2008

Joining a carbon nanotube and a graphene sheet

D. Baowan
University of Wollongong, db898@uow.edu.au

B. J. Cox
University of Wollongong, barryc@uow.edu.au

James M. Hill
University of Wollongong, jhill@uow.edu.au

Joining a carbon nanotube and a graphene sheet

Abstract

This paper is a synopsis of the two least squares approaches developed in [1] for the perpendicular joining of a flat graphene sheet with a carbon nanotube. The two least squares approaches are the variation in the bond length and the variation in the bond angle. These are used to examine the joined structure of a zigzag (8,0) carbon nanotube with a flat graphene sheet. There are sixteen possible distinct defects corresponding to the number of atoms at the (8,0) tube open end, and therefore, in total sixteen joining structures need to be investigated. Moreover, the polygons that occur at the junction are determined and are shown to be consistent with Euler's theorem. Assuming that only pentagons, hexagons and heptagons are acceptable, the number of possible structures is greatly reduced, but there is only one structure that is physically meaningful. These purely geometrical approaches can be formally related directly to a certain numerical energy minimization method used by a number of authors [2-5].

Keywords

Carbon nanotube, Graphene sheet, Joining nanostructures, Variation in bond length, Variation in bond angle

Disciplines

Physical Sciences and Mathematics

Publication Details

This conference paper was originally published as Baowan, D, Cox, BJ and Hill, JM, Joining a carbon nanotube and a graphene sheet, International Conference on Nanoscience and Nanotechnology, ICONN 2008, Melbourne, 25-29 February 2008. Copyright Institute of Institute of Electrical and Electronics Engineers 2008. Original conference paper available here

Joining a carbon nanotube and a graphene sheet

Duangkamon Baowan, Barry J. Cox and James M. Hill
School of Mathematics and Applied Statistics, University of Wollongong, NSW, Australia 2500
Email: db898@uow.edu.au , barryc@uow.edu.au, jhill@uow.edu.au
Tel: +61 (02) 4221 3822, Fax: +61 (02) 4221 4845

Abstract— **This paper is a synopsis of the two least squares approaches developed in [1] for the perpendicular joining of a flat graphene sheet with a carbon nanotube. The two least squares approaches are the variation in the bond length and the variation in the bond angle. These are used to examine the joined structure of a zigzag (8,0) carbon nanotube with a flat graphene sheet. There are sixteen possible distinct defects corresponding to the number of atoms at the (8,0) tube open end, and therefore, in total sixteen joining structures need to be investigated. Moreover, the polygons that occur at the junction are determined and are shown to be consistent with Euler's theorem. Assuming that only pentagons, hexagons and heptagons are acceptable, the number of possible structures is greatly reduced, but there is only one structure that is physically meaningful. These purely geometrical approaches can be formally related directly to a certain numerical energy minimization method used by a number of authors [2-5].**

Keywords-component; Carbon nanotube, Graphene sheet, Joining nanostructures, Variation in bond length, Variation in bond angle

I. INTRODUCTION

Nanotechnology is a major focus in science and technology, and most research in this area deals with chemical, physical and biological issues or a combination of these areas, and very little work has so far been undertaken on mathematical modeling. In this study, we utilize classical applied mathematical modeling procedures and elementary geometrical principles to investigate the perpendicular joining structure between a flat graphene sheet and a carbon nanotube.

For future nano-electronic systems, graphene sheets might be needed as platforms to transmit signals to other materials through carbon nanotubes. The connection of graphene sheets with carbon nanotubes is an interesting problem that may have many potential applications. Here, we examine a particular perpendicular connection of a zigzag (8,0) carbon nanotube and a graphene sheet. Two least squares approaches are employed. These are the variation in the bond length, which seeks to minimize the distance between an atom on the tube open end and an atom on the sheet from the ideal bond length σ, and the variation in bond angle, which involves fixing all the bond lengths to be exactly σ and then minimizing the bond angle. Furthermore, Euler's theorem, which is widely used to determine the geometrical structure for carbon nanostructures [6-9], is utilized to confirm the correctness of the polygons occurring at the junction.

