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Construction of Carbon Nanotube Junctions*

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Diophantic equations are developed for constructing junctions between single wall nanotubes of any chirality and diameter. The solution of these equations makes it possible to find the Descartes coordinates of the carbon atoms in the structures. An example is given for a three terminal junction.

INTRODUCTION

There is a possibility to develop carbon-nanotube-based electronics where truly nanoelectronic architecture can be realized. Namely nanotubes can be applied both as devices and interconnects as well.[1,2] Three-terminal junctions for example are envisaged as units for rectifying elements or transistor components.[3–12] There are several theoretical propositions for various carbon nanotube junctions,[2–11,13–20] but most of them are applied for non chiral ones. We have recently presented an algorithm for constructing junctions between single wall nanotubes of any chirality and diameter[21,22.] This method is suitable only for junctions where the new nanotube branches are attached to already developed ones, and thus there is no possibility in this algorithm to join three various kind of tubes at a junction.

In Ref. 8 a coordinate system was given for describing nanotube junctions and it was applied for connecting two arbitrary nanotubes as for example the two terminal elbow junction.[8,23] In the present paper we shall extend this method for three and more terminal nanotube junctions using the terminology of discrete manifolds.

NANOTUBE JUNCTION AS DISCRETE MANIFOLD

From Euler's theorem follows the following relation for a connected nanotube network with e open ends:[22]

$$\sum_i (6-i)\, n_i = 12(1-g) - 6e \qquad (1)$$

Here g is the genus of the corresponding nanotube network with closed ends and n_i is the number of faces with i vertices. On the corresponding nanotube network with closed ends we mean the original nanotube network plus the half spheres for closing the open ends, where we suppose that each half sphere has six pentagons. For developing Eq. (1) these $6e$ pentagons are removed for opening the tubes. Thus for a three terminal nanotube junction (e = 3 and g = 0) we obtain from Eq. (1):

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

Allowing only one kind of non-hexagonal polygons we obtain that $n_7 = 6$ and $n_i = 0$ for the other non-hexagonal polygons.

* Dedicated to Haruo Hosoya on the occasion of his 70th birthday.

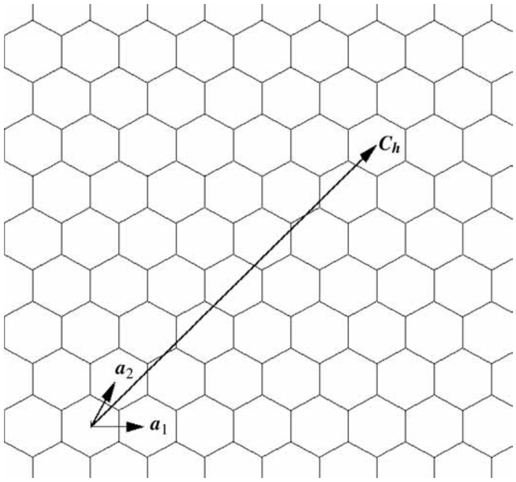

Figure 1. The coordinate system on a graphene sheet. The positions of the hexagons are given with the help of unit vectors $\boldsymbol{a}_1$ and $\boldsymbol{a}_2$. The chiral vector $\boldsymbol{C}_h = m\boldsymbol{a}_1 + n\boldsymbol{a}_2$ describes the nanotube.

A single wall nanotube is a hexagonal network of carbon atoms that has been rolled up to make a cylinder. On a hexagonal graphene sheet G the position of the hexagons are given with the aid of two unit vectors $\boldsymbol{a}_1$ and $\boldsymbol{a}_2$ (Figure 1). These unit vectors join the center of a hexagon with the center of the neighboring hexagons. They are also used for giving the chiral vector $\boldsymbol{C}_h$

$$\boldsymbol{C}_h = m\boldsymbol{a}_1 + n\boldsymbol{a}_2 \tag{3}$$

where m and n are integers. The chiral vector makes equivalence between the hexagons during rolling up the graphene sheet. From this construction follows, that the coordinate system of the sheet can be transferred to the tube as well. Let us suppose that we want to construct a junction between three tubes of parameters

$$\begin{pmatrix} m^1 \\ n^1 \end{pmatrix}, \begin{pmatrix} m^2 \\ n^2 \end{pmatrix} \text{ and } \begin{pmatrix} m^3 \\ n^3 \end{pmatrix}. \tag{4}$$

Each tube has its own coordinate system defined on the corresponding graphene sheets. When these tubes are joined together in a junction we must describe the changing of the local coordinate systems of the neighboring tubes during going from one to the other. This will be given with the help of a discrete manifold.

