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Bond lengths and diameters of armchair single wall carbon nanotubes

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Abstract

CC bond lengths and diameters of armchair single wall carbon nanotubes from (4,4) to (15,15) have been calculated using semi-empirical PM3 and PM5 and density functional PBEPBE and B3LYP methods. The CC bonds are found to be elongated comparatively to those in graphene sheet, 1.421 Å. The bonds directed along the nanotube axis and circumference are elongated differently. The smaller the nanotube index, the larger the bond elongation, but it does not exceed 0.008 Å (0.6% of the graphene sheet value) even for the (5,5) nanotube. We suggest new theoretical relationship between the nanotube diameter, indices, and bond lengths.
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1. Introduction

The structure of an ideal straight, infinitely long single wall carbon nanotube (SWCNT) can be uniquely described by two integers (n, m), which refer to the number of unit vectors of the lattice that are contained in the chiral vector. From the (n, m) indices, one can calculate the diameter of a tube d_t, and other properties of SWCNTs [1]. Besides indices (n, m), an additional parameter that one should know to calculate a nanotube diameter is the CC bond length a_{CC}. Since SWCNT is considered as a graphene sheet rolled up to form a cylinder, the CC bond length in a nanotube is often considered to be equal to that in graphene sheet (measured in bulk graphite), $a_{CC} = 1.421$ Å [2]. For an ideal SWCNT (n, m) with ideal CC bonds, the nanotube diameter is given by the mathematical formula (1) [1]. However, a real nanotube is not cylindrical, but polyhedral (see below). So, we use a prime (′) in formula (1) in order to emphasize that d'_t is

not a diameter of a real nanotube-polyhedron, but that of an ideal nanotube-cylinder,

$$d'_t = a_{CC}\{3(n^2 + nm + m^2)\}^{1/2}/\pi. \tag{1}$$

For armchair SWCNT (n, n) formula (1) is reduced to (2),

$$d'_t = 3na_{CC}/\pi = 0.955na_{CC}. \tag{2}$$

It has been found that the position of some peaks in the Raman spectra [3–6] and bands in the optical absorption and luminescence spectra [7–11] of SWCNTs are directly (or, rather, inversely) related to the nanotube diameter. The dependence of spectra on the nanotube diameter (and chirality) is of significant practical importance for the development of fast, non-destructive, and convenient methods of analysis of SWCNTs mixtures. Few empirical equations have been proposed for the description of the 'band-diameter' dependence in the Raman and optical absorption spectra. And many authors use the 'ideal' value of 1.421 (or 1.42) Å for the CC bond length upon modeling of nanotube properties [5,10,12–14].

However, it is clear that upon rolling up, the CC bonds are distorted, and the degree of the distortion

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should depend on the nanotube curvature (i.e., on the nanotube diameter). Furthermore, the distortion can also depend on the bond orientation relative to the nanotube axis. For example, in an armchair SWCNT there are two types of bonds, directed nearly along the nanotube axis, CC_a, and directed along the nanotube circumference, CC_c, see Fig. 1. The number of CC_a bonds is twice as many as that of CC_c ones.

This appears to be a reason why some authors use a somewhat larger value of 1.44 Å for the CC bond length for calculations of a nanotube diameter and corresponding band positions in the spectra [3,8,15,16]. On the other hand, the smaller value of 1.415 Å is also used [17], and one can find even much lower value of 1.25 Å for this parameter [18].

Since many SWCNTs with different chirality have nearly similar diameters, calculations using different values for the CC bond length (and different empirical equations) result in redefinition of the band positions in the spectra. The same band can correspond to different SWCNTs depending on the equation and the CC bond length used. For example, assuming $a_{CC} = 1.42$ Å and using formula (1), one obtains the values of 12.60 and 15.64 Å for the diameters of (13,5) and (13,10) nanotubes, respectively. However, assuming $a_{CC} = 1.44$ Å, the same diameters are obtained for (12,6) and (16,6) nanotubes, respectively.

