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Topological Description and Construction of Single Wall Carbon Nanotube Junctions*

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Based on Euler´s theorem a topological description will be given for the junctions of carbon nanotubes. Then using the intersection of cylinders an algorithm will be presented for constructing junctions between single wall nanotubes of any chirality and diameter.

INTRODUCTION

Carbon nanotubes[1] are possible candidates for building blocks in nanoscale electronic devices. They can form also very small junctions for electronic circuits in this region. The first theoretical propositions for nanotube junctions[2,3] were published shortly after Iijima's discovery, which were followed by others.[4–16] In Ref. 8 an algebra was given for describing nanotube junctions. There are also several experimental finding on multi wall[17] and single wall Y junctions[18] or other junctions obtained by various methods.[19,20] See a recent review in Ref. 21.

In this paper first we describe the nanotube junctions using the method of Ref. 8 and then an algorithm will be presented and applied for several cases of single wall nanotubes with any chirality and diameter. The final junctions will be described with the help of Schlegel diagrams.

EULER'S THEOREM AND CONSEQUENCES FOR NANOTUBE JUNCTIONS

According to Euler's theorem, for any polyhedron homeomorphic to the sphere S^2 it is stated that the numbers of vertices V, edges E and faces F have the relation

$$F - E + V = 2 \,. \tag{1}$$

In topology, if S is an orientable closed surface, its genus g is the number of handles and its Euler characteristic equals to $F - E + V$. The genus is 0 for the sphere and it is 1 for the torus. The Poincaré formula

$$F - E + V = 2(1 - g) \tag{2}$$

is the generalization of Euler's polyhedron theorem for polyhedrons of higher genus.

* Dedicated to Dr. Edward C. Kirby on the occasion of his 70th birthday.

If n_i is the number of faces with i vertices, and each vertex has 3 neighbors

$$E = \frac{1}{2}\sum_i in_i, \quad V = \frac{2E}{3} = \frac{1}{3}\sum_i in_i, \quad F = \sum_i n_i \quad (3)$$

and thus the Poincaré formula has the following form

$$\sum_i (6-i)n_i = 12(1-g) \quad (4)$$

From this relation follows that the coefficient for n_6 is zero, that is there is no constraint for the number of hexagons. For fullerenes $g = 0$, thus Eq. (4) gives that $n_5 = 12$ if other polygons different of hexagons are not allowed. If we allow heptagons too, from Eq. (4) follows that $n_5 - n_7 = 12$. In Figure 1 we can see the schematic representation of three structures of $g = 0$. They are in order the fullerene (Figure 1a) the nanotube of two closed ends (Figure 1b) and a nanotube junction or a nanotube of three closed ends (Figure 1c). For a fullerene we can suppose that the number of pentagons is 12. The same is valid for a nanotube of two closed ends (Figure 1b) but here we can suppose that the pentagons are at the half spheres. That is there are 6 pentagons at each ends. If we suppose further 6 pentagons at each ends of the structure in Figure 1c, the number of pentagons will be $n_5 = 18$. From the relation $n_5 - n_7 = 12$ follows that $n_7 = 6$. Thus a nanotube junction must have 6 heptagons if other polygons different of hexagons are not allowed. In Figure 2a we can see the schematic representation of a hexagonal nanotube and in Figure 2b the junction of hexagonal nanotubes must have 6 heptagons. Thus a nanotube junction between polyhex nanotubes must have at least 6 heptagons if other polygons are not allowed. The same result was found in Refs. 8 and 14. Using a reasoning as before we can obtain the following relation for a connected nanotube network with e open ends.

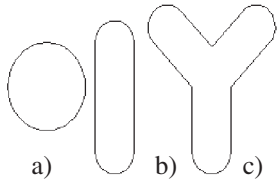

Figure 1. Schematic representation of three structures of $g = 0$. (a) The fullerene; (b) The nanotube of two closed ends; (c) Nanotube junction or a nanotube of three closed ends.