Manifold of a Junction

The manifold is a space that, like the surface of the Earth, can be covered by a family of local coordinate systems. In our case the local coordinate system will be the coordinate system of the hexagonal lattice. Thus we shall use the following definition of manifold:

Let M be the set of polygons on the surface of a nanotube junction constructed from three nanotubes 1, 2 and 3 having covering sets in order U_1, U_2 and U_3 with the relation $M = U_1 \cup U_2 \cup U_3$, where each subset U is in 1 : 1 correspondence $\Phi_U : U \rightarrow G$ with a subset $\Phi_U(U)$ of the graphene sheet G. We require that each $\Phi_{U_i}(U_i \cap U_j)$ be a subset of G. Each pair U, Φ_U defines a coordinate patch on M; to $p \in U \subset M$ we assign the $\begin{pmatrix} m_p \\ n_p \end{pmatrix}$ coordinates of the point $\Phi_U(p)$ in G. For this reason we call Φ_U a coordinate map.

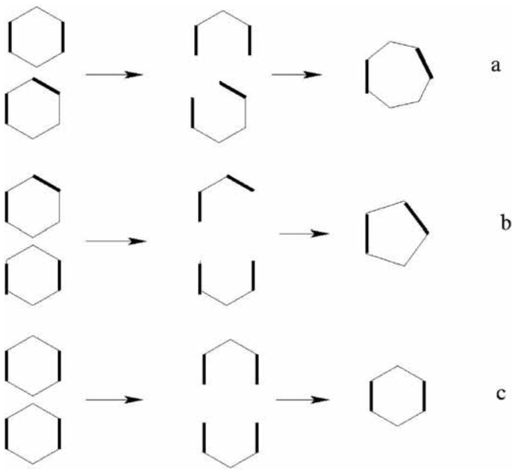

Figure 2. Construction of polygons in set $U_i \cap U_j$. Examples are given for heptagon (a), pentagon (b) and hexagon (c). The cut bonds are marked by thick bonds. In each cases the cut bonds are put in U_i for the upper hexagon and in U_j for the lower one.

For each polygon p in set $U_i \cap U_j$ we suppose that it is constructed from two hexagons $h_i = \Phi_{U_i}(p)$ and $h_j = \Phi_{U_j}(p)$ belonging in order to tubes i and j (Figure 2). That is the polygons in set $U_i \cap U_j$ have the coordinates of their hexagons in the corresponding coordinate map. Thus the construction of the nanotube junction is equivalent with the determination of those $\Phi_{U_i}(p) = h_i$ and $\Phi_{U_j}(p) = h_j$ hexagons that will be used for the construction of the corresponding non-hexagonal polygon p. This will be given by the coordinates of hexagons h_i and h_j on the Φ_U coordinate maps. The coordinates of hexagons h_i and h_j for polygon p will be the same on the two maps because of the gluing condition of the two neighboring tubes. The kind of polygon p will be given by the positions of the cut bonds. We shall use the convention that one of the cut bonds will be in the direction $-\boldsymbol{a}_1$, and the other one will be in the direction $\boldsymbol{a}'_1$, starting from the center of the corresponding polygon. The unit vector $\boldsymbol{a}_1$ is used in the coordinate system for giving the position of the hexagon under study and the new unit vector $\boldsymbol{a}'_1$ belongs to the coordinate system of the next hexagon under study (Figure 3). Thus the local coordinate system might be rotated at each hexagon depending on the position of the cut bonds in polygon $p \in U \subset M$.

