THE SYMMETRICAL BEHAVIOUR OF CARBON NANOTUBES JUNCTIONS

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Abstract We have been developing a mathematical model to predict the mechanical behaviour of carbon nanotubes under loads having different types of structures. In this paper we would like to introduce the behaviour of carbon nanotubes junctions under tensile strain. With an example we display that in a structure the junctions are very important intensifier component. We show the difference between the symmetrical and non-symmetrical junctions. We give an answer, which junctions are symmetrical and which ones are not symmetrical. Under tensile strain the "Y" junctions have different behaviour, if they are symmetric, or not.

Keywords nanotube, mechanical strain, symmetrical, simulation

1 INTRODUCTION

We have found two kinds of examples to the tensile tests of carbon nanotubes in the technical literature. In both cases samples fixed between the needles of microscopes were pulled by atomic force, in one case nanotube bunches [1], in another case multiwall carbon nanotube [2-3]. Beside of test difficulties problem was also the unknown exact structure of the samples tested, it couldn't be known that the measuring concerned for what exactly.

Several research fellows tried to determine the stress-strain diagrams by theoretical way [4-8]. The basic of the methods are always that the atomic forces can be determined as a derivatum of the potential function determining the energy of chemical bounding. The empirical Brenner-potential is used [9] for this now days nearly every-where. The reseats got however differed fairly from time to time there were also differences withes more scales for example in the values of tensile strength calculated [4-8]. The differences derived from the different applications of the Brenner-formulas. Several research fellows noticed namely that as long as the Brenner-formulas can be applied excellently to determine the state of equilibrium at the calculation of atomic forces there are already problems as on the derivate function there are break point and sudden incline changes which can not be explained with the behaviour of chemical bondings. First of all eluding by different ways of this problem caused the great differences at between strength calculated with the Brenner-potential. The best solution to this problem was given by eliminating mathematically the break point the sudden incline changes on the derivate formulas so that in the meantime it remained unchanged the possibility of looking for the equilibrium too. [10]

We have produced a computer program for the simulation algorithm of carbon nanotube structures tensile test in this paper to be able to run in case of great numbers of atoms. We made possible to determine the basic strength properties first of all for nanotube junctions [11-15] and networks [16-18] recommended as never carbon nanostructures by according to newest researches. That is important because in case of carbon nanostructures one of the most interesting characteristic is the high strength and the similarly unusual interesting electric behaviour [19-20].

2 SIMULATION ALGORITHM OF TENSILE TEST

As we calculate also the bonding forces between atoms as derivate of energetic potential function of chemical bondings we think necessary to make known the Brenner- formulas [9]. In this way the energetic potential is described with a rejecting (V_R) and an attractive (V_A) member between i-atom and j-atom to be in r_{ij}-distance from each other:

$$V\left(r_{ij}\right)=V_R\left(r_{ij}\right)-\overline{B}_{ij}V_A\left(r_{ij}\right) \tag{1}$$

where the members are given with the help of D_eS, β and R material factors.

$$V_R = \frac{D_e}{S-1} e^{-\sqrt{2S}\beta(r-R)} f_{ij}\left(r_{ij}\right) \qquad \text{és} \qquad V_A = \frac{D_e S}{S-1} e^{-\sqrt{2/S}\beta(r-R)} f_{ij}\left(r_{ij}\right) \tag{2}$$

The f_{ij} correction function is a formula given by mathematic polynomes. It has got twofold role: partly cuts the attractive and rejecting effects outside a range (rather long) given partly because of its parametric shape the formulas can be matched to measuring results, both functions show their effects at departing from the equilibrium. [10] it was solved by introducing this that there are no break points and sudden incline changes on the derivative of the Brenner-formulas.

