spot.

After finishing the simulations mentioned before I established that the Y branches can be put into two main groups concenring the behaviour against mechanical load. One is the asymmetric group building from different nanotubes. The other great group is the symmetric Y branches, where the type the diameter and length are built from identical nanotubes. The branches deform with the same way and measure to the effect of axial load in this group in case of both the zigzag and the armchair types nanotubes.

3.2. The elasticity of carbon nanotube

I investigated the extreme mechanical properties in my dissertation mentioned in the technical literature too. On of these is the extra elasticity which is more than 1TPa. I loaded one armchair and one zigzag type nanotube in the direction of axis till itt failed with my algorithm to get knowledge that the nanotubes how will behave during tensile process. I observed one-one hexagon ring during tensile process **(Figure 10.)** I show the results of the zigzag type nanotube in diagrams in **Figure 11.** I show the results of the armchair type nanotube in **Figure 12.**

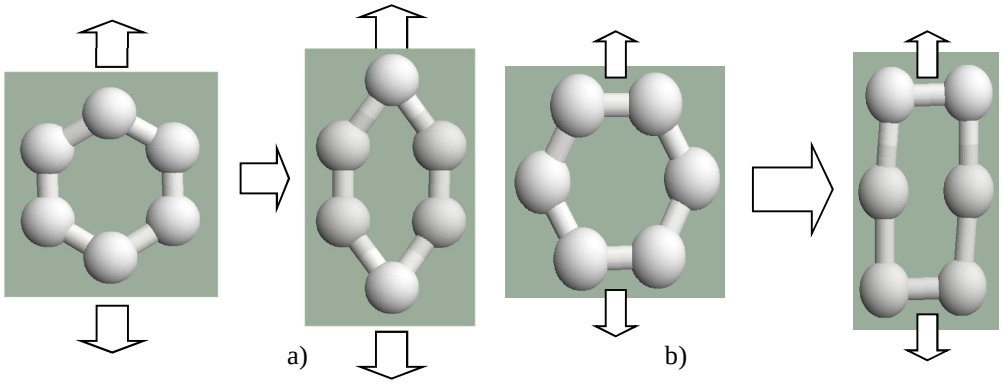


Figure 10. a./ The observed building element of the zigzag type nanotube
b./ The observed building element of the armchair type nanotube

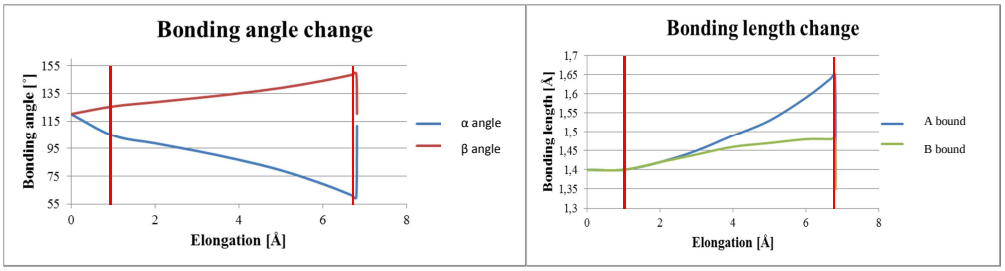


Figure 11. The change of the loading angle and bonding length of the zigzag type nanotube.