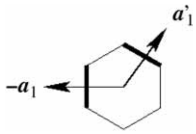

Figure 3. The position of the cut bonds. The unit vector $\boldsymbol{a}_1$ is used in the coordinate system for giving the position of the hexagon under study and the new unit vector $\boldsymbol{a}'_1$ belongs to the coordinate system of the next hexagon under study.

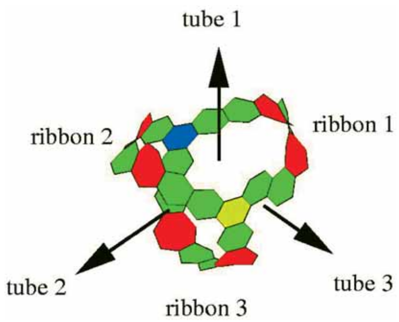

Figure 4. The three ribbons of junction $(U_1 \cap U_2) \cup (U_2 \cap U_3) \cup (U_3 \cap U_1)$ between nanotubes 1, 2 and 3. The two hexagons A and B $\in U_1 \cap U_2 \cap U_3$ are marked in order by colors yellow and blue. The heptagons are red in the figure.

The $(U_1 \cap U_2) \cup (U_2 \cap U_3) \cup (U_3 \cap U_1)$ set of the junction can be described by three ribbons of polygons joined by two hexagons A and B $\in U_1 \cap U_2 \cap U_3$ (Figure 4). Ribbons 1, 2 and 3 belong in order to the sets $(U_3 \cap U_1)$, $(U_1 \cap U_2)$ and $(U_2 \cap U_3)$. The relative positions of these ribbons will be given by the relative direction angles α_{12}, α_{23} and α_{31} on hexagon A and with the relative direction angles β_{12}, β_{23} and β_{31} on hexagon B. We suppose that $\alpha_{ij} > 0$, $\beta_{ij} < 0$ and the unit of angle on the graphene sheet is $\frac{2\pi}{6}$.

We call Φ_{U_i} the first and Φ_{U_j} the second coordinate map if the corresponding ribbon belongs to the set $(U_i \cap U_j)$. The coordinates of the i-th polygons on the first and second map of ribbon k are $\begin{pmatrix} m_i^k \\ n_i^k \end{pmatrix}$. Thus ribbon k is given by the parameters:

$$\begin{pmatrix} m_1^k \\ n_1^k \end{pmatrix} \frac{T_1^{+k}}{T_1^{-k}} \begin{pmatrix} m_2^k \\ n_2^k \end{pmatrix} \frac{T_2^{+k}}{T_2^{-k}} \begin{pmatrix} m_3^k \\ n_3^k \end{pmatrix} \frac{T_3^{+k}}{T_3^{-k}} \cdots \begin{pmatrix} m_{Nk}^k \\ n_{Nk}^k \end{pmatrix} \frac{T_{Nk}^{k}}{T_{Nk}^{k}} \tag{5}$$

where the relative changing of the direction of the unit vector $\boldsymbol{a}_1$ is in order T_i^{-k} and T_i^{+k} on the first and on the second map. The coordinates $\begin{pmatrix} m_1^k \\ n_1^k \end{pmatrix}$ of the first non-hexagonal polygon of the junction is given by the coordinate system of hexagon A and the $\begin{pmatrix} m_{Nk}^k \\ n_{Nk}^k \end{pmatrix}$ coordinates correspond to a hexagon which is neighboring to hexagon B. Thus there are $Nk - 1$ non-hexagonal polygons in ribbon k. From the construction follows that

$$T^- - T^+ = n - 6 \tag{6}$$

for a polygon of n sides. If a ribbon contains only the non-hexagonal polygons and one hexagon which is neighboring to hexagon B, we call it restricted ribbon. If it contains all its polygons we call it unrestricted ribbon.