In this connection, some important questions arise. How large is a distortion of the CC bonds upon rolling up the graphene sheet to a SWCNT? How does it depend on the SWCNT curvature (indices)? What is an error if we neglect the distortion? What is the relationship between nanotube diameter, the CC bond length, and nanotube indices?

There are no direct X-ray structural data on the CC bond lengths in SWCNTs. The only way to get an idea of a possible distortion of the CC bonds and diameter in dependence on the nanotube indices is quantum-chemical calculations.

In the present Letter, we systematically investigate the geometry of SWCNTs using semiempirical and DFT methods. The structures of infinite armchair SWCNTs from (4,4) to (15,15) have been calculated

with full geometry optimization. It is found that the CC bonds in nanotubes are elongated as compared to the value in graphene sheet. The two kinds of bonds in an armchair SWCNT, CC_a and CC_c, are elongated in different ways. The smaller the nanotube index, the larger the bond elongation. However, even for the (5,5) nanotube, the elongation does not exceed 0.008 Å (according to both semiempirical and DFT data), that is 0.6% relative to the graphene sheet value of 1.421 Å. Thus, the value of 1.44 Å for the CC bond length in armchair SWCNTs is an overestimation.

Due to the fact that a real nanotube is not cylindrical, the theoretical relationship (1) between the nanotube diameter, indices and bond length is broken. Calculated data enable us to put forward a new Eq. (5), which differs from the formula (1) by the presence of a free term and a reduced value of the coefficient before n.

2. Computational methods

Geometric structures of infinite nanotubes have been calculated with full geometry optimization using the semiempirical PM3 and PM5 methods and density functional theory (DFT) methods, the hybrid density functional B3LYP (Bercke's three-parameter nonlocal-exchange functional with the non-local correlation functional of Lee, Yang, and Parr), and the gradient-corrected correlation functional PBEPBE (functional of Perdew, Burke and Ernzerhof) with periodic boundary conditions (PBC) with the 3-21G*, 6-31G, 6-31G*, 6-311G* basis sets. All calculations were performed by employing the quantum chemical program packages MOPAC 2002 [19] and GAUSSIAN 03 [20].

The optimization was performed under symmetry constraints, all atoms were assumed to have the same radial distance from the nanotube axis, and all CC_a and CC_c bond lengths were set to be equal within the two groups of bonds. In semiempirical calculations, we used the nanotube fragment consisting of 20 layers (sections) of carbon atoms.

3. Results and discussion

Table 1 presents the following parameters of armchair SWCNTs: heat of formation per carbon atom ΔH_f^c, the length of the bond directed along the nanotube axis CC_a and along the nanotube circumference CC_c, and the nanotube diameter d_t, calculated by different methods. For comparison, the nanotube diameter, calculated for an ideal rolled-up cylinder of graphene sheet using formula (1) and the CC bond lengths of 1.42 and 1.44 Å, are also shown.

ΔH_f^c is the quantity, which determines the thermodynamic stability of SWCNTs of different diameters.
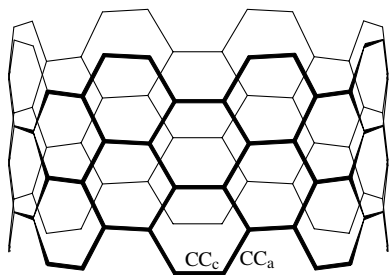

Fig. 1. Geometry of an armchair nanotube with two types of bonds, CC_a and CC_c.

Table 1
Parameters of armchair single wall carbon nanotubes: heat of formation per carbon atom ΔH_f^c, the lengths of bonds directed along the nanotube axis CC_a and nanotube circumference CC_c, and the nanotube diameter d_t, calculated by different methods