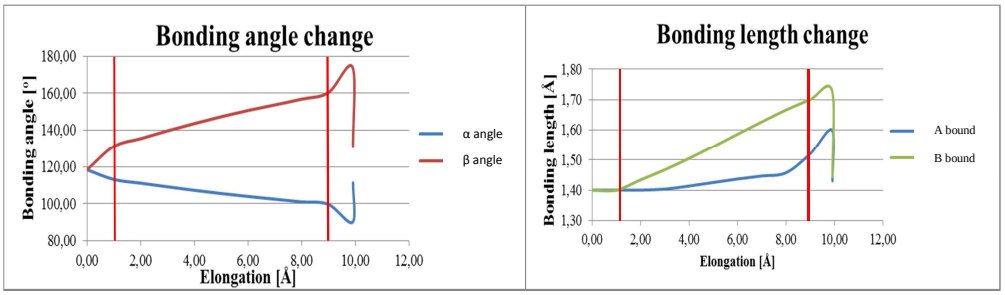
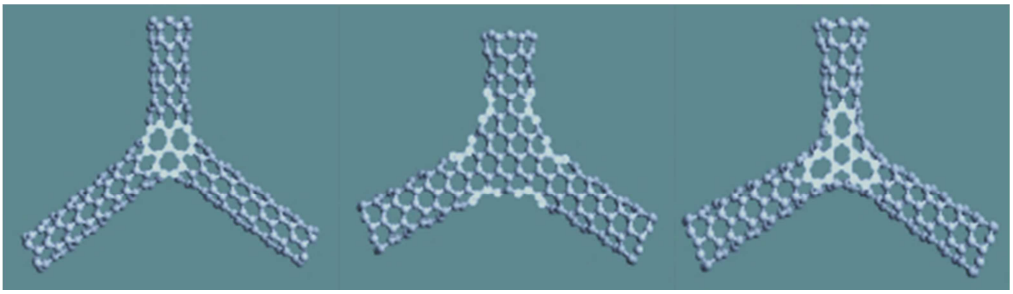


Figure 12. The change of the bonding angle and bonding length of the armchair type nanotube

I established from the running off results, that in both cases three parts can be distingvished. Between 0-1 Å there is a sleep changing part at the bonding angles, while the bonding length diagram doesn't on the next part both diagrams change uniformly as far as another sleep part. This spot is different at the two types. This is that spot to be exceeded the nanotube loses its elasticity. Before this spot the nanotube recovers it original dimension if the load is eliminated, afterwards doesn't recover. I establsihed that the bonding angles turn into the load direction sooner and after heir length start to grow.

3.3. Tensile diagram of the carbon nanotube Y branch

I discussed the elasticity of nanotubes previously. Now I make known the other extreme high mechanical characteristic of nanotubes, their outstanding tensile strength. This characteristic can be extended to every direction of the space with the help of Y branches. I established during modelling of branches that the structure construction influences the weak spot of the structure. I investigated how is influenced the mechanical load capacity if the structure is modified. The objects of my investigation were also Y branches, I made two modifications only from structure standpoint. One is a topological transfromation, the other is an atom take in **(Figure 13.)**.



a) b) c)

Figure 13. a./ Base structure
b./ Transformed structure
c./ Final result of modifying with atom take in.

I loaded the structures with the same simulated load in all cases. The modifyed correction function was altered with $R_t = 1,9$; $f_t = 0,2$ value pairs in all cases. I analysed and interpreted the maximum loads used in the technical literature. I presented the results in a diagram **(Figure 14.)**

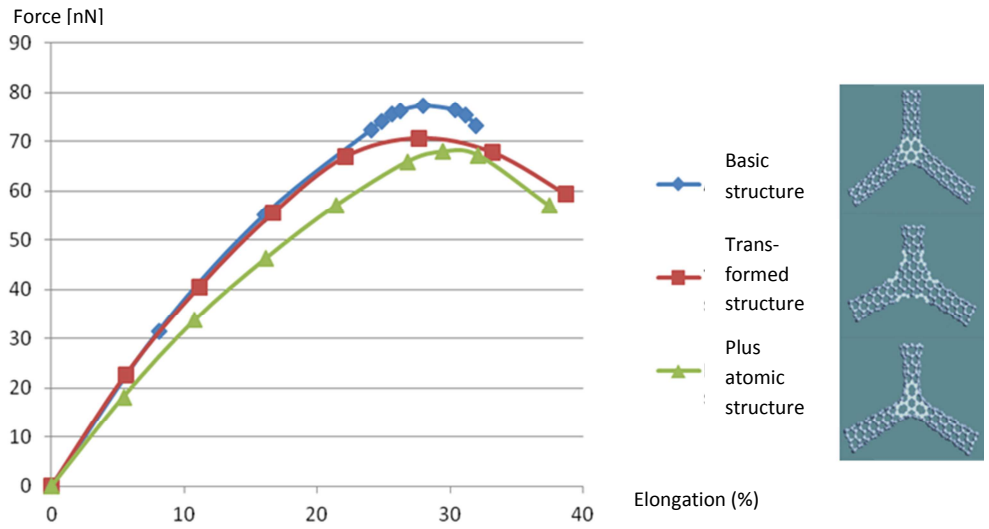


Figure 14. The three tensile – diagrams

I calculated the tensile strength (Belytschko, 2002) of all three structures besides the results got.