Diophantic Equations for Nanotube Junctions

Let

$$s(\tau) = \frac{2}{\sqrt{3}} \sin\left(\frac{\pi}{3}\tau + \frac{2\pi}{3}\right) \tag{7}$$

be a function of the integer variable τ. The range of $s(\tau)$ contains only the integers –1, 0 and 1. Then if the transformation O^τ rotates the coordinate system by the angle τ then the coordinates $\begin{pmatrix} m_i^k \\ n_i^k \end{pmatrix}$ of a polygon will be changed according to the relation

$$O^\tau \begin{pmatrix} m_i^k \\ n_i^k \end{pmatrix} = \begin{pmatrix} m_i^k s(\tau) + n_i^k s(\tau+1) \\ m_i^k s(\tau-2) + n_i^k s(\tau-1) \end{pmatrix}. \tag{8}$$

It is convenient to introduce new variables as

$$\sigma_0^k = \tau_0^k = 0, \tag{9}$$

$$\sigma_{i+1}^k = \sigma_i^k + T_{i+1}^{+k} \tag{10}$$

and

$$\tau_{i+1}^k = \tau_i^k + T_{i+1}^{-k}. \tag{11}$$

The variables σ_i^k and τ_i^k are rotation angles of the local coordinate systems relative to the local coordinate system of hexagon A on the ribbon k.

In tube 1 the coordinates of hexagon B can be given by vector $\boldsymbol{v}_1$ on ribbon 1 and by vector $\boldsymbol{v}_2$ on ribbon 2 in the following way.

$$\boldsymbol{v}_1 = \sum_{i=1}^{N1} O^{\sigma_{i-1}^1} \begin{pmatrix} m_i^1 \\ n_i^1 \end{pmatrix} + O^{\sigma_{N1}^1} \begin{pmatrix} 1 \\ 0 \end{pmatrix} \tag{12}$$

$$\boldsymbol{v}_2 = \sum_{i=1}^{N2} O^{\tau_{i-1}^2 + \alpha_{12}} \begin{pmatrix} m_i^2 \\ n_i^2 \end{pmatrix} + O^{\sigma_{N2}^1 + \alpha_{12}} \begin{pmatrix} 1 \\ 0 \end{pmatrix} \tag{13}$$

As tube 1 has the parameters $\begin{pmatrix} m^1 \\ n^1 \end{pmatrix}$ it is true that

$$\boldsymbol{v}_1 - \boldsymbol{v}_2 = O^{\varphi_1} \begin{pmatrix} m^1 \\ n^1 \end{pmatrix} \tag{14}$$

where the original coordinate system for the coordinates in Eq. (3) is rotated by the angle φ_1 in constructing the vectors $\boldsymbol{v}_1$ and $\boldsymbol{v}_2$.

The parameters β_{12}, β_{23} and β_{31} must fulfill the following joining conditions at hexagon B:

$$O^{\sigma^1_{N1}+\beta_{12}}\begin{pmatrix}1\\0\end{pmatrix} = O^{\tau^2_{N2}+\alpha_{12}}\begin{pmatrix}1\\0\end{pmatrix}. \quad (15)$$

That is

$$\sigma^1_{N1} + \beta_{12} - \tau^2_{N2} - \alpha_{12} = 0 \quad \mathrm{mod}(6)\,. \quad (16)$$

The same relations can be obtained for the other tubes too. Applying in Eqs. (12–14) the relation of Eq. (8) for each tubes we obtain the following diophantic equations:

$$\sum_{i=1}^{N1}(m_i^1 s(\sigma^1_{i-1})+n_i^1 s(\sigma^1_{i-1}+1))+s(\sigma^1_{N1})-$$
$$\sum_{i=1}^{N2}(m_i^2 s(\tau^2_{i-1}\alpha_{12})+n_i^2 s(\tau^2_{i-1}+\alpha_{12}+1))-$$
$$s(\tau^2_{N2}+\alpha_{12}) = m^1 s(\varphi_1)+n^1 s(\varphi_1+1)\,; \quad (17)$$

$$\sum_{i=1}^{N1}(m_i^1 s(\sigma^1_{i-1}-2)+n_i^1 s(\sigma^1_{i-1}-1))+s(\sigma^1_{N1}-2)-$$
$$\sum_{i=1}^{N2}(m_i^2 s(\tau^2_{i-1}+\alpha_{12}-2)+n_i^2 s(\tau^2_{i-1}+\alpha_{12}-1))-$$
$$s(\tau^2_{N2}+\alpha_{12}-2) = m^1 s(\varphi_1-2)+n^1 s(\varphi_1-1)\,; \quad (18)$$

