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## The role of the atomic force function in molecular mechanics simulations for carbon nanostructures

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**Abstract.** Molecular mechanics studies were performed on structures consisting of Y junctions of carbon nanotubes. Tensile simulations were run on the same structure, wherein atomic force functions of various shape were used. According to the numerical test results the behavior of the structure, the failure site and the failure process could be determined irrespective of the shape of the force function.

### 1. Introduction

Because of their derivation from graphene structures (winding of graphene ribbon) carbon nanotubes may be materials with a strength value approaching the theoretical maximum achievable in solids. Direct determination of the strength of carbon nanotubes has been performed on multiwall carbon nanotubes (MWCNT) (Demczyk 2002, Yu 2000a), and on bundles of single wall carbon nanotubes (SWCNT) (Yu 2000b). One can say of such experiments that these are very cumbersome and expensive tests that can be performed on simple carbon structures and the accuracy of the tests, thus the correctness of the obtained results is not yet clear.

In order to determine the tensile strength of individual carbon nanotubes theoretically the methods of molecular mechanics are used. The basis of this is that the interatomic binding forces can be calculated from the gradient of the potential function describing the energetics of chemical bonds. In most of such calculation the empirical Brenner potential (Brenner, 1990, 2002) has been used (Belytschko 2002, Mylvaganam 2004, Duan 2007, Fu 2008, Agrawal 2008).

In the original Brenner formulae at a certain interatomic distance there is a discontinuity in the potential function which causes problems in the atomic force function because of the sudden change of the slope. Neither this sudden slope change, nor the multiplication of the maximum atomic force due to the slope change can be explained by physical reasons.

In order to avoid the sudden change of slope a correction function has been introduced (Zsoldos 2009). The correction function has been defined by polynomials having adjustable parameters, and by means of these freely adjustable parameters the atomic force function can be fitted to the test results. As, however, the accuracy of the test results is not known, the usefulness of adjustment to the test results has not been decided either.

In this work it is investigated how can molecular mechanics simulations using the Brenner potential be used for the study of more complicated carbon nanostructures, such as Y junctions.



## 2. Algorithm

In the modified Brenner formulae they were used the following correction function (Zsoldos 2009):

$$f_{ij}(r) = \begin{cases} f_1(r), & R_1 \leq r \leq R_T \\ f_2(r), & R_T < r \leq R_2 \end{cases} \quad (1)$$

where  $R_T$  is the position of the inflection point between  $R_1$  and  $R_2$ ,  $r$  is the interatomic distance between two neighbor atoms.

$f_1(r)$  and  $f_2(r)$  functions defined in two distinct intervals are polynomials of the fourth and third order respectively:

$$f_1(r) = a_0 + a_1r + a_2r^2 + a_3r^3 + a_4r^4, \quad f_2(r) = b_0 + b_1r + b_2r^2 + b_3r^3 \quad (2)$$

The coefficients of the polynomials have been determined by fitting them to the Brenner potential:

$$b_3 = \frac{f_T}{2(R_2 - R_T)^3}, \quad a_4 = \frac{3f_T - 3 + 6b_3(R_2 - R_T)^2(R_T - R_1)}{(R_T - R_1)^4} \quad (3)$$

$$a_3 = \frac{4a_4[R_T^3 - R_1^3 - 3R_T^2(R_T - R_1)] + 3b_3(R_2 - R_T)^2 + d}{3(R_T - R_1)^2} \quad (4)$$

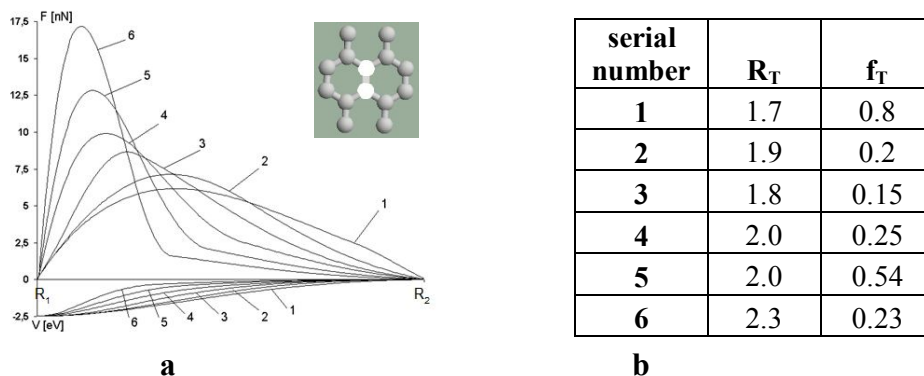
$$b_2 = -3b_3R_T, \quad a_2 = -3a_3R_T - 6a_4R_T^2, \quad a_1 = d - 2a_2R_1 - 3a_3R_1^2 - 4a_4R_1^3 \quad (5)$$

