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1 Introduction

As nanotubes can be applied both as devices and interconnects as well, there is a possibility to develop carbon nanotube based electronics where truly nanoelectronic architecture can be realized [1, 20]. Based on the geometric intersection of cylinders, we have recently presented an algorithm for constructing junctions where the new nanotube branches are attached to already developed ones [21–23]. In Ref. [7] an algebra was given for describing nanotube junctions where the authors used their method to characterize given structures. They constructed only the relative simple two-tube junctions as the inversion of their procedure. Based on their idea and using the terminology of manifolds we have developed diophantic equations for constructing junctions between single wall nanotubes of any chirality and diameter [24]. In the present paper an algorithm will be given for the solution of these equations.

2 Method and results

Nanotubes, characterized by the integers m, n and thus by the chiral vector $C_{\mathrm{h}} = m\boldsymbol{a}_1 + n\boldsymbol{a}_2$ can be imagined as rolled up graphene sheets, where the two unit vectors $\boldsymbol{a}_1$ and $\boldsymbol{a}_2$ show from the center of a hexagon to the center of the neighboring hexagons. We suppose that $\boldsymbol{a}_2$ is obtained by $+60°$ rotation of $\boldsymbol{a}_1$. If we have three tubes we have also three coordinate systems as well. By constructing the junction one have to tell in which way can we go from one coordinate system to the other. As we suppose that the non hexagonal polygons are at the boundaries of the coordinate systems each of them have two coordinates originated from the two neighboring tubes. The common non hexagonal and hexagonal polygons can be visualized as three ribbons, where the polygons are given by the local coordinates and the corresponding rotations of the local coordinates.

Figure 1 shows an example for constructing junction between the tubes (10,0), (10,1) and (10,2). In the center is a yellow hexagon with the coordinates (0,0). There is an other yellow hexagon at the right side of the figure for representing the hexagon with the coordinate (10,0). If we rotate this coordinate system by 120° we turn to the coordinate system of the second tube and can find an other yellow hexagon at the upper left corner with the coordinates (10,1). An other rotation by 120° gives the coordinate

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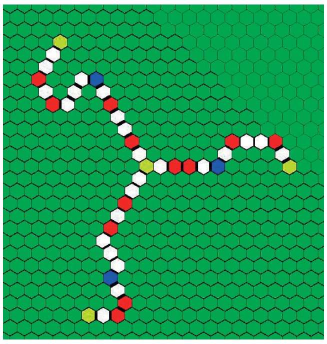

Fig. 1 (online colour at: www.pss-b.com) Representation of the three ribbons for construction of a junction between the nanotubes (10,0), (10,1) and (10,2), see the text.

system of the third tube and the yellow hexagon at the lower part of the figure with the coordinates (10,2). Now after constructing the three tubes (10,0), (10,1) and (10,2) we can draw on each of them the corresponding ribbons according to Fig. 1. Let us cut these tubes along the ribbons and keep the upper part of the tubes. These half tubes can be joined together at the yellow and the blue hexagons. Namely the three ribbons intersect each others at the yellow and blue hexagons. After joining in order the cut bonds we can obtain the junction of Fig. 2. Usually there are various possibilities for joining three nanotubes. Energy optimizing procedures can give the most stable structures. Here we give only an example where the three pairs of heptagons are in symmetric positions yielding about 120° branch angles.

In Fig. 2 it can be seen that the red hexagons turned to be the heptagons after joining together the three tubes and the white hexagons became hexagons after joining together the three pieces. The ribbons of Fig. 1 can be given by the parameters

$$\begin{pmatrix} m_1^k \\ n_1^k \end{pmatrix} \frac{T_1^{+k}}{T_1^{-k}} \begin{pmatrix} m_2^k \\ n_2^k \end{pmatrix} \frac{T_2^{+k}}{T_2^{-k}} \begin{pmatrix} m_3^k \\ n_3^k \end{pmatrix} \frac{T_3^{+k}}{T_3^{-k}} \cdots \begin{pmatrix} m_{Nk}^k \\ n_{Nk}^k \end{pmatrix} \frac{T_{Nk}^k}{T_{Nk}^k}, \tag{1}$$

where $\begin{pmatrix} m_i^k \\ n_i^k \end{pmatrix}$ are the relative coordinates of the i-th polygon on ribbon k and T_i^{+k} is the rotation of the coordinate system of the tube k. The unit of rotation is 60°. As each ribbon is between two tubes, ribbon k belongs to tube k (upper tube) and to the other neighbouring tube (lower tube) as well. The rotation on this neighbouring tube is T_i^{-k}. Thus $\frac{T_2^{+k}}{T_2^{-k}} \begin{pmatrix} m_3^k \\ n_3^k \end{pmatrix}$ means the rotation of the vector $\begin{pmatrix} m_3^k \\ n_3^k \end{pmatrix}$ by the angle T_2^{+k} on the upper and by the angle T_2^{-k} on the lower tube concerning ribbon k.