$$\sum_{i=1}^{N2}(m_i^2 s(\sigma^2_{i-1})+n_i^2 s(\sigma^2_{i-1}+1))+s(\sigma^2_{N2})-$$
$$\sum_{i=1}^{N3}(m_i^3 s(\tau^3_{i-1}+\alpha_{23})+n_i^3 s(\tau^3_{i-1}+\alpha_{23}+1))-$$
$$s(\tau^3_{N3}+\alpha_{23}) = m^2 s(\varphi_2)+n^2 s(\varphi_2+1)\,; \quad (19)$$

$$\sum_{i=1}^{N2}(m_i^2 s(\sigma^2_{i-1}-2)+n_i^2 s(\sigma^2_{i-1}-1))+s(\sigma^2_{N2}-2)-$$
$$\sum_{i=1}^{N3}(m_i^3 s(\tau^3_{i-1}+\alpha_{23}-2)+(n_i^3 s(\tau^3_{i-1}+\alpha_{23}-1))-$$
$$s(\tau^3_{N3}+\alpha_{23}-2) = m^2 s(\varphi_2-2)+n^2 s(\varphi_2-1)\,; \quad (20)$$

$$\sum_{i=1}^{N3}(m_i^3 s(\sigma^3_{i-1})+n_i^3 s(\sigma^3_{i-1}+1))+s(\sigma^3_{N3})-$$
$$\sum_{i=1}^{N1}(m_i^1 s(\tau^1_{i-1}+\alpha_{31})+n_i^1 s(\tau^1_{i-1}+\alpha_{31}+1))-$$
$$s(\tau^1_{N1}+\alpha_{31}) = m^3 s(\varphi_3)+n^3 s(\varphi^3+1)\,; \quad (21)$$

$$\sum_{i=1}^{N3}(m_i^3 s(\sigma^3_{i-1}-2)+n_i^3 s(\sigma^3_{i-1}-1))+s(\sigma^3_{N3}-2)-$$
$$\sum_{i=1}^{N1}(m_i^1 s(\tau^1_{i-1}+\alpha_{31}-2)+n_i^1 s(\tau^1_{i-1}+\alpha_{31}-1))-$$
$$s(\tau^1_{N1}+\alpha_{31}-2) = m^3 s(\varphi_3-2)+n^3 s(\varphi_3-1)\,; \quad (22)$$

and from Eq. (16) the joining conditions are:

$$\sigma^1_{N1}+\beta_{12}-\tau^2_{N2}-\alpha_{12}=0 \quad \mathrm{mod}(6)\,; \quad (23)$$

$$\sigma^2_{N1}+\beta_{23}-\tau^3_{N3}-\alpha_{23}=0 \quad \mathrm{mod}(6)\,; \quad (24)$$

$$\sigma^3_{N3}+\beta_{31}-\tau^1_{N1}-\alpha_{31}=0 \quad \mathrm{mod}(6)\,. \quad (25)$$

EXAMPLE

We shall construct the junction between the following three chiral nanotubes:

$$\begin{pmatrix}m^1\\n^1\end{pmatrix}=\begin{pmatrix}9\\6\end{pmatrix},\ \begin{pmatrix}m^2\\n^2\end{pmatrix}=\begin{pmatrix}8\\7\end{pmatrix} \text{ and } \begin{pmatrix}m^3\\n^3\end{pmatrix}=\begin{pmatrix}10\\5\end{pmatrix}. \quad (26)$$

Now we have to solve the Eqs. (17–22) with the joining conditions Eqs. (23–25) for the restricted ribbons. Depending on the needs of the special problem one can construct various junction between three nanotubes. If we want to make a junction with the minimal number of non-hexagonal polygons, from Eq. (2) follows that it will have $n_7 = 6$ heptagons. We put 2 heptagons on each ribbon having symmetrical relative positions, that is:

$$N1 = N2 = N3 = 3 \quad (27)$$

and

$$\alpha_{12} = \alpha_{23} = \alpha_{31} = -\beta_{12} = -\beta_{23} = -\beta_{31} = 2\,. \quad (28)$$

