# UNIAXIAL STRESS EFFECTS FOR SINGLE- AND DOUBLE-WALLED CARBON NANOTUBES

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## Introduction

The wrapping of a graphene layer around an axis to form a carbon nanotube provokes nonplanarity, introducing what we term « alignment defects » [1]. Such defects are related to the band gaps in a 1D-tight binding scheme. The influence of uniaxial stress on the electronic properties is analyzed and evidence is put forward of possible experimentally observable semiconductor to metal transitions under compression for single- and double-walled nanotubes.

## Single-walled carbon nanotubes

Among the stable morphologies observed for single-walled nanotubes, two types designated « zigzag » (Figure 1) and « armchair » stand out (Figure 2).

The zigzag carbon nanotubes are small gap semi conductors with gaps G varying as $1/n^2$ if n=3q : G= $6.91/n^2$ (in eV) and larger gap semiconductors with gaps varying as 1/n if n=3q ± 1 : G= 11.59/n (in eV). For radii R >6 angstroems, the gap is so small that such tubules may be classified as « quasi-metallic ».

The (n,n) armchairs are metallic. The DOS shows no forbidden energy in the whole spectral range (Figure 3).

## Double-walled carbon nanotubes

The double-walled carbon nanotubes studied here are supposed built up from only armchair and zigzag species.

We observe that the interactions between the two constitutive coaxial cylinders of a double-walled carbon nanotube are smaller than that between the graphene layers in graphite. The basic electronic properties of each constituent cylinder are unaffected by the other even though the detailed energy dispersion relations do depend on the interlayer interactions.

Since metallic behavior is expected for single-walled carbon armchair nanotubes, all double-walled tubes containing an armchair tubule will also be metallic. In the case of double-walled zigzag-zigzag tubes, it is the smaller bandgap cylinder (the outer) which conditions the overall E(k) behavior and thus the electronic properties.

## Effects of uniaxial stress on carbon nanotubes

An uniaxial, homogeneous deformation of carbon nanotubes along their axes is created by uniaxial stress $\sigma$. We computed the $\pi$-electronic band structure under both uniaxial traction ($\sigma$ >0) and uniaxial compression ($\sigma$ <0) using a tight-binding hamiltonian.

For (n=3q,0) single-walled zigzag-zigzag carbon nanotubes the gap increases with uniaxial traction : $G=0.01\sigma+6.91/n^2$ ($\sigma$ in GPa). The pressure $\sigma_t$ characterizing the transition between semiconductor and metallic behavior [2] is related to n by $\sigma_t=-652/n^2$. If n=3q ± 1, $G=\pm 0.0065\sigma+11.59/n$. The transition pressure is related to n by $\sigma_t=\mp 1785/n$.

The armchair tubules being metallic and remaining so under uniaxial stress applications, the armchair-armchair double-walled carbon nanotubes will not be further treated.

For the zigzag-armchair (armchair-zigzag) tubes, the electronic properties are due to the outer (inner) armchair tubule, and all these compounds are metallic and the application of uniaxial stress again has no effect on the gaps of the double-walled tubules.

We are thus left with only the zigzag-zigzag double-walled tubules. It is the smaller bandgap cylinder (the outer) which conditions the overall E(k) behavior and thus the electronic properties. Table 1 summarizes the data concerning the gaps and transition pressures of selected combinations with an outer zigzag tubule (Figure 4).

## Conclusions

We have shown that because of the weak coupling between inner and outer cylinders in a double-walled carbon nanotube, it is the smaller gap component which dictates the overall electronic properties. Thus all double- or multi-walled tubules, comprising an armchair type are expected to be metallic, and only zigzag–zigzag combinations may still be semiconducting. Application of uniaxial stress can modify the band gap, and thus certain nanotubes may manifest a semiconductor to metal transitions.

## References

[1] Heyd R., Charlier A., McRae E., Charlier M.-F., Phys Rev B 1997 ;56 :9958-9963
[2] Heyd R., Charlier A., McRae E., Phys Rev B 1997 ;55 :6820-6826
[3] Charlier A., McRae E., Heyd R., Charlier M.-F., submitted to Journal of Physics : condensed matter.