SWCNT	ΔH_f^c	CC_a (Å)	CC_c (Å)	d_t (Å)	Method	$d'_{t(1.42)}$[a] (Å)	$d'_{t(1.44)}$[a] (Å)
(4,4)	9.34	1.424	1.429	5.518	PM3	5.424	5.500
		1.437	1.442	5.571	PBEPBE/3-21C*		
		1.435	1.439	5.566	PBEPBE/6-31C*		
		1.432	1.435	5.546	PBEPBE/6-311C*		
		1.432	1.439	5.546	B3LYP/6-31G		
		1.429	1.435	5.546	B3LYP/3-21G*		
(5,5)	6.88	1.423	1.426	6.854	PM3	6.780	6.875
	6.30	1.420	1.425	6.842	PM5		
		1.435	1.438	6.762	PBEPBE/3-21G*		
		1.428	1.431	6.844	B3LYP/3-21G*		
	5.54				Estimated[b]		
(6,6)	5.58	1.422	1.424	8.198	PM3	8.136	8.251
(8,8)	4.30	1.421	1.423	10.895	PM3	10.848	11.001
(9,9)	3.96	1.420	1.423	12.246	PM3	12.204	12.376
(10,10)	3.72	1.420	1.422	13.598	PM3	13.560	13.751
		1.433	1.434	13.717	PBEPBE/3-21G*		
(12,12)	3.40	1.420	1.422	16.305	PM3	16.272	16.501
(15,15)	3.15	1.420	1.422	20.368	PM3	20.340	20.626
Graphene sheet	2.8		1.420	(∞)	PM3		
	2.2		1.417		PM5		
			1.430		PBEPBE/3-21G*		
			1.429		PBEPBE/6-31G*		
			1.427		PBEPBE/6-311G*		
			1.425		B3LYP/6-31G		
			1.424		B3LYP/3-21G*		
	1.96[c]		1.421		Experimental		

[a] Diameters $d'_{t(1.42)}$ and $d'_{t(1.44)}$ were calculated by formula (1) for ideal cylindrical nanotubes using the CC bond length of 1.42 and 1.44 Å, respectively.

[b] Estimated from B3LYP/6-311G*-calculated heats of formation of capped finite-length (5,5) armchair SWCNTs [30].

[c] Calculated based on the heat of wetting for graphite [21].

Experimentally, ΔH_f^c is zero by definition for bulk graphite and 1.96 kcal/mol for a single graphene sheet, according to empirical estimates for the van der Waals interactions between the graphite layers [21]. As one could expect, ΔH_f^c decreases with the nanotube diameter (index) increasing; the calculated PM3 data can be fitted by the inverse second-order polynomial (see Fig. 2):

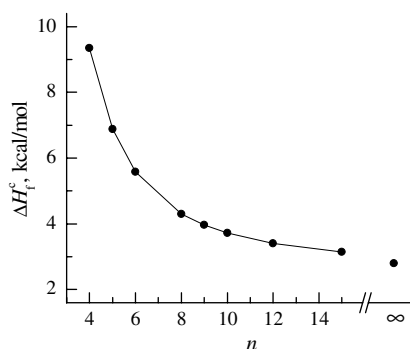$$\Delta H_f^c = (2.65 \pm 0.01) + (106.5 \pm 0.5)/n^2 \text{ kcal/mol}, \quad (3)$$

Fig. 2. PM3-calculated heat of formation per carbon atom (ΔH_f^c) vs. the nanotube index (n) for armchair SWCNTs (n, n). The limiting value calculated for graphene sheet is also shown.

with the correlation coefficient of 0.9999 and the standard error of 0.03 kcal/mol. Here, the free term corresponds to the ΔH_f^c of graphene sheet ('a nanotube with infinite diameter') and is close to the value calculated by the same method (Table 1).

To compare the relative thermodynamic stability of different kinds of nanotubes (armchair, zigzag, chiral), it is useful to correlate the relative heat of formation of a nanotube with its diameter,

$$\Delta H_f^c = (2.61 \pm 0.03) + (203.0 \pm 1.7)/d_t^2 \text{ kcal/mol}. \quad (4)$$

Here, the correlation coefficient is 0.9998 and the standard error is 0.05 kcal/mol. It should be noted that, according to a simple theory, the ratio of strain energies of nanotubes is close to the reciprocal square of the ratio of the corresponding tube radii [22].