From Eq. (6) follows that $T^- - T^+ = 1$ for heptagons and $T^- - T^+ = 0$ for the hexagons. That is the τ_i^k values can be calculated from the σ_i^k ones. As there are only 6 diophantic equations for the 24 polygon coordinates and the σ_i^k parameters, there is a great liberty for the positions of the non-hexagonal polygons. Let us choose the following coordinates (Eq. (5)) for ribbons 1 and 2 in the tube 1:

$$\begin{pmatrix}3\\-1\end{pmatrix}\frac{0}{1}\begin{pmatrix}2\\-1\end{pmatrix}\frac{-1}{0}\begin{pmatrix}2\\0\end{pmatrix}\frac{0}{0} \quad \text{(restricted ribbon 1)} \qquad (29)$$

$$\begin{pmatrix}3\\0\end{pmatrix}\frac{-1}{0}\begin{pmatrix}1\\1\end{pmatrix}\frac{0}{1}\begin{pmatrix}1\\0\end{pmatrix}\frac{0}{0} \quad \text{(restricted ribbon 2)}\,. \qquad (30)$$

In Figure 5 we can see ribbons 1 and 2 on tube 1 of coordinates $\begin{pmatrix}m^1\\n^1\end{pmatrix}=\begin{pmatrix}9\\6\end{pmatrix}$.

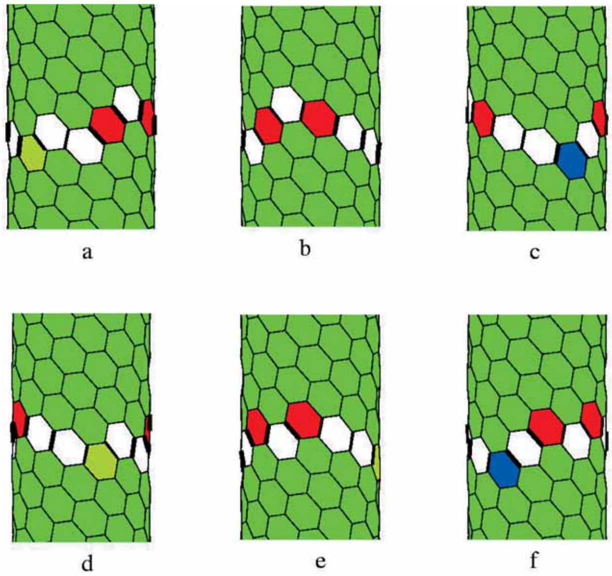

Figure 5. Ribbons 1 and 2 for tube 1. They are seen from azimuthal angles $\varphi = 0$ (a), $\varphi = 60$ (b), $\varphi = 120$ (c), for ribbon 1 and $\varphi = -60$ (d), $\varphi = -120$ (e), $\varphi = -180$ (f) for ribbon 2. The two hexagons A and B $\in U_1 \cap U_2 \cap U_3$ are marked in order by colors yellow and blue. The heptagons are red and the ribbon hexagons are white in the figure. Only the heptagons and the neighboring ribbon hexagons to hexagon B belong to the restricted ribbon.

We put hexagon B in antipodal position to hexagon A on the tube surface.

The positions of the heptagons of ribbon 1 are chosen somewhere on the intersection line between tubes 1 and 3. In the same way are chosen the heptagons on ribbon 2 using the intersection line between the tubes 2 and 1. We suppose that the $T^{+}(T^{-})$ parameters generate unit vectors $\boldsymbol{a}'_1$ pointing to the next polygon for ribbons of Eqs. (29,30).