$$\sigma_{\max} = \frac{F_{\max}}{\pi D t} \cdot 4$$

where:

F_{max} – is the maximum force, that can be read from the diagram
D – is the nanotube diameter
t – is distance between grafen planes

The tensile strength of the nanotube structure in the base case:

$$\sigma_{\max} = \frac{F_{\max}}{\pi D t} \cdot 4 = \frac{77,1939 \cdot 10^{-9} \cdot 4}{\pi \cdot 4,701 \cdot 10^{-10} \cdot 3,4 \cdot 10^{-10}} = 153,73\, GPa$$

The tensile strength of the structure in the transformed case:

$$\sigma_{\max} = \frac{F_{\max}}{\pi D t} \cdot 4 = \frac{70,7001 \cdot 10^{-9} \cdot 4}{\pi \cdot 4,701 \cdot 10^{-10} \cdot 3,4 \cdot 10^{-10}} = 140,80\, GPa$$

The tensile strenght of the structure in the modified with plus atom case

$$\sigma_{\max} = \frac{F_{\max}}{\pi D t} \cdot 4 = \frac{68,0040 \cdot 10^{-9} \cdot 4}{\pi \cdot 4,701 \cdot 10^{-10} \cdot 3,4 \cdot 10^{-10}} = 135,43\, GPa$$

I summed up my statements connected with the branches in one table. I introduce a force factor to the filling in the table, by which I give symbol to the nanotube types to be in the structures and by which I determine their loadabilities. An order of rank can be set with this number among different nanotube types. This factor is the ψ which I determined with the following method.

$$\Psi = \frac{F_{sz}}{F_{kk}}$$

where:

F_{sz}: is the maximum force effecting the structure in the moment of failure to be parallel with the nanotube axis

F_{kk}: the force taking place in the critical (failed) bonding to the effect of the maximum force in the structure, naturally this is the same in all cases, as to put on end to the bonding between two carbon atoms needs always the same force (13,453 nN).

The maximum load effecting the structure at te calculations always has to be parallel with the axis of the setting nanotube, the structure is always loaded with axial forces. At the same time not any projection of the force rising in the critical bonding has not to be calculated as the maximum of the force between two atoms is interpreted to all directions of spherical surface.

Table 1. comparing the load capacity of nanotubes

	ψ_{basic}	$\psi_{transformed}$	ψ_{plus}
$Y_{zig-zag}$	5,73	5,25	5,05
$Y_{armchair}$	4,21	-	-

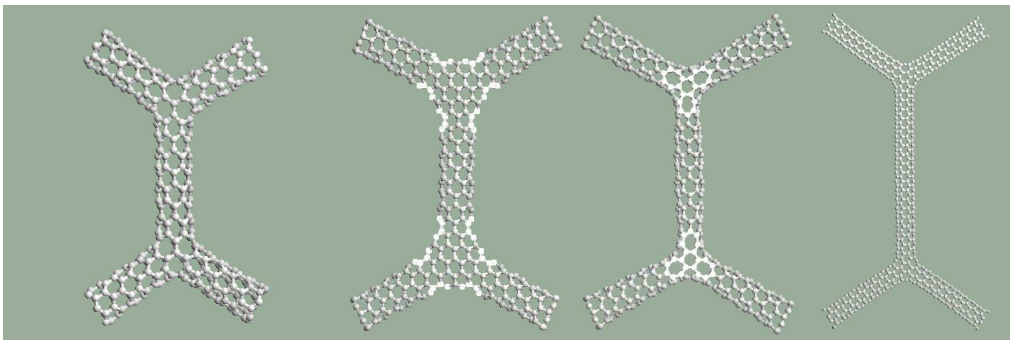
ψ_{basic} : Value concerning the base structure
$\psi_{transformed}$: Value concerning the transformed structure
ψ_{plus} : Value concerning the plus structure

I established from data of the table that the nanotubes setting up the structure have got different load capacity. Hereby the armchair type nanotubes will always be weaker at the asymmetric Y branches. This derives from that the topological modifications of the zigzag type nanotubes are also stronger than the branch set up form armchair type nanotubes.

