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Abstract

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A polyhedral model for carbon nanotubes

Barry J. Cox and James M. Hill

A new structural model accounts for the curvature inherent in their cylindrical shape.

Carbon nanotubes hold considerable research interest due to their high thermal and electrical conductance and tensile strength. The conventional nanotube model[1] is based on rolling a sheet of graphene—a single layer of graphite with a hexagonal lattice—into a cylinder. However, this model neglects the effect of rolling, which introduces an asymmetry not present in the graphene sheet, on the bond lengths and bond angles. As a result, the conventional model incorrectly predicts geometric parameters such as unit length and tube radius.

The smaller the radius of the carbon nanotube, the larger the effect of curvature. Small nanotubes have been investigated by several authors, both with theoretical, *ab initio* calculations[2] as well as experimental growth of carbon nanotubes in zeolite channels.[3] We have proposed a new model[4] that accounts for curvature and agrees very well with *ab initio* results[2] without intensive computation.

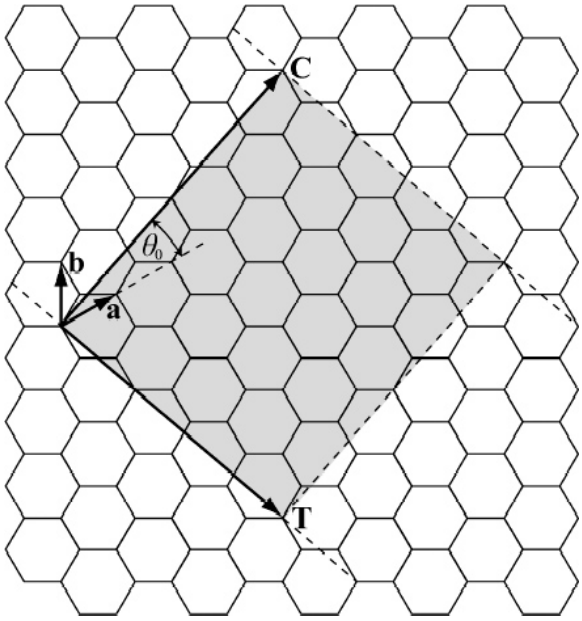

Figure 1. *The conventional model describes a carbon nanotube as a graphene sheet, rolled into a cylinder described by basis vectors* **a** *and* **b**, *chiral angle* θ_0, *chiral vector* **C** *and translation vector* **T**. *The figure is drawn for a* $(4, 2)$ *nanotube, and the shaded section is one unit cell.*

Approach

As illustrated in Figure 1, carbon nanotubes are classified by the chiral vector numbers (n, m) that characterise the orientation of the hexagons in a corresponding graphene sheet. Atoms in the graphene that are separated by the chiral vector $\mathbf{C} = n\mathbf{a} + m\mathbf{b}$ (where **a** and **b** form a non-orthogonal basis for the sheet) represent to the same atom in the nanotube.

In the conventional model, the length of the chiral vector, $|\mathbf{C}|$, is the circumference of the cylinder, and its direction relative to the first basis vector **a**, is the chiral angle θ_0. The translation vector, **T**, whose length defines the nanotube unit cell length, is perpendicular to **C**.

This model tacitly assumes that all bond lengths are equal and all bond angles remain 120°. However, the rolling-up process modifies both the lengths and angles. We postulated that, in the cylindrical state, all bond lengths and all bond angles are equal in the cylindrical state, but may differ from their values in graphene. These postulates lead to a 'polyhedral' model, in which atoms are arranged in a tessellation of right triangular pyramids, as shown in Figure 2. We deduced how the angles and lengths depend on the chirality of the nanotube of interest, and derived precise expressions for the chiral angle, bond angle, radius and unit cell length.

Results

Figures 3 and 4 show the relative difference in radius and unit length between the conventional and new model for nanotubes of different chirality, corresponding to different values of θ_o. Zigzag nanotubes—those with $m = 0$—are the most sensitive to curvature.

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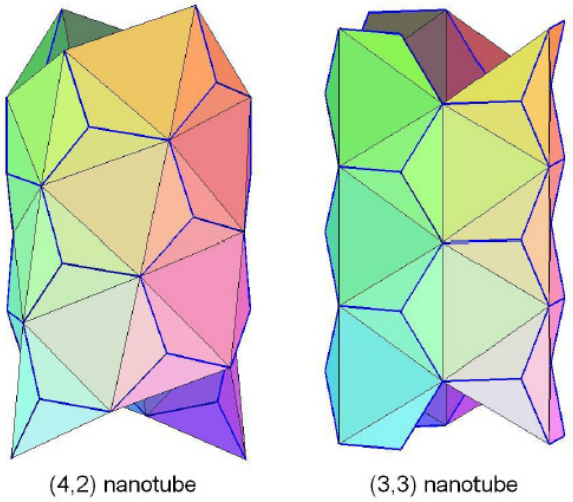

Figure 2. *The new model represents carbon nanotubes as polyhedra, with an atom at every vertex.*