$$b_1 = d - 2b_2R_2 - 3b_3R_2^2, \quad a_0 = 1 - a_1R_1 - a_2R_1^2 - a_3R_1^3 - a_4R_1^4, \quad b_0 = -b_1R_2 - b_2R_2^2 - a_3R_2^3 \quad (6)$$

$f_T$  in the expressions for the coefficients of the polynomials is the value of the correction function at the inflection point (at  $R_T$ ). Variables  $R_T$  and  $f_T$  are freely adjustable parameters.

In this work it has been investigated how does the behavior of carbon nanostructures change, if the shape of the potential energy function and, consequently the shape of atomic force function is varied.

When varying the shape of the energy potential function and the atomic force function 7 different cases were investigated. In the first case the  $f_{ij}(r)$  function was removed from the Brenner formula, i.e. it was assumed that its value is 1 in each case. In the next 6 cases 6 different value pairs were selected for  $R_T$  and  $f_T$  for the  $f_{ij}(r)$  correction function, thus we generated 6 different atomic force functions. Figure 1 shows these 6 different cases. The differences between the energy potential functions are smaller, the variation of the free parameters in the atomic force function, however, results in more drastic changes. The question is really relevant: what changes are caused by the variation of the atomic force function in the behavior of carbon nanostructures?



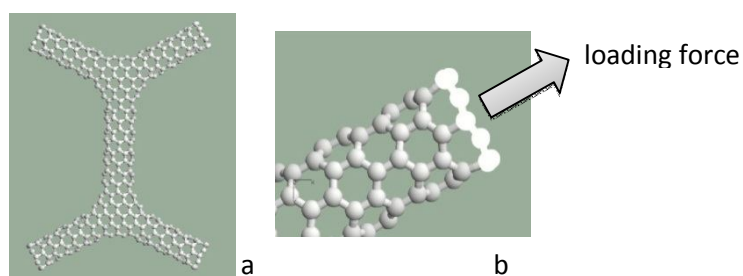
**Figure 1:** a.) Below the abscissa the energy potential function, above the abscissa the atomic force function is shown, calculated between two adjacent atoms (indicated by white color) b.) Freely chosen parameters of the correction function.

### 3. Tensile simulation of carbon nanotube Y junction

Seven tensile simulations were performed by using the atomic force functions described in the previous paragraph. The tensile simulations were performed on the same structure consisting of two Y junctions opposing each other, as shown in Fig. 2a. These models of opposing Y junctions were built from zigzag type nanotubes, the chiral vector being (6, 0). During the tensile simulation axial tensile forces were applied at the ends of the four straight tube portions, as shown in Fig. 2b. Simulations were run until the appearance of deformation (failure).

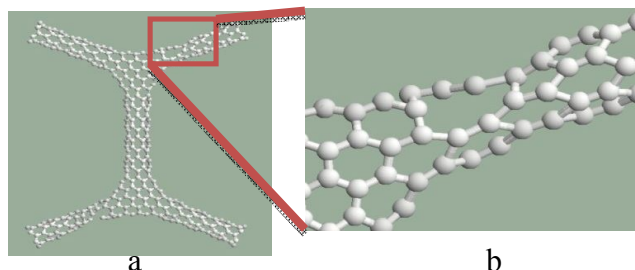
In the first case the original Brenner potential was used, where the effect of “cutting” or correction function was not taken into account, its value was assumed to be invariably 1. During the tensile simulation process the position was identified where the structure was deformed.

Afterwards the effect of the correction function was determined using 6 different pairs of the freely chosen parameters. By this set of simulations we wanted to explore how much is it necessary to adjust the atomic force functions to exact experimental results in order to determine the weakest points.