3.4. Carbon nanotube structures

The following step towards the networks if these Y barnches are fitted so if the structures to is put periodically side by side then a network develops.

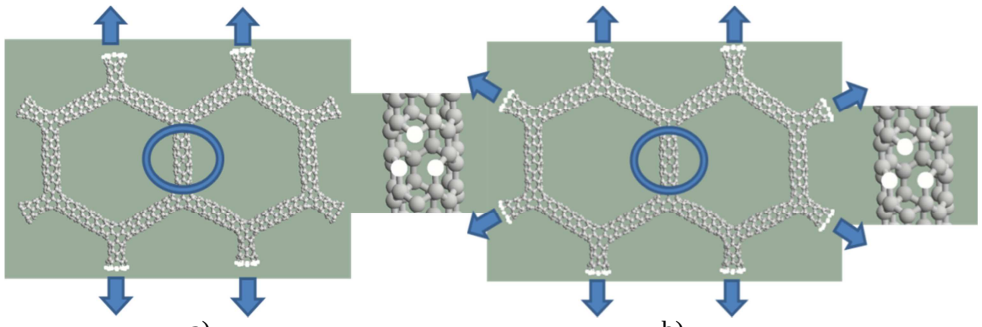
I show these models in **Figure 15**. I investigated four types structures in this case, too. The aim of simulations here is also to find the weak spot of the structure.



a) b) c) d)

Figure 15. a./ Network element set up from base model; **b./** Transformed model **c./** Reinforced with atom take in; **d./** Armchair type network part

After runnings off I established that in all cases the weak spot of the structures can be found beside the heptagon rings. I still make on step towards the networks in the followings and I investigate the structure with multidirectional loads. I show the structure investigated in **Figure 16**. I put the loads to the structure either parallel or from more directions simulated with this the different mechanical loads. I also modified the structures becaues I produced vacancies (unoccupied places, where there are no atoms) inside them.

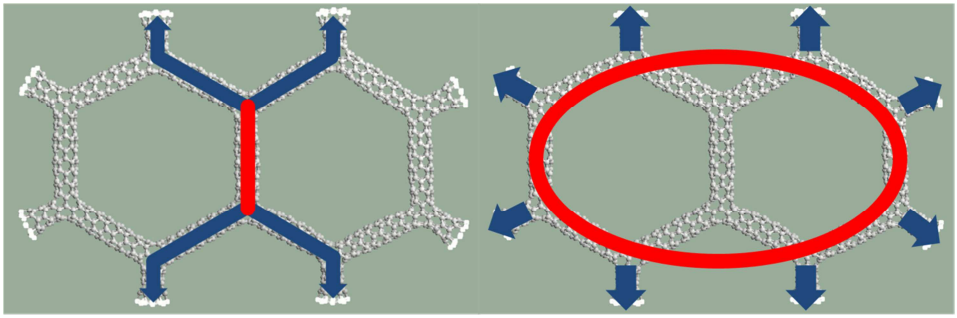


a) b)

Figure 16. Part of the nanotube network, stressing the vacancy. **a./** With parallel load; **b./** With multidirectional load

I made two establishings from the results of simulations. The first is that the internal stresses developed so that the failure happened on the middle

nanotube part on the intact structure and on the structure with vacancy, too. In the second case when the load was multidirectional then my structure divided into two parts concerning the load-bearing. To one internal part, where the stresses show that this part of the structure hasn't got such load than the other part. The other part is a ring to be found on the border of the structure. The failure will happen on this ring. I also established here thath the primary failures can be found beside the heptagon rings in both cases. I show the two cases results in **Figure 17.** where I emphasized with red colour those places where the internal stress is high and the failure happened.