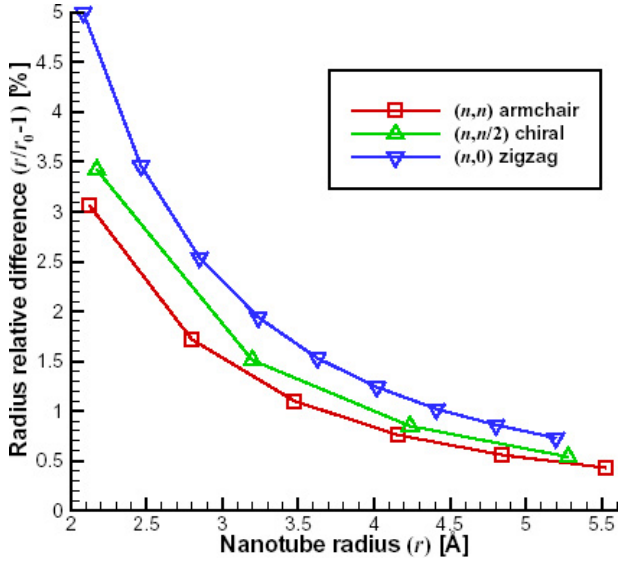

Figure 3. *The radius, r, predicted by the polyhedral model differs from the conventional radius, r_0. The three curves show the relative difference for families of carbon nanotubes with different chirality: zigzag $((5,0) to (13,0))$, chiral $((4,2) to (10,5))$, and armchair $((3,3) to (8,8))$.*

Figure 5 shows the bond angle for nanotubes of various radius and chirality. Unlike the radius and unit length, the bond angle is not sensitive to chirality differences.

Table 1 shows the conventional radius, r_0, the radius predicted by the 'polyhedral' model, r, and that determined by Cabria, et al.[2]. The new model agrees very well with the *ab initio* results, and is a considerable improvement over the conventional formula for small radius nanotubes.

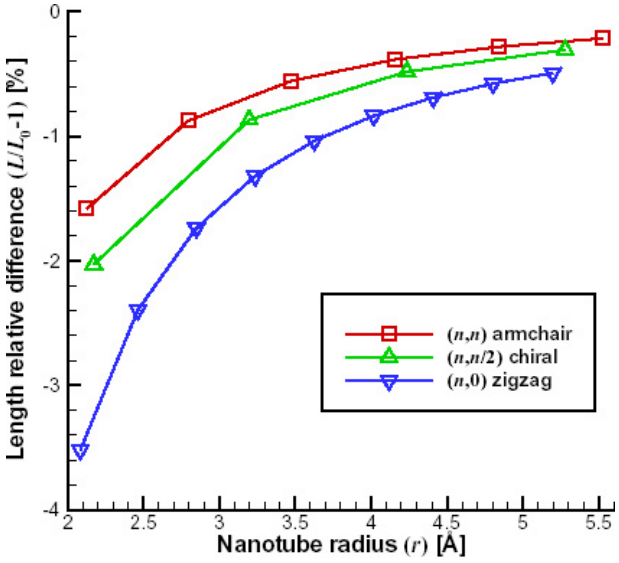

Figure 4. *The predicted unit-cell length also differs between polyhedral and conventional models, shown for the same nanotubes as in Figure 3.*

Table 1. *Comparison of radii from conventional model, polyhedral model, and* ab initio *calculations*[2].

nanotube	r_0 (Å)	r (Å)	Cabria, et al.[2] (Å)
(4,0)	1.59	1.71	1.71
(3,2)	1.73	1.81	1.8
(4,1)	1.82	1.92	1.91
(5,0)	1.98	2.08	2.06
(3,3)	2.06	2.13	2.12
(4,2)	2.10	2.17	2.17
(5,1)	2.21	2.29	2.28
(6,0)	2.38	2.46	2.45
(4,3)	2.41	2.47	2.46

Conclusions

We have proposed a new "polyhedral" model for carbon nanotube geometry, whose predictions agree well with *ab initio* studies. In contrast to the *ab initio* approach, the analytical calculations can be performed in seconds, and the model provides an understanding of the detailed structure of carbon nanotubes that cannot be gained from a purely numerical study. We have used

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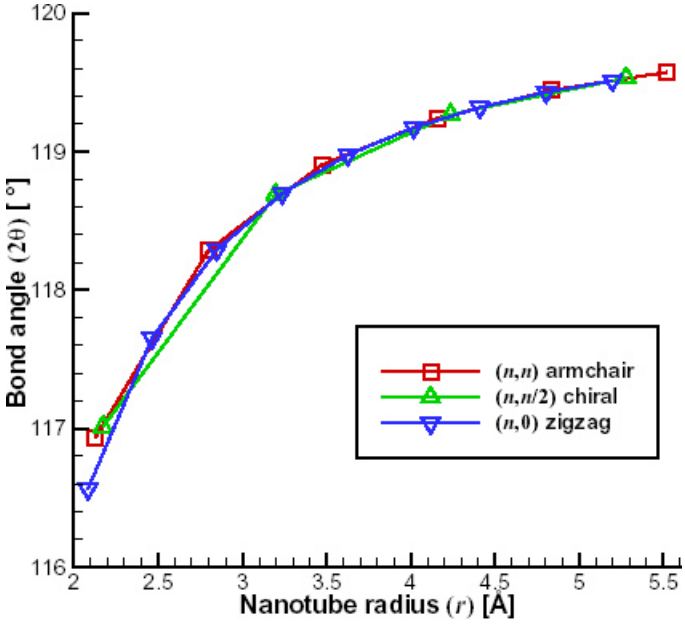

Figure 5. *Bond angles for the same nanotubes as in Figures 3 and 4. In the conventional model the angle is always* 120°.

this model to investigate ring-like cage molecules of carbon[5] and we are presently applying it to carbon-nanotube junctions.

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