We also comment that our two approaches are directly related to the computer simulations of [2-5], which minimize the quadratic potential energy per bond given by

$$E = \frac{1}{2}k_r(r-r_0)^2 + \frac{1}{2}k_\theta(\theta-\theta_0)^2 + \frac{1}{2}k_\tau(1-\cos(n\phi-\phi_0)), \quad (1)$$

where k_r, k_θ and k_τ are certain bond stretching, bending angle and torsional constants, respectively, r_0, θ_0 and φ_0 are the equilibrium values of the bond length, bond angle and ideal phase angle for this bond type, respectively, and n is an integer. In general, from the above equation our variation in bond length approach corresponds to taking the bond stretching energy, and similarly, our variation in bond angle approach corresponds to taking only the angle bending energy into account.

The variation in bond length is detailed in the following section. Sixteen possible distinct defects on the flat graphene sheet, which can be considered as a platform to connect the (8,0) carbon nanotube, are classified in section II. Once the two structures are joined, Euler's theorem is utilized to determine the most likely physical structure and the result is presented in section III. In section IV, the chosen configuration from section III is reconsidered using the variation in bond angle approach. Finally, a summary is given in section V.

II. VARIATION IN BOND LENGTH

Firstly, we employ a least squares approach to the bond length. The basic idea is that we seek to minimize the variation in distance between an atom on the tube open end and the adjoining atom on the sheet from the ideal bond length σ, which is taken to be 1.42 Å. We assume that the atom positions on the tube end and the graphene sheet are fixed. There are eight atoms on a (8,0) tube end that must be connected to the tube by two carbon bonds, so that they require one more bond to complete the sp^2 structure. Consequently, the defect on the graphene sheet must have eight atoms which each require one further bond to complete the structure, and there are sixteen possible defects to which the (8,0) tube might be joined which are shown in Figure 3.

In Cartesian coordinates (x, y, z), the flat graphene sheet is assumed to be located in the (x, y) plane, and the ith atom on the sheet is assumed to have the position vector $\mathbf{a}_i = (a_{xi} + X, a_{yi} + Y, 0)$. The sheet is allowed to move in both the x- and y-directions by the distances X and Y, respectively, which can be either positive or negative. The position vector of the ith atom

on the tube is assumed to be given by $\mathbf{b}_i = (b_{xi}, b_{yi}, l)$ where l is the assumed spacing between the tube and the sheet in the positive z-direction. Moreover, we suppose that the tube can be rotated by an angle θ. Adopting a least squares approach, we determine X, Y, l and θ which minimize the function

$$f(X,Y,l,\theta) = \sum_{i=1}^{8} (|\mathbf{a}_i - \mathbf{b}_i| - \sigma)^2, \qquad (2)$$

where $|\mathbf{a}_i - \mathbf{b}_i|$ is the Euclidean distance between an atom on the tube end and an atom on the sheet. The numerical values for the least squares function f and the number of polygons P_n, where n is the number of sides occurring at the junctions, are shown in Table 1.

TABLE 1. Values of function f (Å^2) and polygons P_n

Configuration #	f	P_5	P_6	P_7	P_8	P_9
1	0.0239	-	4	2	2	-
2	0.2092	1	3	1	3	-
3	0.0018	-	4	2	2	-
4	0.0676	1	2	3	2	-
5	1.2631	2	-	4	2	-
6	0.0817	-	2	6	-	-
7	0.0729	1	1	5	1	-
8	0.0020	1	2	3	2	-
9	0.0592	2	2	-	4	-
10	0.0793	2	1	2	3	-
11	0.5513	2	-	5	-	1
12	0.2498	2	-	4	2	-
13	0.0404	2	1	2	3	-
14	0.6005	3	-	2	2	1
15	0.5262	3	-	2	2	1
16	0.5284	4	-	-	2	2

III. EULER'S THEOREM

In this section, we begin by considering Euler's theorem which states that;

$$F + V - E = \chi, \qquad (3)$$

where F, V and E denote the number of faces, vertices and edges for the given polyhedron and χ is the Euler characteristic. Since any surface which is homeomorphic to a sphere has an Euler characteristic of 2, all the polygons occurring at the connecting sites need to satisfy the relation:

$$2P_4 + P_5 - P_7 - 2P_8 - 3P_9 = 12. \qquad (4)$$

However, a square ring is believed to be very unstable for a carbon network [6] and experimentally defects in the carbon nanotube are observed to have only pentagons and heptagons [8]. Therefore, only configuration #6 meets these requirements and the resulting three dimensional structure is shown in Figure 2(a).