a) b)

Figure 17. The structures with load and the internal stresses high values are emphasized with red colour.
a./ In case of parallel load; **b./** In case of multidirectional load

3.5. Tensile modelling of carbon nanotube networks

I reached in the last part of my dissertation to carry out the tensile simulation of a whole network. I expected the final result of the simulation based on my previously mentioned establishings. I loaded my network from more directions but each load was unit and axial. I show these loads and structure in **Figure 18**.

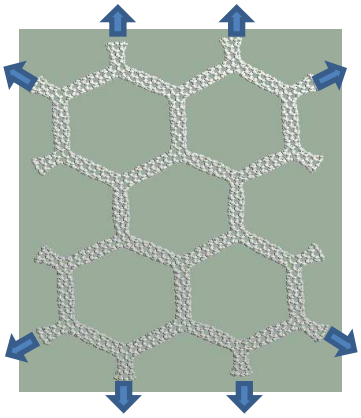


Figure 18. Carbon nanotube network with loads

After finishing my investigations I established that this network behaved similarly with the structures till now. I observed here also the dissection ensued to the effect of the multidirectional load mentioned in the previous chapter. The internal structure and the external ring also developed. During my dissertation I established in all cases that the failure spots on the structure can always be found in the neighbourhood of heptagon rings. I proved this with the investigation of the network, too. I show my result in **Figure 19.** and **Figure 20**.

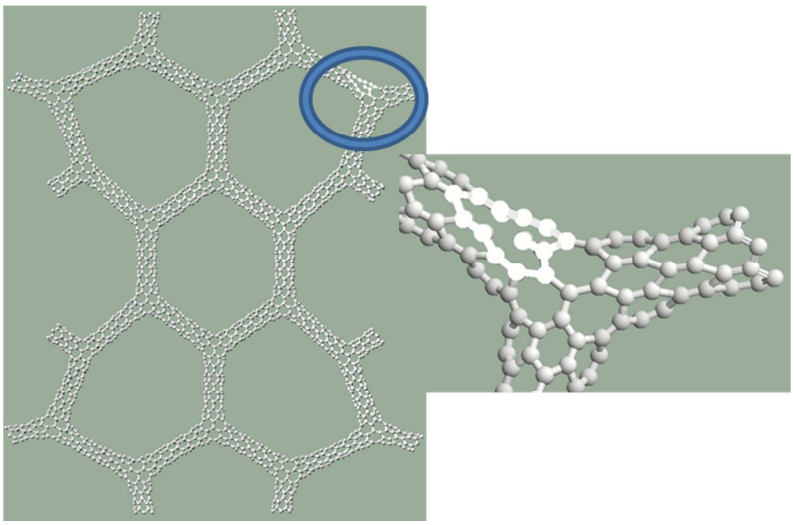


Figure 19. The primary failure spot on the network

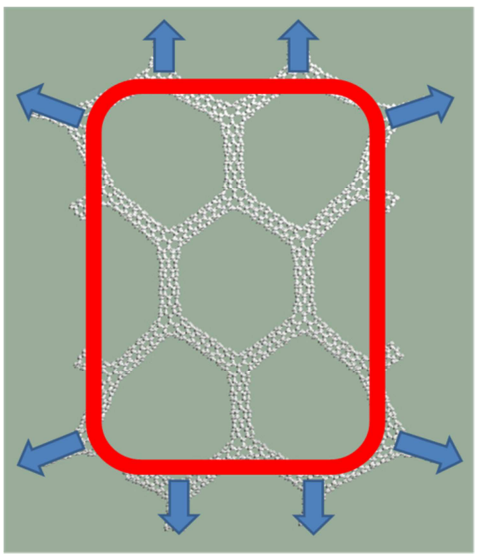


Figure 20. The ring to be found on the network on which the failure spots appeared.