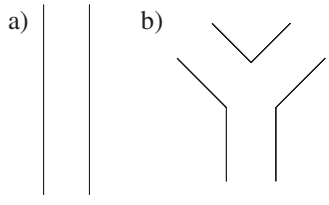

Figure 2. Schematic representation of (a) nanotube and (b) nanotube junction of open ends.

$$\sum_i (6-i)n_i = 12(1-g) - 6e \quad (5)$$

Here g is the genus of the corresponding nanotube network with closed ends. The interior carbon atoms are three-connected and the polygons obtained by opening the ends are not counted in the summation. Let us turn back to the nanotube junction of three ends ($e = 3$) and $g = 0$. In this case Eq. (5) can be written as:

$$3n_3 + 2n_4 + n_5 - n_7 - 2n_8 - 3n_9 - 4n_{10} - 5n_{11} - 6n_{12} - 7n_{13} - \ldots = -6 \quad (6)$$

Triangles, squares or pentagons alone can not fulfill the condition of a nanotube junction. If we want to use only one type of polygons we need 6 heptagons, 3 octagons, 2 nonagons or 1 dodecagon. There are other possibilities using several polygons.

NANOTUBE JUNCTION AS INTERSECTION OF CYLINDERS

Usually the single wall nanotube is a hexagonal network of carbon atoms that has been rolled up to make a cylinder. The unit vectors of this graphene sheet are $\boldsymbol{a}_1 = a(\sqrt{3}/2, 1/2)$ and $\boldsymbol{a}_2 = a(\sqrt{3}/2, -1/2)$. The unit cell contains two atoms at positions (0,0) and $(a/\sqrt{3},0)$. A parallelogram can be constructed from the super cell vectors $\boldsymbol{b}_1 = m\,\boldsymbol{a}_1 + n\,\boldsymbol{a}_2$ and $\boldsymbol{b}_2 = p\,\boldsymbol{a}_1 + q\,\boldsymbol{a}_2$ where m, n, p and q are integers. Usually the chiral vector $\boldsymbol{b}_1$ determines the type of the nanotube and the length is given by the translation vector $\boldsymbol{b}_2$. In our case the super cell will be rectangular. That is $p = -k(m + 2n)$ and $q = k(2m + n)$ with the positive integer k. After rolling up this super cell a nanotube is obtained with a radius of

$$r = \frac{a\sqrt{3m^2 + 3mn + 3n^2}}{2\pi}. \quad (7)$$

We want to find the junction between the nanotubes (m_1, n_1) and (m_2, n_2). As the nanotube can be thought of as a cylinder having the hexagonal network on its surface, the junction will be determined with the help cylinders' intersection. In our notation the line of intersection on the first cylinder is intersection 1 and on the second cylinder is intersection 2. The (u, v) Descartes coordinates with horizontal and vertical axes $\boldsymbol{b}_1$ and $\boldsymbol{b}_2$ for intersection 1 on the rectangle of the first cylinder are:

$$u = r_1\varphi_1 \quad (8)$$

$$v = \frac{-r_2\cos(\pi - \varphi_2) + r_1\cos(\varphi_1)\cos(\alpha)}{\sin(\alpha)} - \frac{r_1}{\tan(\alpha)} \quad (9)$$

and

$$v = \frac{-r_2\cos(\varphi_2) + r_1\cos(\varphi_1)\cos(\alpha)}{\sin(\alpha)} - \frac{r_1}{\tan(\alpha)} \quad (10)$$

with

$$\varphi_2 = \arcsin\left(\frac{r_1 \sin(\varphi_1) - d}{r_2}\right) \tag{11}$$

where (r_1, φ_1) and (r_2, φ_2) are the cylindrical coordinates of cylinders 1 and 2. The angle and distance between the axis of the two cylinders are in order a and d. The value $d \neq 0$ correspond to the case where the cylinder axes are not intersecting. It is supposed further that

$$r_2 \leq r_1, \quad d \leq |(r_1 - r_2)| \tag{12}$$

and

$$\arcsin\left(\frac{d - r_2}{r_1}\right) \leq \varphi_1 \leq \arcsin\left(\frac{d + r_2}{r_1}\right). \tag{13}$$