According to relations of Eqs. (23–25) we could chose the parameters as well. Substituting in Eqs. (17–22) the known data of Eqs. (29–30) for ribbons 1 and 2, the obtained diophantic equations give the missing parameters of ribbon 3. In this way we have found the following parameters for ribbon 3:

$$\begin{pmatrix}2\\0\end{pmatrix}\frac{-1}{0}\begin{pmatrix}3\\0\end{pmatrix}\frac{0}{1}\begin{pmatrix}2\\0\end{pmatrix}\frac{0}{0} \quad \text{(restricted ribbon 3)}\,. \qquad (31)$$

Now the missing hexagons can be place easily and thus we obtain the full description of ribbons 1, 2 and 3 in the following way:

$$\begin{pmatrix}1\\0\end{pmatrix}\frac{-1}{-1}\begin{pmatrix}1\\0\end{pmatrix}\frac{1}{1}\begin{pmatrix}1\\0\end{pmatrix}\frac{0}{1}\begin{pmatrix}1\\0\end{pmatrix}\frac{-1}{-1}\begin{pmatrix}1\\0\end{pmatrix}\frac{0}{1}\begin{pmatrix}1\\0\end{pmatrix}\frac{0}{0}\begin{pmatrix}1\\0\end{pmatrix}\frac{0}{0}$$

$$\text{(ribbon 1)} \qquad (32)$$

$$\begin{pmatrix}1\\0\end{pmatrix}\frac{0}{0}\begin{pmatrix}1\\0\end{pmatrix}\frac{0}{0}\begin{pmatrix}1\\0\end{pmatrix}\frac{0}{1}\begin{pmatrix}1\\0\end{pmatrix}\frac{-1}{-1}\begin{pmatrix}1\\0\end{pmatrix}\frac{0}{1}\begin{pmatrix}1\\0\end{pmatrix}\frac{0}{0}$$

$$\text{(ribbon 2)} \qquad (33)$$

$$\begin{pmatrix}1\\0\end{pmatrix}\frac{0}{0}\begin{pmatrix}1\\0\end{pmatrix}\frac{-1}{0}\begin{pmatrix}1\\0\end{pmatrix}\frac{0}{0}\begin{pmatrix}1\\0\end{pmatrix}\frac{0}{0}\begin{pmatrix}1\\0\end{pmatrix}\frac{0}{1}\begin{pmatrix}1\\0\end{pmatrix}\frac{0}{0}\begin{pmatrix}1\\0\end{pmatrix}\frac{0}{0}$$

$$\text{(ribbon 3)} \qquad (34)$$

In Figure (5) we presented ribbons 1 and 2 of Eqs. (32, 33) on the tube 1. In the same way we can draw ribbons 2 and 3 on tube 2, and ribbons 3 and 1 on the tube 3 using Eqs. (32–34). After cutting the thick bonds on the tubes they were joined together and after conjugate gradient relaxation with Brenner potential[24] we obtained the junction of Figure (6).

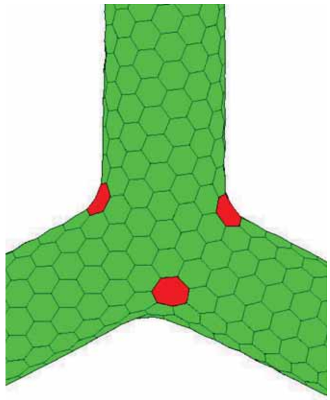

Figure 6. Junction between three chiral nanotubes of parameters $\begin{pmatrix}m^1\\n^1\end{pmatrix}=\begin{pmatrix}9\\6\end{pmatrix}$, $\begin{pmatrix}m^2\\n^2\end{pmatrix}=\begin{pmatrix}8\\7\end{pmatrix}$ and $\begin{pmatrix}m^3\\n^3\end{pmatrix}=\begin{pmatrix}10\\5\end{pmatrix}$

CONCLUSIONS

We have developed diophantic equations for constructing three terminal nanotube junctions. Similar equations can be written down for other junctions as well and usually there are several solutions for these equations and one junction can be described with different parameters too. There are also algebraic solutions which do not fulfill the geometric conditions. It is possible for example that an algebraic solution describes self intersecting ribbons. The number and distribution of various kind of non hexagonal polygons determines the geometric an electronic properties of the junctions. Applying the present algorithm various junctions can be constructed and the best can be found for special problems under study.