4. New scientific results

No. 1. Thesis: I showed with the molecular mechanical simulation of carbon nano structures that the determination of the structure weak cross-section remains exact during modifying with the correction function of the Brenner-potencial function. Therefore this statement is important became the energetic potential functions of chemical bondings are defined exatly only still in the neighbourhood of equilibrium place nowdays.

No. 2. Thesis: I showed with the simulations of load tests of straight carbon tubes that he high elasticity can be explained beside the cange of bond length with the characteristic changes of bond angles, with the turning into the load direction of the bondings, too. The tensile simulations show that turning of bondings starts sooner as long as the change of bond lenght develops only later.

No. 3. Thesis: I established with using molecular mechanical simulation that the failure always happened at the armchair type nanotubes at the asymmetric Y branches containing the chosen zigzag and armchair type nanotubes having the smallest diameter difference.

No. 4. Thesis: I showed with the running off series of molcular mechanical tensile – simulations that the heptagon rings determine exatly the weak cross-section to be found in the structure of carbon nanotube Y branches. The weakest place that is the primary failures are in the direct neighbourhood of heptagon rings in a carbon nano structure.

No. 5. Thesis: I established that after the structural modifications (transfer of heptagon rings) of the Y branches containing indentical carbon nanotubes and after molecular mechanical investigations that there is no considerable difference in mechanical characteristic between branches having different modal point structures but having the same diameter tubes.

No. 6. Thesis: I showed that by changing the topological structure in the modal point of Y branch, namely by moving the heptagon rings the weak spot also displaces.

No. 7. Thesis: I established during molecular mechanical investigations of larger networks that structures behaviour in two ways to the effect of tensile load. Due to parallel load the stresses rising in the structure destruct the structure on that nanotube part in the neighbourhood of heptagon rings where the forces are concentrated. The structure loaded from more directions splits to two parts, one internal part where the stresses are lower and to and external ring which takes the great part of the load hereby the failure spots will be in this part.

5. Conclusions and proposals

The algorithm worked out by me estimates the characteristic of sturcures against mechanical load based on expermental calculation method. The specimen of experiment test carried out in laboratory couldn't be determined till now. It can be conlcuded to the characteristic of nanotube that the typ can be calculated form the diameter can be taken out respectively. Therefore from this the use of algorithm can be used to estimate the characteristic of structures with constructed nanotubes having determined type in advance.

During investigationg nanotube structures it was proved unambigously that due to the topological set of armchair type nanotubes (there are such bonds int he structure which are axial) this type is the weakest. I came to the conclusion investigationg the mechanical characteristic of structures that the position of heptagon rings to be found inevitably in the structure don't influence the mechanical load capacity considering the whole structure. However they influence certianly the weak spot of the structure such way that the primary failure happened in the direct neighbourhood of the heptagon rings.

Concerning the elasticity of nanotubes I established that the elongation of a nanotube what is made up of. The deformation consists of two main parts.

The atomic bonds to be found in the nanotube turn into the direction of load in the first part until the atoms approaching to one another don't reach that place in the structure where the attracting and repelling effects to each other still compensate one another. The departion of atoms from each other, namely the bond length starts increasing, happens in the second part.

The behaviour of the carbon nano structure against the mechanical load can't be similar to the macro materials. The set of networks can be divided to two parts. In every case there is an internal part of the body and there is a shell structure that surrounds this body and which takes greater part of the load. The failure sports develop on this shell.

The development of the sicence will make it possible to produce suitable structure to the explicity set target from nanotubes. In this case these structure will be designed in such way as whatever tool or jig used today. The calculation method of my algorithm can be the basis for a later developed 3D-al design software. The structures built from carbon nanotubes will be possible to make models with this software to load with different mechanical loads respectively. The load capacity will be possible to estimate and the set of structure will be possible to modify for the sake of the aim.

6. Summary

Y branching in carbon nanotubes is of paramount importance because of at least two features:

- As Y branches contain 3 joint tube elements, they may become the basic units of molecular electronics provided that a proper industrial production technology is found. It has been proved in the literature that in the case of carbon nanostructures molecular size transistors may consist of Y branches.
- The extremely high strength of carbon nanotubes is due to the very strong covalent bonds of graphene. They exhibit this extremely high strength only in the axial direction. Carbon nanotube branching can be a structural unit which, organized into a network might allow the extension of extreme strength into various spatial directions.