The new PM5 method has been shown to predict heats of formation with higher accuracy as compared to PM3 [23]. The present calculations also confirmed this conclusion; see the data for graphene sheet and the (5,5) nanotube (Table 1). On the other hand, as one can see from Table 1, PM3 reproduces better than PM5, within 0.001 Å, the CC bond length in graphene sheet. At the PBEPBE level in the row of the basis sets

3-21G*–6-31G*–6-311G*, the calculated CC bond length in graphene sheet decreases from 1.430 to 1.427 Å. When passing from the PBEPBE to B3LYP functionals with the 3-21G* basis set, the CC bond length in graphene sheet decreases from 1.430 to 1.424 Å (Table 1). The B3LYP/3-21G* calculated CC bond length is 0.003 Å longer than the experimental value for graphite, 1.421 Å.

All the methods used predict that the two kinds of the C–C bonds, CC_a and CC_c (see Fig. 1), have different lengths (Table 1). The difference between the CC_a and CC_c bond lengths decreases with the nanotube diameter increasing; the length of each kind of bond approaches that in graphene sheet, see Fig. 3a. The largest deviations from the graphene CC bond length are predicted for the small-diameter nanotubes. For example, at the PBEPBE/3-21G* level, as compared to graphene sheet, the CC_c bond length increases by 0.004, 0.008, and 0.012 Å for the nanotubes (10,10), (5,5), and (4,4), respectively (Table 1). Nearly the same increase of the CC_c bond length is predicted at the B3LYP/3-21G* level: by 0.007 and 0.011 Å for the nanotubes (5,5) and (4,4), respectively. At the PM3 level, the CC_c bond length in the nanotube (4,4) exceeds that in graphene

sheet by 0.009 Å, and the CC_a bond length – by 0.005 Å. Already starting from the nanotube (9,9), the CC_a bond length is equal to that in graphene sheet.

One can pay attention to an interesting aspect of nanotube geometries, namely, the ratio between the CC bond length and the nanotube diameter. Despite the CC bond lengths for all nanotubes are close to 1.42 Å, the diameter of the (5,5) nanotube is close to the value estimated by formula (1) using $a_{CC} = 1.44$ Å and for the (4,4) nanotube even exceeds this value (Table 1). This can be clearly seen in Fig. 3b where the relative diameters $(d'_t - d_t)$ are plotted as a function of the nanotube index.

To explain the discrepancy between the optimized diameter and that calculated by formula (1), one should take into consideration the conditions, at which formula (1) was derived. Upon rolling up the graphene sheet, the length of the chiral vector is equated with the perimeter of the circle whose diameter is marked as d'_t in Fig. 4. However, a real nanotube is not cylindrical, but polyhedral, and the nanotube cross-section is not circular, but polygonal. Therefore, the length of the chiral vector is equal to the perimeter of a polygon, whereas the nanotube diameter is a diameter of the circumcircle, d_t in Fig. 4. The relationship between these two diameters is $d'_t < d_t$. For armchair SWCNTs with even n, the nanotube diameter is equal to the main diagonal of the polygon and can be 'measured' as the distance between two opposite carbon atoms, as shown in Fig. 4 for SWCNT (4,4). For armchair SWCNTs with odd n, there are no diagonally opposite carbon atoms, see SWCNT (5,5) in Fig. 4. The nanotube diameter can be obtained as twice the radius, i.e., the distance of a carbon atom from the nanotube axis.

Fig. 5 shows the dependence of the PM3 calculated diameter on the nanotube index. The data obtained can be fitted by a linear polynomial,