It is taken into account the effect of local surroundings of atoms (first and second coordination sphere) and the different angles of bondings with the help of B_{ij} -factor:

$$B_{ij} = \left[1 + \sum_{k(\neq i,j)} G(\theta_{ijk}) f_{ik}(r_{ik})\right]^{-\delta} \tag{3}$$

where Θ_{ijk} is the angle of i-j and k-bondings, G given with a_0, c_0, d_0 material factors respectively:

$$G(\Theta) = a_0\left[1 + \frac{c_0^2}{d_0^2} - \frac{c_0^2}{d_0^2 + (1+\cos\Theta)^2}\right] \tag{4}$$

The factor in (1) formula:

$$\overline{B}_{ij} = \left(B_{ij} + B_{ji}\right)/2 \tag{5}$$

The steps of simulation algorithm of tensile test:

We have developed a computer program for the algorithm:

1. Giving the carbon nano-structure with the Table of appropriate point coordinates of atoms, unloaded, static condition.
2. Moving the atoms to be in the place of load in the load direction with small distance. (The displacement degree is so small it doesn't disturb the equilibrium calculations of the next step.)
3. Calculation of the new equilibrium (minimizing the Brenner-formula): confirming the atoms to be in the place of fixation and displaced in the previous step, the atoms between them are relaxed until to be calculated the equilibrium.
4. Calculation of bonding forces.
5. Repeating the previous three steps until the structure is damaged or niptures (if certain bonding in the structure reaches critical bond length, which is 1.7 Å).
6. Naturally it is sufficient to calculate the bonding forces at the weakest place (cross section) as this place however will be knows only during pulling because the forces can be expediently calculated from the tables put down after the steps, too. Finally we represent the resultant of bonding forces added vectorial at the weakest cross section in the function of elongation and this will be the tensile-test diagram.

After carrying out the chechings needed we started out research work by running the algorithm on a nanotube-structure. The aim of the research work is to carry out tensile-tests of carbon nano-structures with a lot of atoms mentioned in the introduction by the new simulation means. This structure is a Y-junction which branches are built up from zig-zag type nano-tubes in this case. Here we could determine that the angular arragement between branches is 120^0. We show the snaps of pulling-simulation in Figure 1. On the left Figure we show a basic starting structure. In the middle already the axial pulled structure can be seen. On the right Figure we displayed the moment before damage. The most loaded bonding in this structure reaches the critical bond-length at this moment (1,7A). (Figure 2.)

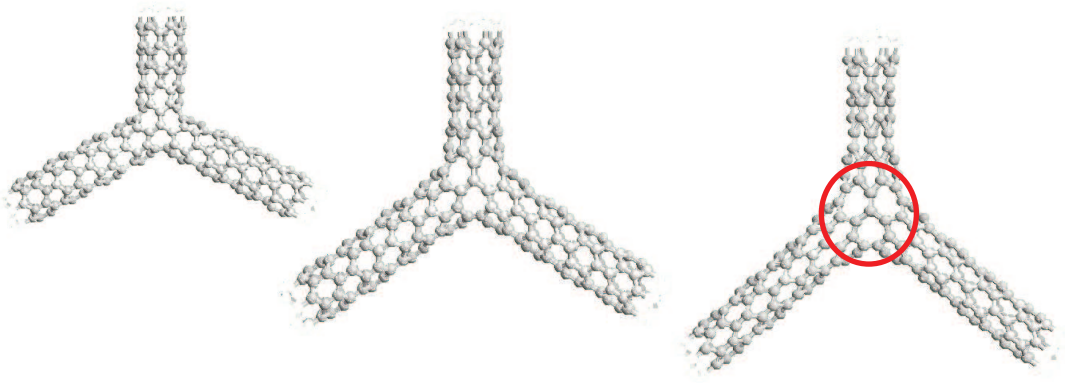

Figure 1. Snaps from the symmetric Y-junction pulling

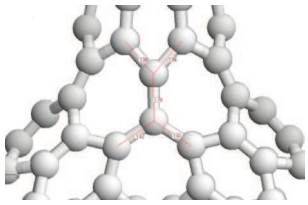

Figure 2. Critical bond-length (1.7 Å) inside of node

We show the results of runs carried out on asymmetric structure in Figure 3 and 4, where the tensile-test snaps of carbon nanotube Y-junction can be seen. The pulling takes place in the axial direction of tubes. According to the first appreciation still only can be decided that this structure will not rupture inside of node the bonding nomely here start to elongate in the greatest amount.