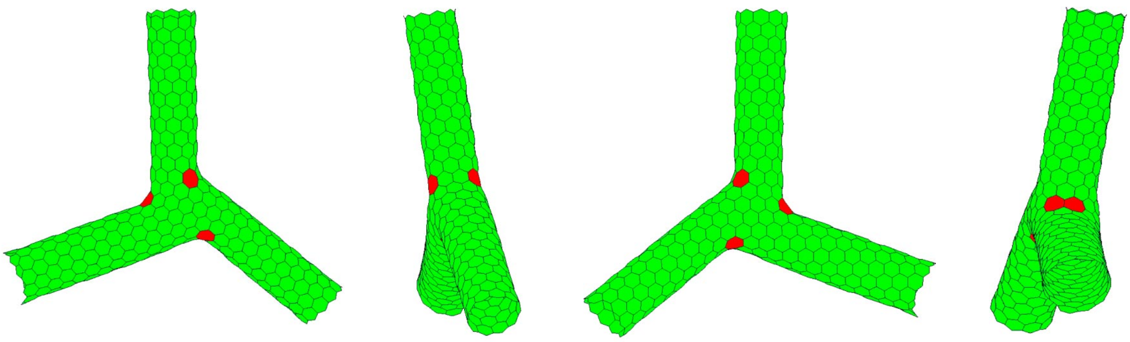

Fig. 2 (online colour at: www.pss-b.com) Junction 1 between the tubes (10,0), (10,1) and (10,2). Front view (a), left view (b), back view (c) and right view (d).

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For a polygon of n sides $T^- - T^+ = n - 6$. In Ref. [24] we have developed the following equations for the junction of three tubes with the parameters $\begin{pmatrix} m^1 \\ n^1 \end{pmatrix}$, $\begin{pmatrix} m^2 \\ n^2 \end{pmatrix}$ and $\begin{pmatrix} m^3 \\ n^3 \end{pmatrix}$:

$$\sum_{i=1}^{N1}(m_i^1 s(\sigma_{i-1}^1) + n_i^1 s(\sigma_{i-1}^1 + 1)) + s(\sigma_{N1}^1) - \sum_{i=1}^{N2}(m_i^2 s(\tau_{i-1}^2 + \alpha_{12}) + n_i^2 s(\tau_{i-1}^2 + \alpha_{12} + 1))$$
$$- s(\tau_{N2}^2 + \alpha_{12}) = m^1 s(\varphi_1) + n^1 s(\varphi_1 + 1)\,, \tag{2}$$

$$\sum_{i=1}^{N1}(m_i^1 s(\sigma_{i-1}^1 - 2) + n_i^1 s(\sigma_{i-1}^1 - 1)) + s(\sigma_{N1}^1 - 2) - \sum_{i=1}^{N2}(m_i^2 s(\tau_{i-1}^2 + \alpha_{12} - 2) + n_i^2 s(\tau_{i-1}^2 + \alpha_{12} - 1))$$
$$- s(\tau_{N2}^2 + \alpha_{12} - 2) = m^1 s(\varphi_1 - 2) + n^1 s(\varphi_1 - 1)\,, \tag{3}$$

$$\sum_{i=1}^{N2}(m_i^2 s(\sigma_{i-1}^2) + n_i^2 s(\sigma_{i-1}^2 + 1)) + s(\sigma_{N2}^2) - \sum_{i=1}^{N3}(m_i^3 s(\tau_{i-1}^3 + \alpha_{23}) + n_i^3 s(\tau_{i-1}^3 + \alpha_{23} + 1))$$
$$- s(\tau_{N3}^3 + \alpha_{23}) = m^2 s(\varphi_2) + n^2 s(\varphi_2 + 1)\,, \tag{4}$$