The same notation is used for the (u, v) coordinates of intersection 2 on the second cylinder rectangle. That is

$$u = r_2 \varphi_2 \tag{14}$$

$$v = \frac{-r_1 \cos(\varphi_1) + r_2 \cos(\varphi_2) \cos(\alpha)}{\sin(\alpha)} - \frac{r_1}{\sin(\alpha)} \tag{15}$$

with

$$\varphi_1 = \arcsin\left(\frac{r_2 \sin(\varphi_2) + d}{r_1}\right) \tag{16}$$

where $-\pi \leq \varphi_2 \leq +\pi$.

EXAMPLES

Here we shall construct junctions between the nanotubes $(m_1, n_1) = (18, 2)$ and $(m_2, n_2) = (10, 5)$. Equation (1) gives the corresponding radii $r_1 = 7.36$ Å and $r_2 = 5.11$ Å using the $a = 1.421$ Å carbon-carbon distance in the graphene sheet. In our first example the angle and distance between the nanotube (cylinder) axes are in order $\alpha = 70°$ and $d = 2.0$ Å. In Figure 3 can be seen the line of intersection made by the cylinder of the second nanotube on the super cell of the first one and Figure 4 shows the line of intersection on the other rectangle. Each lines cut several carbon-carbon bonds. The vertical and horizontal translations of the intersection lines correspond to axial rotations or translations of the cylinders. With the help of these transformations the number of cut bonds

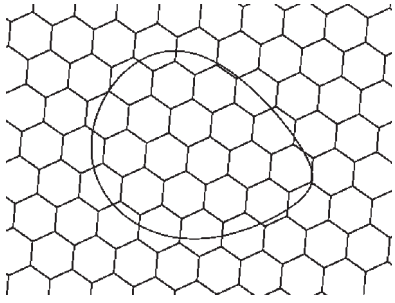

Figure 3. The line section of the (10, 5) nanotube cylinder on the super cell rectangle of the (18, 2) nanotube.

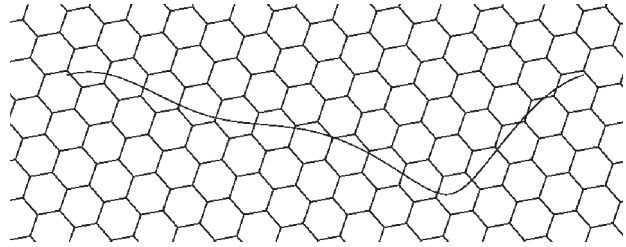

Figure 4. The line section of the (18, 2) nanotube cylinder on the super cell rectangle of the (10, 5) nanotube.

are changing and our purpose is looking for such positions where their number is the same on each cylinders. After cutting out the interior part of the first intersection and the lower part of the second one the two nanotubes can be joined together by the corresponding half bonds. The positions and order of these bonds can be described by the angles φ_2 and the nanotubes will have little distortions if the two joined atoms of the new bonds have nearly the same φ_2.

This algorithm provides a nanotube junction where each carbon atoms have three neighbors.