Figure 3. The critical bond-length and the damage on an asymmetric junction respectively

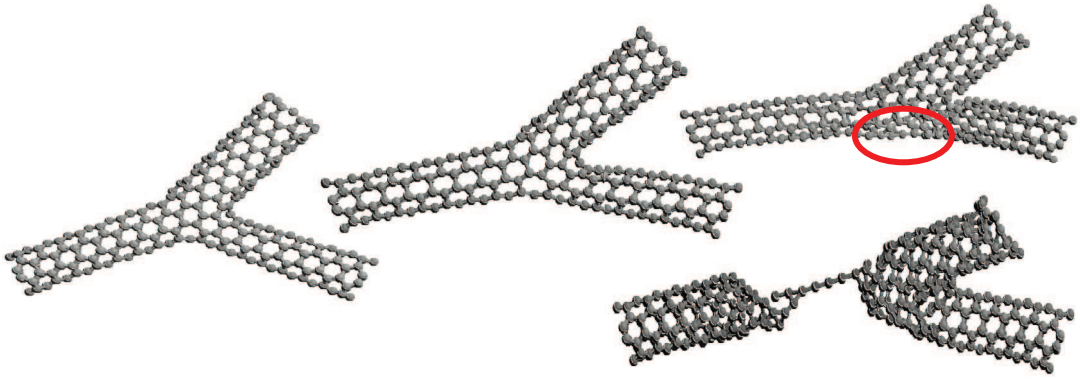

Figure 4. The critical bond-length and the damage on an another asymmetric junction respectively

2.2 Symmetric calculating method

During examining nanotube junctions lights was thrown that the symmetry has got a great effect to its strength properties

This paper sums up the results reached in the theme concerning the searching of axial symmetries of planar configurations and examining the similarity of 2D-al configurations.

2.2.1. Method

We search the symmetric axis of the configuration examined that we are scanning the plane with the hot direct lines passing through of the centre of gravity.

During scanning we set out from that theses whereas all symmetrical axes have to pass through on the centre of gravity. We carry out a calculation method for all direct line passing the centre of gravity which results we put down. By evaluating of data got this way we select the spot of approximating and exact symmetry. We display the results presenting in diagram. During evaluating the diagram we examine the local maximum values.

During our research work we have drawn up a symmetry searching algorithm, (Figure 5.) which by it is known in technical literature and can be applied in case of configurations with multiple complex outline, too.

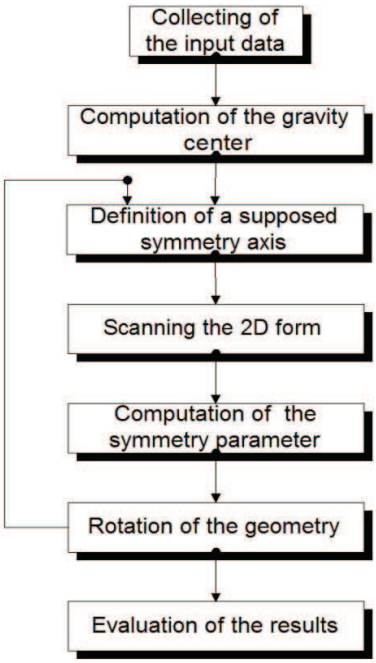

Figure 5. The algorithm

2.2.2. Calculating the symmetry-parameter

The Z symmetry-parameter shows the approximation to the axial symmetry in numerical form. This is a number between 0 and 1, it can be a certain grade of the symmetry characteristic. We introduce the following Z_k parameter for the definition referring to the k. scanning level:

The calculation of Z_k is simple in that case when on one scanning one-one intersection derives on the both sides of the axis. With the Figure Z. symbols:

$$Z_k = 1 - \frac{abs(b-j)}{b+j} \tag{6}$$

Where:

b: marks the left-hand side distance measured from symmetry axis of the perimeter section.

j: marks the right-hand side distance measured from the symmetry axis of the perimeter section.

The Z_k is designed so if the section of configuration with the measuring direct line given is exatly symmetrical to the axis supposed, then b=j, this Z_k=1. The better the configuration approximate to the symmetric the move it will be nearer the Z_k to 1 (figure 6).