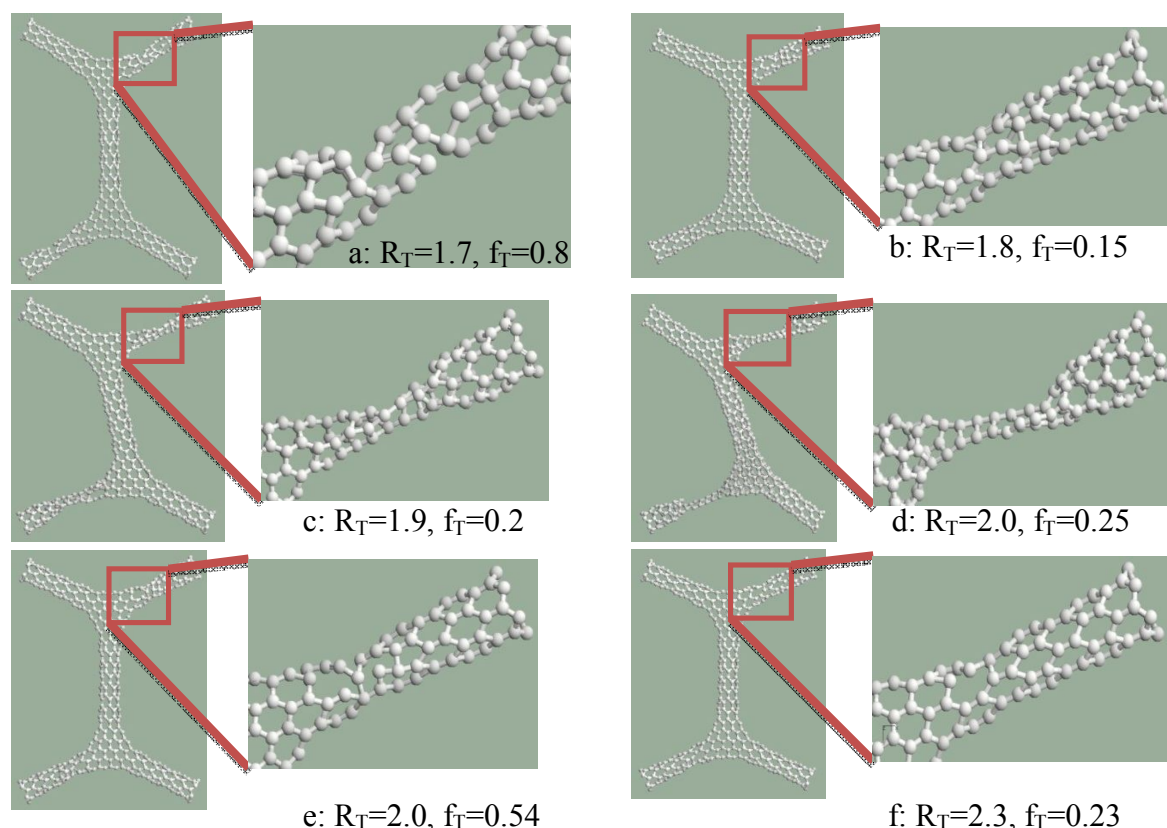
**Figure 2:** a.) the initial structure b.) The axial force applied at the ends of the straight portions of the tubes

Fig. 3 shows the results of the calculation run with the original Brenner potential. The run was finished when the failure site was identified on the structure. This state was achieved when the elongation in all 4 branches reached 11.26 Å. This corresponds to 38% elongation. From the geometry of the structure it follows that two, symmetrically occurring failures can be observed. The deformations did not appear in the junction sites (nodes) but in the straight tube portions. It can be seen at higher magnification that certain bonds broke, some others are rearranged.



**Figure 3:** a.) The failed structure investigated by the original Brenner potential, b.) At higher magnification one can see the broken bonds

In the following the results of the runs performed using the correction functions determined by the 6 freely chosen parameter pairs mentioned above are shown (see Figs. 4a-4f).



**Figure 4:** Results of the calculations performed using correction functions determined by different pairs of parameters

During the test runs it has been established that the failure occurs at the same structural unit, even at the same location (in the neighborhood of the same atoms). In all cases the deformation developed at the location observed in the first run.

## Conclusions

Molecular mechanics methods are applicable to find the failure site of carbon nanotube structures. The atomic force functions derived from energetic potential functions can be used without fitting to measured data. The shape of the atomic force function does not modify the failure location.

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