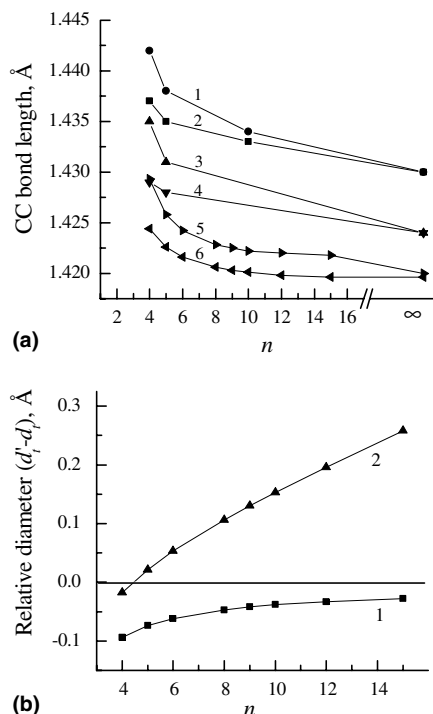$$d_t = (0.101 \pm 0.009) + (1.350 \pm 0.001)n \text{ Å}, \quad (5)$$

Fig. 3. (a) CC bond length vs. the nanotube index (n) for different kinds of bonds: CC_a (2,4,6) and CC_c (1,3,5), calculated at the PBEPBE/3-21G* (1,2), B3LYP/3-21G* (3,4) and PM3 (5,6) levels. The values for graphene sheet are shown as limiting ones. (b) Relative armchair SWCNT diameter $(d'_{t(1.42)} - d_t)$, curve (1) and $(d'_{t(1.44)} - d_t)$, curve (2) vs. the nanotube index (n), where d_t is the PM3-optimized diameter, $d'_{t(1.42)}$ and $d'_{t(1.44)}$ are the diameters calculated by formula (1) using the CC bond length of 1.42 and 1.44 Å, respectively.
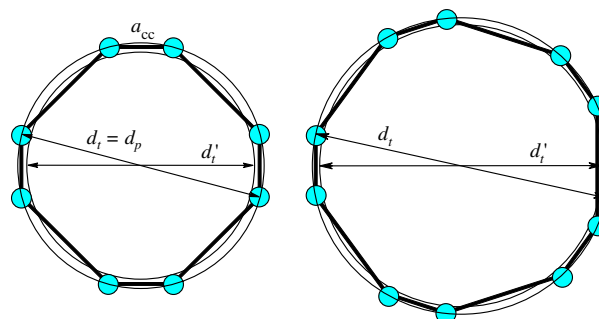
Fig. 4. Cross-sectional cuts of (4,4) and (5,5) SWCNTs; d_t is the diameter of the real optimized tube, d'_t is the diameter calculated by formula (1) for an ideal cylindrical tube, d_p is the main diagonal of a polygon (for the (4,4) SWCNT it is an octagon).
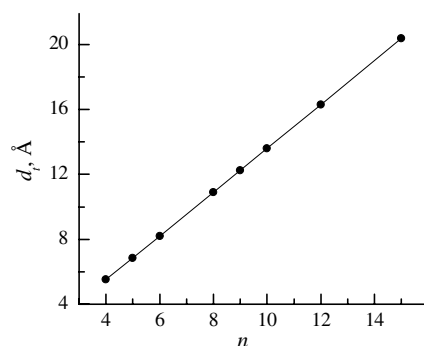
Fig. 5. PM3-calculated nanotube diameter (d_t) vs. the nanotube index (n) for armchair SWCNTs (n, n).

with the correlation coefficient of 0.99999 and the standard error of 0.010 Å. Appearance of a free term in Eq. (5) as compared to formula (2) obviously is a result of the non-cylindrical structure of a nanotube and appears due to a deviation of the CC bond length from the ideal one for the smaller diameter nanotube. The coefficient before n is close to that calculated by formula (2) using $a_{CC} = 1.42$ Å: $0.955 * 1.42 = 1.356$.

It is noteworthy to compare the results obtained here with other theoretical calculations. As was already mentioned above, calculations of energetics and electronic properties (band-gap value, density of states (DOS), frontier molecular orbital distribution) of nanotubes are often performed under fixed geometry using $a_{CC} = 1.42(1)$ [12,13,24–28] or 1.44 Å [15,22]. There are scarce and conflicting data in the literature on the optimized CC bond lengths and nanotube diameters calculated by various quantum-chemical methods.