IV. VARIATION IN BOND ANGLE

In this section we examine the variation in bond angle approach. We attempt to minimize the variation of the bond angle at each connection site from the maximum normal physical value for both the sheet and the tube. For the graphene sheet, the bond angle is assumed to be 120˚, while the bond angle for the (8,0) nanotube is taken from the new model of carbon nanotubes which properly incorporates the curvature of Cox and Hill [10] and which is found to be 118.70˚.

Since the atomic networks on both the sheet and the tube are formed from hexagonal rings, a general procedure to determine the position vectors of all atoms at the junction is given by:

i. Find the point **M** which is the mid-point of $\mathbf{A}_1$ and $\mathbf{A}_2$,

ii. Find the vector $\mathbf{U} = \mathbf{MA}_3$,

iii. Find the unit vector $\mathbf{V} = \mathbf{A}_1\mathbf{A}_2/|\mathbf{A}_1\mathbf{A}_2|$ which is perpendicular to **U**,

iv. Determine the vector **W** which is perpendicular to both **U** and **V** and has the same magnitude as **U**; namely $\mathbf{W} = \mathbf{U} \times \mathbf{V}$,

v. The atom position is then given by $\mathbf{M} + \mathbf{U}\cos\theta + \mathbf{W}\sin\theta$,

where $\mathbf{A}_1$, $\mathbf{A}_2$ and $\mathbf{A}_3$ are the atoms position as shown in Figure 1. The atom $\mathbf{A}_3$ which is the joining position can move around a circular path and whose position is determined by an angle θ. Moreover, each bond length which joins between an atom on the tube to one on the sheet is restricted to be 1.42 Å. We refer the reader to Baowan et al. [1] for the full details of this method.

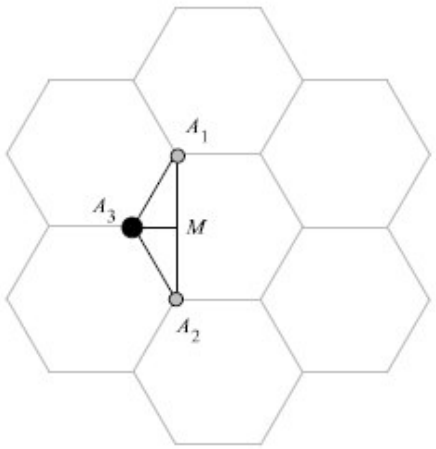

Figure 1. Position vectors for the variation in bond angle approach.

Here, we examine the joining of the (8,0) tube with the defect #6 identified as the most likely configuration from the

bond length approach. Again by using the minimization process, the three dimensional structure is shown in Figure 2(b).

We comment that in terms of the variation in bond length, all bond lengths on the tube and the sheet are fixed. However, the bond lengths which connect between the atoms at the tube open end and the atoms on the sheet may vary from the assumed bond length σ, which means that the variation in bond length approach affects both the bond stretching and the bond angle terms in the energy equation (1). On the other hand for the variation in bond angle approach, all the bond lengths are fixed and only the bond angle varies, and therefore, the bond stretching term will always be zero.

From Figure 2, it is clear that the two approaches give very similar structures in terms of the atom locations. In order to give a more mathematical measure to the difference between the atom locations, we determine the mean absolute error for which we obtain a difference in bond length of 26.19%. However, the theoretical structures examined here have yet to be confirmed either experimentally or by molecular dynamics simulation.

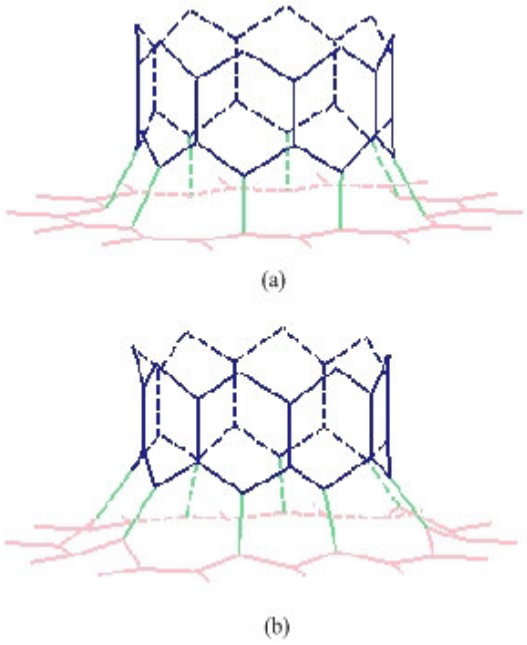

Figure 2. Three dimensional illustrations for (8,0) connection with grapheme sheet by (a) variation in bond length and (b) variation in bond angle.