In most of the cases, however, the number of non hexagonal polygons is not the ideal. We made systematic searches in order to find the ideal case of six heptagons (that is $n_7 = 6$). For the parameters of $\alpha = 70°$ and $d = 2.0$ Å we could not find a junction of six heptagons. The junction we have found contains seven heptagons and one pentagon ($n_7 = 7$ and $n_5 = 1$) Figure 5. Although

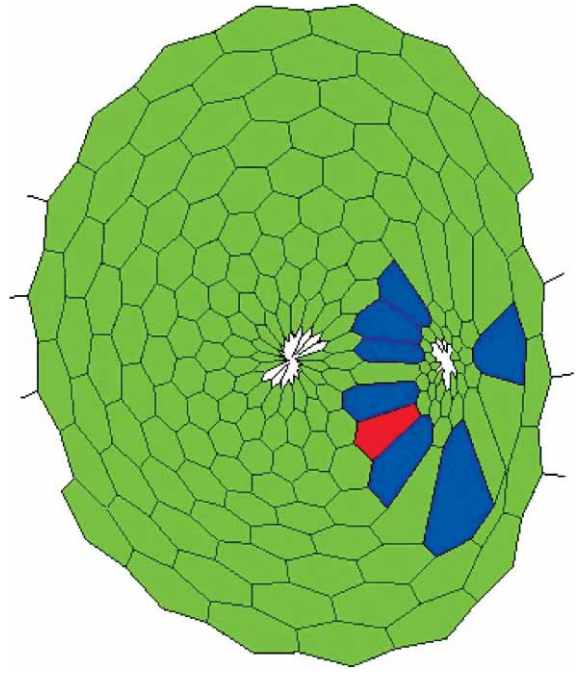

Figure 5. The Schlegel diagram of a junction between nanotubes $(m_1, n_1) = (18, 2)$ and $(m_2, n_2) = (10, 5)$ with the parameters $\alpha = 70°$, $d = 2.0$ Å, $n_5 = 1$ and $n_7 = 7$.

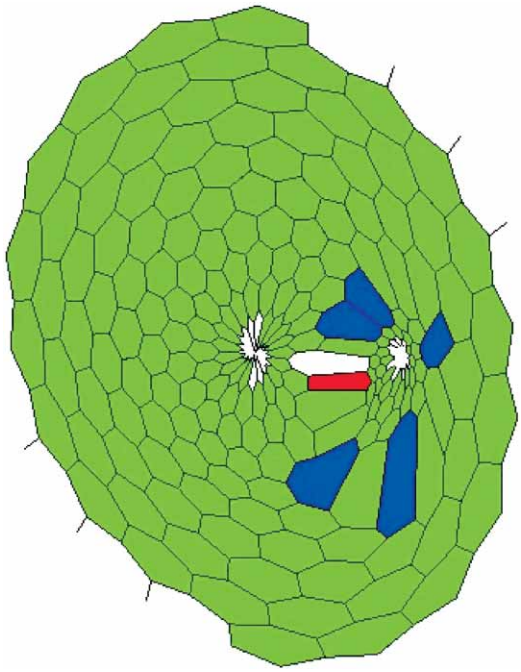

Figure 6. The Schlegel diagram of a junction between nanotubes $(m_1, n_1) = (18, 2)$ and $(m_2, n_2) = (10, 5)$ with the parameters $\alpha = 90°$, $d = 2.0$ Å, $n_5 = 1$, $n_7 = 5$ and $n_8 = 1$.