$$\sum_{i=1}^{N2}(m_i^2 s(\sigma_{i-1}^2 - 2) + n_i^2 s(\sigma_{i-1}^2 - 1)) + s(\sigma_{N2}^2 - 2) - \sum_{i=1}^{N3}(m_i^3 s(\tau_{i-1}^3 + \alpha_{23} - 2) + n_i^3 s(\tau_{i-1}^3 + \alpha_{23} - 1))$$
$$- s(\tau_{N3}^3 + \alpha_{23} - 2) = m^2 s(\varphi_2 - 2) + n^2 s(\varphi_2 - 1)\,, \tag{5}$$

$$\sum_{i=1}^{N3}(m_i^3 s(\sigma_{i-1}^3) + n_i^3 s(\sigma_{i-1}^3 + 1)) + s(\sigma_{N3}^3) - \sum_{i=1}^{N1}(m_i^1 s(\tau_{i-1}^1 + \alpha_{31}) + n_i^1 s(\tau_{i-1}^1 + \alpha_{31} + 1))$$
$$- s(\tau_{N1}^1 + \alpha_{31}) = m^3 s(\varphi_3) + n^3 s(\varphi_3 + 1)\,, \tag{6}$$

$$\sum_{i=1}^{N3}(m_i^3 s(\sigma_{i-1}^3 - 2) + n_i^3 s(\sigma_{i-1}^3 - 1)) + s(\sigma_{N3}^3 - 2) - \sum_{i=1}^{N1}(m_i^1 s(\tau_{i-1}^1 + \alpha_{31} - 2) + n_i^1 s(\tau_{i-1}^1 + \alpha_{31} - 1))$$
$$- s(\tau_{N1}^1 + \alpha_{31} - 2) = m^3 s(\varphi_3 - 2) + n^3 s(\varphi_3 - 1)\,, \tag{7}$$

$$\begin{aligned} &\sigma_{N1}^1 + \beta_{12} - \tau_{N2}^2 - \alpha_{12} = 0 \mod (6),\\ &\sigma_{N2}^2 + \beta_{23} - \tau_{N3}^3 - \alpha_{23} = 0 \mod (6),\\ &\sigma_{N3}^3 + \beta_{31} - \tau_{N1}^1 - \alpha_{31} = 0 \mod (6). \end{aligned} \tag{8}$$

Here we have $\sigma_0^k = \tau_0^k = 0$, $\sigma_{\mathrm{i}+1}^k = \sigma_{\mathrm{i}}^k + T_{\mathrm{i}}^{+k} +$ and $\tau_{i+1}^k = \tau_i^k + T_i^{-k}$.

The expression $s(\tau) = 2/\sqrt{3}\,\sin((\pi/3)\tau + (2\pi/3))$ is a function of the integer variable of τ. The φ_i are generated rotation angles. The number of polygons on ribbon k is N_k. The relative positions of the ribbons are given by the relative direction angles α_{12}, α_{23} and α_{31} on the yellow hexagon and with the relative direction angles β_{12}, β_{23} and β_{31} on the blue hexagon of Fig. 1. We suppose that $\alpha_{ij} > 0, \beta_{ij} < 0$.

Thus the algorithm for constructing a nanotube junction between three nanotubes is the following:

(1) according to the Euler relation [21–24] $3n_3 + 2n_4 + n_5 - n_7 - 2n_8 - 3n_9 - 4n_{10} - 5n_{11} - 6n_{12} - 7n_{13} - \ldots = -6$ we decide the number of non-hexagonal polygons (n_i is the number of faces with i vertices);

(2) we construct Eqs. (2)–(8) for these non-hexagonal polygons plus the hexagons neighbouring to the blue hexagons;

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(3) in Eqs. (2)−(8) we suppose that $T_i^{+k} = 0$ and $\varphi_1 = \varphi_2 = \varphi_3 = 0$;

(4) we solve Eqs. (2)−(8) using Gauss elimination;

(5) we chose an algebraic solution of Eqs. (2)−(8) which is also a geometric solution. A solution is geometric if step (6) can be realized;

(6) we extend the solution of point (5) by the ribbon hexagons as well. For hexagons the relation $T^- - T^+ = 0$ is valid.

3 Conclusions

In this work we have shown that using diophantic equations Descartes coordinates can be constructed for three carbon nanotubes of any chirality. We have presented our algorithm using the nanotubes (10,0), (10,1) and (10,2). The final coordinates were obtained by using conjugate gradient method for interactions obtained from Brenner potential [25].

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