V. SUMMARY

Two least squares approaches are undertaken here to determine the joined structure between a flat graphene sheet and a zigzag (8,0) carbon nanotube. The composite structure is regarded as a possible future nanoelectromechanical device to transmit signals to other materials which employs the sheet as a platform. In this study, sixteen distinct defects on the sheet, corresponding to the number of the atoms at the (8,0) tube open end, are proposed. All the bond lengths for both the sheet and the tube are assumed to be σ = 1.42 Å, the bond angle of the sheet is taken to be 120˚, and the bond angle for the (8,0) tube is the value proposed in the new geometric model of carbon nanotubes by Cox and Hill [10] which is 118.70˚.

The variation in bond length approach is employed to minimize the deviations of the joining distances between atoms on the tube open end and atoms on the sheet from the ideal bond length σ. On the other hand, for the variation in bond angle method, we fix all the bond lengths to be σ and then seek to minimize the bond angles from the physical bond angle values. We comment that both variation approaches are closely related to the bonded energy equation that is widely used by a number of authors [2-5]. Furthermore, Euler's theorem is utilized to verify the polygons which occur at the connection site, and it can be shown that the polygons obtained are all compatible with Euler's theorem. However, we note that such theoretical structures have yet to be confirmed either experimentally or by molecular dynamics simulations. Finally, we note that the corresponding problem for the perpendicular joining of a boron nitride nanotube and a boron nitride sheet is examined in the recent paper [11]. However, due to the alternating boron and nitrogen atoms in boron nitride structures, the defined defects are more complicated, and the mathematical ideas developed there are quite different to those elucidated here.

ACKNOWLEDGMENT

The support of the Australian Research Council, both through the Discovery Project Scheme and for providing an Australian Professorial Fellowship for JMH is gratefully acknowledged.

REFERENCES

[1] D. Baowan, B. J. Cox, and J. M Hill, "Two least squares analyses of bond lengths and bond angles for the joining of carbon nanotubes to graphenes," Carbon, vol. 45, pp. 2972-2980, 2007.

[2] W. D. Cornell, P. Cieplak, C. I. Bayly, I. R. Gould, et al., "A second generation force field for the simulation of proteins, nucleic acids, and organic molecules," J. Am. Chem. Soc., vol. 117, pp. 5179-5197, 1995.

[3] C. Li, and T. –W. Chou, "A structural mechanics approach for the analysis of carbon nanotubes," Int. J. Solids Struct., vol. 40, pp. 2487-249, 2003.

[4] Y. Jin, and F. G. Yuan, "Simulation of elastic properties of single-walled carbon nanotubes," Comp. Sci. Technol., vol. 63, pp. 1507-1515, 2003.

[5] T. Natsuki, K. Tantrakarn, and M. Endo, "Effects of carbon nanotube structures on mechanical properties," vol. 79, pp. 117-124, 2004.

[6] H. W. Kroto, "The stability of the fullerenes C_n, with n=24, 28, 32, 36, 50 and 70," Nature, vol. 329, pp. 529-531, 1987.

[7] H. Terrones, and A. L. Mackay, "The geometry of hypothetical curved graphite structures," Carbon, vol. 30, pp. 1251-1260, 1992.

[8] T. W. Ebbsene, and T. Takada, "Topological and sp^3 defect structures in nanotubes," Carbon, vol. 33, pp. 973-978, 1995.

[9] A. Maiti, C. J. Brabec, and J. Bernholc, "Kinetics of metal-catalyzed growth of single-walled carbon nanotubes," Phys. Rev. B, vol. 55, pp. R6097-R6100, 1997.

[10] B. J. Cox, and J. M. Hill, "Exact and approximate geometric parameters for carbon nanotubes incorporating curvature," Carbon, vol. 45, pp. 1453-1462, 2007.

