# FROM POLYACETYLENE TO CARBON NANOTUBES

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## Introduction

First we evaluate the elastic constants and give an analytic expression of the deformation potential energy for both the armchair and zigzag tubules using a modified polyacetylene model. Secondly we examine in detail the behavior of the gap for the zigzag tubules as a function of radius.

## Deformation potential energy

The conformal mapping[1] of a single-layer graphite sheet, designated "graphene", to form a zigzag tubule[2-3] ($N_y$,0) induces angular distortion and therefore what we term an "alignment defect" of the orbitals involved in the $\sigma$ bonds.

If A and $B_i$ are two carbon atoms in the same graphene plane, distant from each other by $d_i$, the alignment defect $\delta\theta_{AB_i}$ induced by rolling the plane to form the tubule causes a total elastic energy per orbital

$$e^{\sigma_{AB_i}}_{total,tubule}=\frac{1}{2}C^{tubule}_{\sigma}(\delta\theta_{AB_i})^2 \qquad (1)$$

where $C^{tubule}_{\sigma}$ is the torsion constant of the $\sigma_{AB_i}$ bonds. If we denote by W the potential energy of deformation associated with the conformal mapping which transforms the graphene into a zigzag tubule, then we observe that $W_{AB_1}=W_{AB_2}$ since $|\ \delta\theta_{AB_1}\ |=|\ \delta\theta_{AB_2}\ |$ and $W_{AB_3}=0$ since $\delta\theta_{AB_3}=0$.

For an armchair tubule, the $\sigma_{AB_3}$ bond is perpendicular to the tubule's axis. Thus $\sigma_{AB_1}$ and $\sigma_{AB_2}$ are symmetrically deformed and to a lesser extent: consequently, the alignment defect of each orbital is also less than that encountered for $\sigma_{AB_3}$. In conclusion: $W_{AB_1}=W_{AB_2}$ and $W_{AB_3\neq}0$.

## Total energy per 1-D cell

The hamiltonian is a modified Su[4-5] et al's formulation used for polyacetylene. The total energy is then evaluated as given by:

$$E^{tubule}_{total}(\delta\theta)=-2\frac{\Omega_{tubule}}{2\pi}\int_{1ZB}E_{tubule}(\mathbf{k},\delta\theta)d\mathbf{k}$$

$$+N_{tubule}e^{\sigma_{AB}}_{total,tubule}(\delta\theta) \qquad (2)$$

$\Omega_{tubule}$ is the length of the unit cell.
To determine the form of the operator $W_{AB}(\delta\theta)$ which allows minimizing the total energy per unit cell $e_{total}^{armchair}(\delta\theta)$ for a value of $\delta\theta$ corresponding to a given tubule, we have tried several different forms based on Taylor series development of $W_{AB}(\delta\theta)$ in the neighbourhood of graphene's planar condition. In the absence of experimental values linking tubule chirality to electronic properties, we took as a reference the values proposed by Hamada et al[1] and Moussaddar et al[6] to evaluate $C_\sigma^{tubule}$ and $\alpha_{(n_1,n_2)}^{tubule}$. This leads to finding a variation in potential energy which varies as $R^{-2}$: $W^{zigzag}=\frac{3.52}{N_y^2}$; the coupling coefficient $\alpha_{(n_1,n_2)}^{tubule}$ varies from one tubule to another as a function of the tubule diameter, confirming the correlation indicated above: $\alpha_{(N_y,0)}^{zigzag}=\frac{2.16}{N_y}$.For armchair tubules $C_\sigma^{armchair}=\frac{7}{4}C_\sigma^{zigzag}=3.5eV$, $W^{armchair}=\frac{1.08}{N_x^2}$ and $\alpha_{(N_x,N_x)}^{armchair}=\frac{1.05}{N_x}$.

## Conclusions

We would like to underline some important points here. First we recall that for $N_y$=3q-1, 3q or 3q+1, the allowed k-lines closest to the Brillouin zone corner pass respectively through, below and above the point K. The discrete energy level which furnishes the gap for each type of zigzag tubule is that which corresponds to m=q and these gaps therefore are determined by:

- for $N_y$=3q-1 :
$E_g=2\alpha_0[1-2(1+\frac{W_{AB_1}}{\alpha_0})\cos\frac{q\pi}{3q-1}]$;
- for $N_y$=3q, $E_g=2W_{AB_1}$
- for $N_y$=3q+1,
$E_g=2\alpha_0[1-2(1+\frac{W_{AB_1}}{\alpha_0})\cos\frac{q\pi}{3q+1}]$.

The introduction of curvature allows predicting nonzero gaps for the zigzag tubules $N_y$=3q: $E_g(N_y)=\frac{7.2}{N_y^2}$eV. And, if $N_y \neq 3q$, then $E_g(N_y)=\frac{11.6}{N_y}$eV, in agreement with the results of Saito et al[7] and Olk et al[8]. For the armchair tubules, there is no gap opening near the Fermi energy. Our deformation potential couples the alignment defect of the orbitals participating in the $\sigma$ bonds with the $\pi$ electrons..

## References


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