For a finite-length open-ended (4,4) SWCNT, DFT at the B3LYP/6-31G* level predicts $a_{CC} = 1.414$ Å and $d_t = 5.488$ Å [29]. Hou at al. [29] did not comment on the fact that, despite the calculated bond length is smaller than 1.42 Å, the nanotube diameter coincides with that (5.50 Å) estimated using the CC bond length of 1.44 Å (see the explanation above). Cioslowski et al. [30] used the same B3LYP method (but with the 6-311G* basis set) for optimization of capped finite-length fragments of (5,5) SWCNT. They did not report the optimized geometry but pointed out to a mismatch between the diameters of the caps and the main body of the nanotube. Van Lier et al. [31] also determined the dependence of a closed (end-capped) nanotube diameter on the fragment length; the calculated diameters (at the HF/6-31G* level) are 7.06 and 6.88 Å for C_{80} and C_{150} fragments of the (5,5) nanotube, respectively. Wu et al. [32] found that the bond length in optimized open-end finite-length nanotube fragments depends on the position of the bond relative to the fragment end; for example, in the (5,5) nanotube the CC bond length varies from 1.413 to 1.452 Å (the B3LYP/3-21G data).

The geometry of the (6,6) nanotube was calculated by different DFT methods and varies depending on the approximation used. The local density approximation (LDA) predicts all the CC bonds to be the same and $a_{CC} = 1.466$ Å [33] that appears to be an overestimation. Agrawal et al. [34], using the generalized gradient approximation (GGA), obtained $a_{CC} = 1.422$ Å and $d_t = 8.194$ Å, that is close to our data.

Sun et al. [35] calculated a series of infinite armchair and zigzag nanotubes using GGA DFT with periodic boundary conditions. Two different bond lengths were found in both types of nanotubes. For the armchair series, all possible relations were obtained, $CC_a > CC_c$, $CC_a = CC_c$, or $CC_a < CC_c$, depending on the nanotube index. The largest deviation from the graphene bond length is 0.008 Å for the (5,5) SWCNT and decreases with the increasing diameter. Unfortunately, the authors [35] did not report the values of optimized nanotube diameters, instead, they calculated d_t' using formula (1) and $a_{CC} = 1.42$ Å.

Summarizing, the presence of certain differences in CC bond lengths in different directions of SWCNT was reported in the literature earlier, however, this phenomenon has not been completely understood and systematized. The results of our calculations carried out with periodic boundary conditions complement the previous theoretical results for nanotubes obtained without PBC. The analysis of the literature given above shows that, at present, the data on 'accurate' diameters of SWCNT are practically absent. Moreover, this issue is often avoided in the discussion, perhaps, because the results of quantum chemical calculations do not coincide with those obtained using commonly accepted formulas. It is clear now that this disagreement is related to the differences of the CC bond lengths in SWCNT and in the graphene sheet and also, as we have demonstrated here, to the non-cylindrical geometry of the nanotubes.

4. Conclusion

Taking into account our results and those obtained by the other authors one can make the following general conclusions.

Rolling up the graphene sheet into an armchair SWCNT leads to the CC bond elongation. The two kinds of bonds in an armchair SWCNT, directed nearly along the nanotube axis and directed along the nanotube circumference, are elongated in different ways. The smaller the nanotube index, the larger the bond elongation. However, even for the (5,5) nanotube, the elongation does not exceed 0.008 Å (according both to semiempirical and DFT data), that is 0.6% relative to the graphene sheet value of 1.421 Å. Thus, the value of 1.44 Å for the CC bond length in armchair SWCNTs is an overestimation.

A real nanotube is not cylindrical, therefore the nanotube cross section is not circular, but polygonal. Because of this, the theoretical relationship (1) between the nanotube diameter, indices, and the bond length is broken. Based on the PM3 data, for an armchair SWCNTs (n, n), the nanotube diameter is related to the nanotube index by the following equation:

$$d_t = (0.101 \pm 0.009) + (1.350 \pm 0.001)n \text{ Å},$$

that differs from the theoretical formula (1) by the presence of a free term and a reduced value of the coefficient before n.

Acknowledgements

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