[11] D. Baowan, B. J. Cox, and J. M. Hill, "Junctions between a boron nitride nanotube and a boron nitride sheet," Nanotechnology, vol. 19, pp. 075704, 2008.

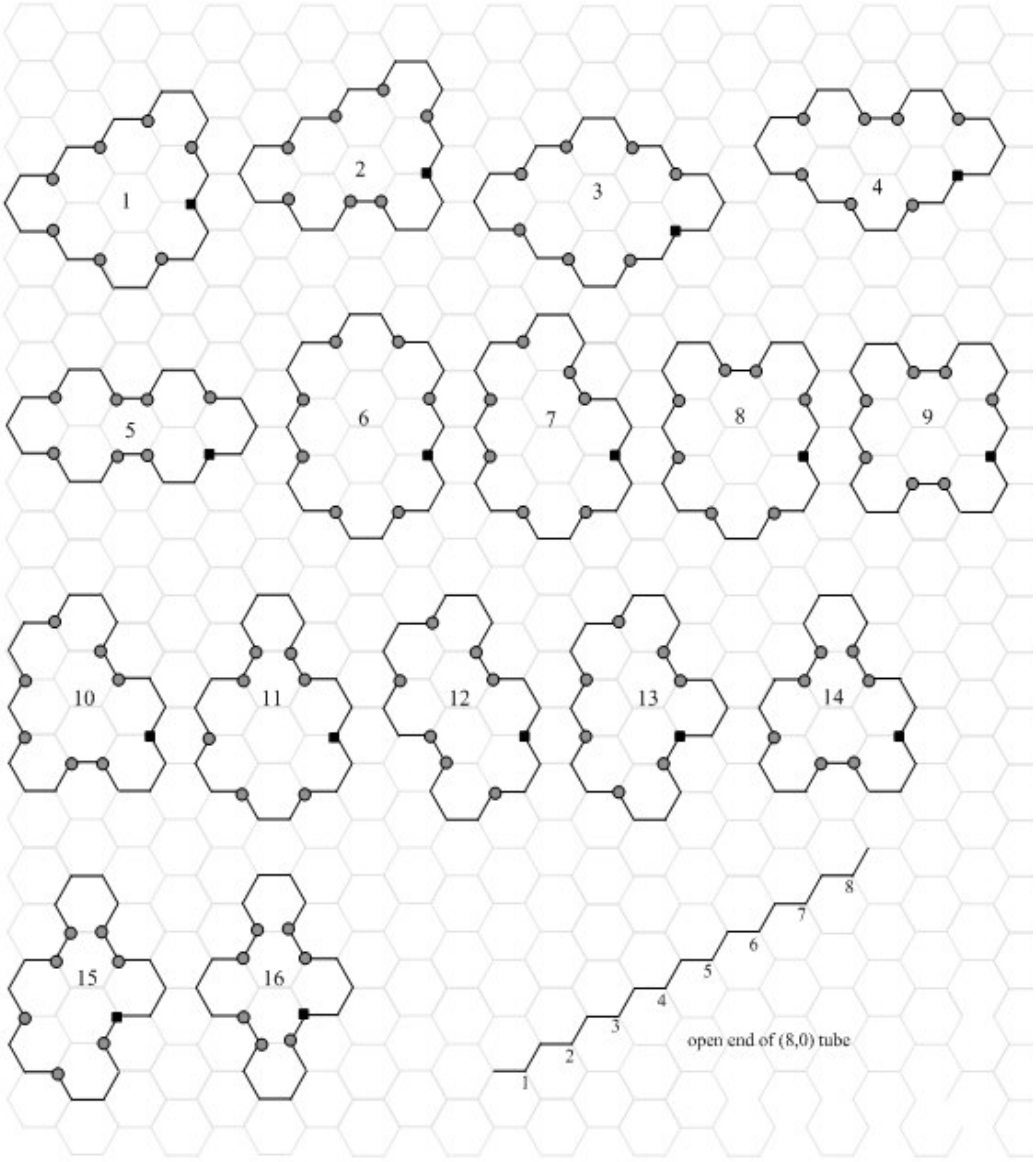

Figure 3. Sixteen possible defects which require another eight bonds for sp^2 network where a black square is the first atom on the sheet.