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REFERENCES

1. H. Xu, *Nature Mater.* **4** (2005) 649–650.
2. P. R. Bandaru, C. Dario, S. Jin, and A. M. Rao, *Nature Mater.* **4** (2005) 663–666.
3. L. A. Chernozatonskii, *Phys. Lett*. **A 172** (1992) 173–176.
4. L. Chico, V. H. Crespi, L. X. Benedict, S. G. Louie, and M. L. Cohen, *Phys. Rev. Lett*. **76** (1996) 971–974.
5. M. Menon and D. Srivastava, *Phys. Rev. Lett.* **79** (1997) 4453–4456.
6. V. H. Crespi, *Phys. Rev.* **B 58** (1998) 12671–12671.
7. G. Treboux, P. Lapstun, and K. Silverbrook, *Chem. Phys. Lett*. **306** (1999) 402–406.
8. S. Melchor, N. V. Khokhriakov, and S. S. Savinskii, *Mol. Eng***. 8** (1999) 315–344.
9. A. N. Andriotis, M. Menon, D. Srivastava, and L. Chernozatonkii, *Appl. Phys. Lett*. **79** (2001) 266–268.
10. A. N. Andriotis, M. Menon, D. Srivastava, and L. Chernozatonkii, *Phys. Rev. Lett*. **87** (2001) 066802 1–4.
11. A. N. Andriotis, M. Menon, D. Srivastava, and L. Chernozatonkii, *Phys. Rev.* **B 65** (2002) 165416 1–12.
12. L. P. Bíró, Z. E. Horváth, G. I. Márk, Z. Osváth, A. A. Koós, A. M. Benito, W. Maser, and Ph. Lambin, *Diam. Relat. Mater.* **13** (2004) 241–249.
13. M. Terrones, F. Banhart, N. Grobert, J.-C. Charlier, H. Terrones, and P. M. Ajayan, *Phys. Rev. Lett.* **89** (2002) 75505 1–4.
14. V. Meunier, M. B. Nardelli, J. Bernholc, T. Zacharia, and J.-C. Charlier, *Appl. Phys. Lett.* **81** (2002) 5234–5234.
15. E. C. Kirby, *MATCH-Commun. Math. Comp. Chem.* **48** (2003) 179–188.
16. S. Melchor and J. A. Dobado, *J. Chem. Inf. Comput. Sci.* **44** (2004) 1639–1646.
17. M. Yoon, S. Han, G. Kimm, S. B. Lee, S. Berber, E. Osawa, J. Ihm, M. Terrones, F. Banhart, J.-C. Charlier, N. Grobert, H. Terrones, P. M. Ajayan, and D. Tomanek, *Phys. Rev. Lett.* **92** (2004) 75504 1–4.
18. I. Zsoldos, Gy. Kakuk, T. Réti, and A. Szász, *Modeling Simul Mat. Sci. Eng.* **12** (2004) 1251–1266.
19. I. Zsoldos, Gy. Kakuk, J. Janik, and L. Pék, *Diam. Relat. Mater* **14** (2005) 763–765.
20. M. V. Diudea and Cs. L. Nagy, *Periodic Nanostructures*, Springer, 2007.
21. I. László, *Fullerenes, Nanotubes, Carbon Nanostruct.* **13** (2005) 535–541.
22. I. László, *Croat. Chem. Acta* **78** (2005) 217–221.
23. S. Melchor and J. A. Dobado, *J. Chem. Inf. Comput. Sci*. **44** (2004) 1639–1646.
24. D. W. Brenner, *Phys. Rev.* **B 42** (1990) 9458–9471.

SAŽETAK

Konstruiranje spojeva između ugljikovih nanocijevčica

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U radu su izvedene diofantske jednadžbe za konstrukciju spojeva između jednostrukih nanocijevčica proizvoljne kiralnosti i promjera. Rješenje ovih jednadžbi omogućava određivanje prikladnih trodimenzionalnih koordinata ugljikovih atoma u takvim strukturama. Prikazan je primjer sa spojem triju nanocijevčica.