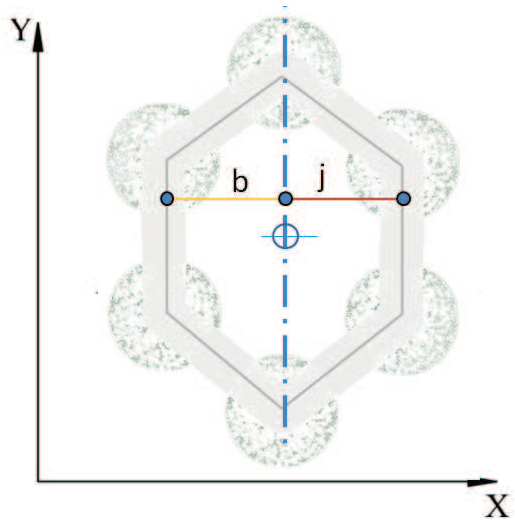

Figure 6. Explanation of measuring section

The more unfavourable situation is regarding to symmetry when the measuring section hasn't got a match on the opposite side of the axis, that is b>0 and j=0, or b=0 and j>0, then Z_k =0, the smallest value.

As in the (6) connection the quotient of geometric dimension occurs, Z_k is a nondimensional number, its value does not depend on geometrical size.

If on a scanning level there are more than two intersections (with Figure 7. markings b_1 , $b_2 \ldots . b_n$; j_1 , $j_2 \ldots . j_m$) then we place the b_1 and j_1 values into pairs and we form the Z_k value with (6) connection from this. If I suppose that more intersections are on the left-hand side: n>m. then the planning into pairs has to be made so, that beginning from b_{m+1} the b_i (i= m+1,… n) pair should be always j_i =o (i=m+1,…n). The Z_k value in general case is the average of expressions formed of pairs calculated according to (6).

$$Z_k = \frac{1}{n}\sum_{i=1}^{n}\left(1 - \frac{abs(b_i - j_1)}{b_i + j_i}\right) \tag{7}$$

The Z parameter formed, from the Z_k average of symmetry parameter

$$Z = \frac{\sum_{k=1}^{n} Z_k}{N} \tag{8}$$

where:

N: marks the number of scanning levels from timely $Y_{\max}$ to $Y_{\min}$. As we form Z value by averaging according to (z), (8), Z keeps the original characteristic of Z_k values:

- Z can take up values in (0,1) interval ,
- Z = 1 is the most favourable (exact) case of symmetry,
- Z=0 is the most unfavourable case regarding to symmetry,
- The values between 0 and 1 correspond to the approximate symmetry all the better the nearer is Z value to 1.
- Z is a nondimensional number and its value does not depend on the dimension of plane figure only it depends on its shape.

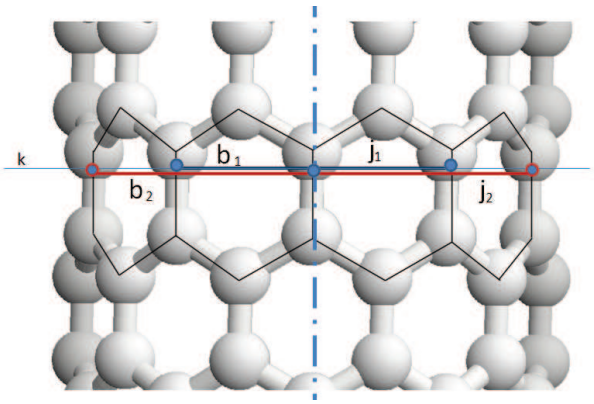

Figure 7. The explanation of Z_k parameter in case of optional complication.

3 CONCLUSIONS

We have developed a method to examine nanotube junctions.

Based on this method the nanotubes can be divided into two groups based on the symmetry theory, into symmetric and asymmetric configurations. It is possible to search the symmetry axis of the junction by a one axial symmetry rearching method. We search for such configurations with theoretical tensile-test of nanotubes that are optimized against pulling load. The structure of nanotube junctions have got near such strength properties than the tubes connected to it.

We have established that the symmetric and asymmetric junctions behave differently to the effect of mechanical loads. The symmetric junctions get damaged inside of node while the asymmetric junctions get damaged at the node and of the nanotube border. We have determined a quick and exact calculating method to distinguish at these nanotube structures. This program determines exatly whether the nanotube structure is symmetrical or arymmetrical.

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