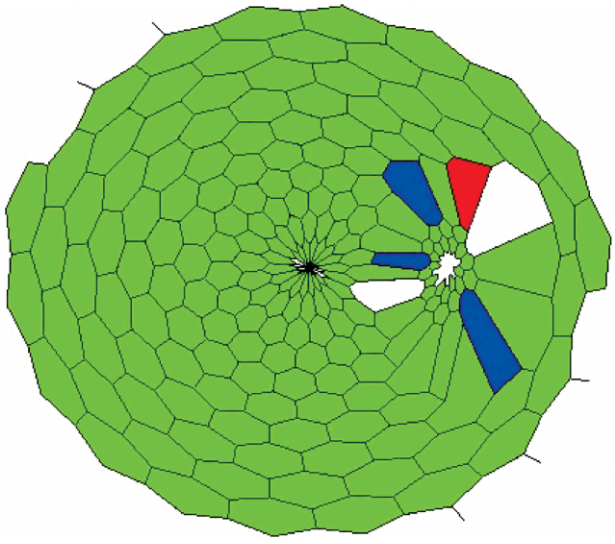

Figure 7. The Schlegel diagram of a junction between nanotubes $(m_1, n_1) = (18, 2)$ and $(m_2, n_2) = (10, 5)$ with the parameters $\alpha = 60°$, $d = 0.0$ Å, $n_5 = 1$, $n_7 = 3$ and $n_8 = 2$.

decreasing α we could not found any junction with low number of non hexagonal polygons, the parameters $\alpha = 90°$ and $d = 2.0$ Å provided the junction of Figure 6. It has one pentagon, five heptagons and one octagon ($n_5 = 1$, $n_7 = 5$ and $n_8 = 1$). In Figure 7 we can see a junction of one pentagon three heptagons and two octagons ($n_5 = 1$, $n_7 = 3$ and $n_8 = 2$) with the parameters $\alpha = 60°$ and $d = 0.0$ Å. An ideal case of $n_7 = 6$ was found for $\alpha = 90°$ and $d = 0.0$ Å (see Figure 8.).

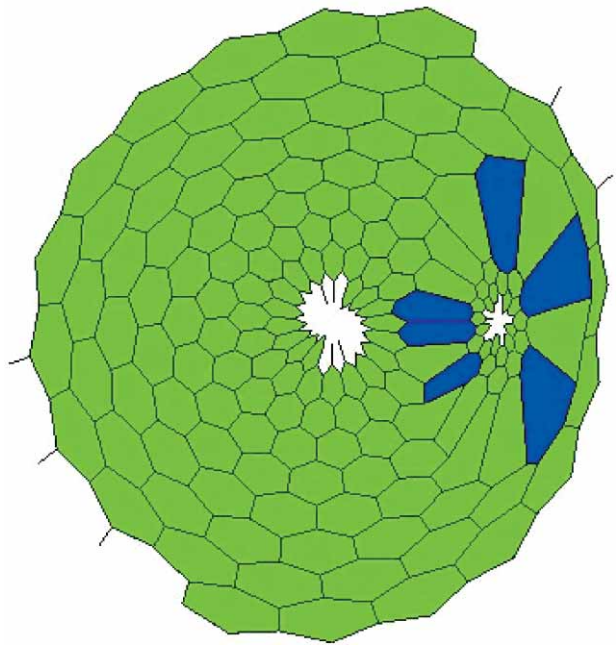

Figure 8. The Schlegel diagram of a junction between nanotubes $(m_1, n_1) = (18, 2)$ and $(m_2, n_2) = (10, 5)$ with the parameters $\alpha = 90°$, $d = 0.0$ Å, and $n_7 = 6$.

In each cases the final structure was constructed with the help of a molecular mechanics method based on the Brenner potential.[22]

CONCLUSIONS

We have shown that using only geometrical reasoning realistic nanotube junctions can be constructed. It was found that by changing the positions and angles between nanotube axes, several junctions can be generated between any kind of single wall carbon nanotubes. As the electronic properties depend on the junctions, a systematic search by parameter variations could reach to special nanotube networks with new useful properties. The method of cylinder intersection can be generalized for intersection of other surfaces too, thus the it can be generalized for constructing junction between any kind of carbon surfaces.

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SAŽETAK

Topologijski opis i konstrukcija spajanja ugljikovih nanocijevi s jednom stjenkom

István László

Dan je topologijski opis, temeljen na Eurelovu teoremu, spojišta ugljikovih nanocijevi. Zatim je prikazan, uporabom sjecišta cilindara, algoritam za konstrukciju spojišta između ugljikovih nanocijevi s jednom stjenkom i bilo kojom kiralnošću i bilo kakvim dijametrom.