This work aims at the investigation of the latter problem, the mechanical properties of carbon nanotube Y branches and of networks consisting of them. Tensile simulations were performed by molecular mechanical algorithm first on carbon nanotube Y branches then on smaller or larger network structures consisting of Y branches. The basis of the algorithm was that the atomic force can be determined as the gradient of an energetic potential function describing the chemical bonds. The Brenner potential was chosen for the calculations. The Brenner potential is an empirical equation, but the fitting to the experimental data is proven only in the immediate neighborhood of the equilibrium structure. In the tensile simulations, however, parts of the potential function farther from the equilibrium position are also needed. In such cases however, only an order of magnitude agreement with the experimental data can be achieved nowadays. In the first part of my work therefore I had to investigate what kind of problems can be solved realistically with the presently available precision of the molecular mechanical algorithm. I found that it is possible to study realistically the failure process of the given carbon nanostructure, it is possible to identify the weak sites and it is possible to compare the failure of various structures.

Tensile simulations of Y branches of various structures have been performed. It was found that the failure is determined by the topology of the structures, weak spots occurred in the immediate neighborhood of 7-membered rings.

During the tensile simulations the changes in bond length and bond angle values were monitored. It was found that in the first stage of the process the bonds turn towards the load direction, bonds become elongated only later, these two phenomena together explain the extreme elasticity of carbon nanostructures.

7. Publications in connection with the theme of doctoral dissertation

Lectorated articles in foreign language:

Pataki, T., Zsoldos, I., Molecular mechanics simulations on carbon nanotube Y-junctions, Fullerens, Nanotubes and Carbon Nanostructures, 2014 (under review) (IF.: 0.76*)

Pataki, T., Kári-Horváth, A. , Szakál, Z. , Drawing process of carbon nanotube "Y" junctions, MECHANICAL ENGINEERING LETTERS: R AND D : RESEARCH AND DEVELOPMENT 10, 2013 pp. 140-144.

Pataki, T., Kári-Horváth A., Carbon nanostructures behaviour on the strength of different atomic force function, MECHANICAL ENGINEERING LETTERS: R AND D : RESEARCH AND DEVELOPMENT 9, 2013 pp. 112-117.

Pataki, T., Zsoldos, I., Loading simulations of carbon nanotube junctions; MATERIALS SCIENCE FORUM 729: 2012 pp. 162-168.

Pataki, T., Szakál, Z., The symmetrical behaviour of carbon nanotubes junctions, SUSTAINABLE CONSTRUCTION & DESIGN 2, 2011 pp. 128-133.

Zsoldos, I., Kakuk, Gy., **Pataki, T.,** Theoretical Models for Some Possible Elements of Carbon Nanotubes Networks; MECHANICAL ENGINEERING LETTERS: R AND D : RESEARCH AND DEVELOPMENT 3, 2009 pp. 120-132.

Pataki, T., Kakuk, Gy., Zsoldos I., Dynamical Behaviour of Carbon Nanotube, DIAMOND AND RELATED MATERIALS 15, 2006 pp. 288-291., (IF.:1,935)

Lectorated articles in Hungarian language:

Pataki T., Nanoszerkezetek Szakítóvizsgálatának Szimulációja; GÉP 2011/1-2, 2011 oo. 64-66.

Pataki T., Szakál Z., Polimerek erősítésére alkalmas szén nanoszerlezetek mechanikai teherbírásának vizsgálata, Műanyag és Gumi 2014/3, 2014 oo. 112-114.

Pataki T., Molekuláris szimulációk szén nanoszerkezeteken, Anyagok világa 2014/3-4, 2014 8 o. (megjelenés alatt)

Pataki T., Kári-Horváth A., Műanyag alkatrészek erősítésének módszerei szén nanoszerkezetekkel, GÉP 2014/3, 2014 oo. 38-41.