**Table 1.** Selection of inner (n,0) single-walled carbon nanotubes for double-walled zigzag-zigzag tubules. G is the gap near the Fermi energy, and $\sigma_t$ the semi-conductor metal transition pressure.

| n | G in eV | $\sigma_t$ in GPa |
|---|---|---|
| 9 | 0.085 | -8.0 |
| 12 | 0.048 | -4.5 |
| 15 | 0.030 | -2.9 |
| 18 | 0.021 | -2.0 |
| 21 | 0.015 | -1.4 |

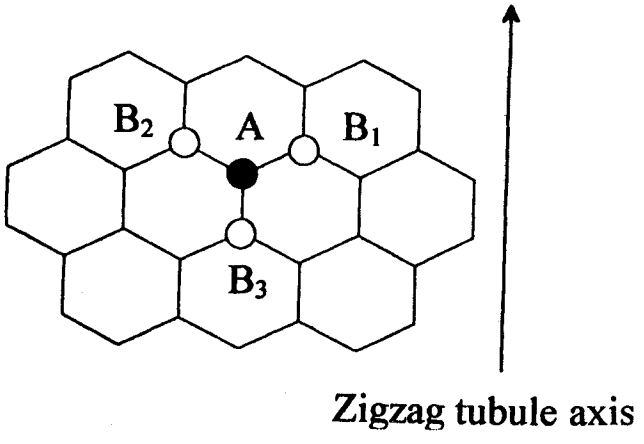


**Figure 1**. Zigzag single-walled carbon nanotube

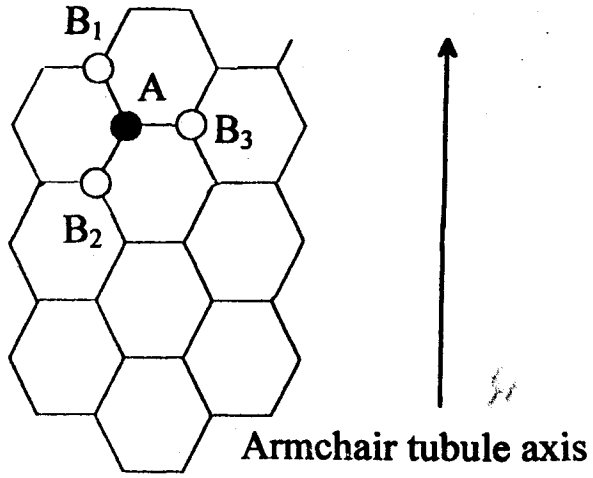


**Figure 2**. Armchair single-walled carbon nanotube

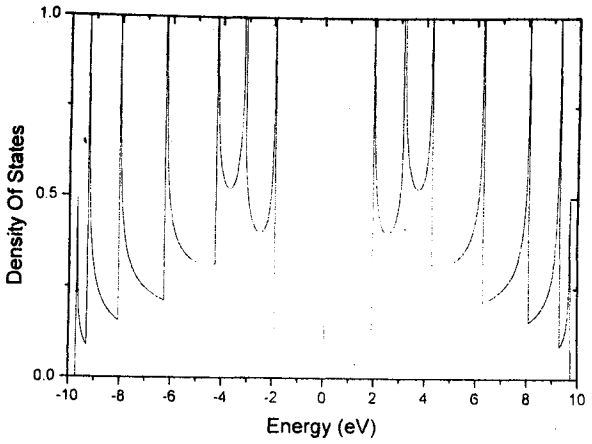


**Figure 3**. Density of states versus energy for a (5,5) armchair metallic tubule

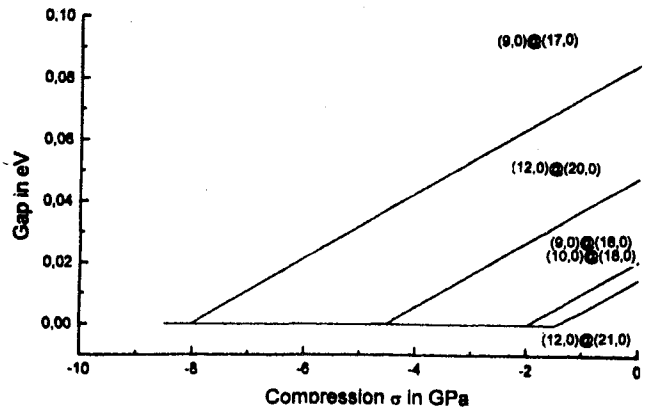


**Figure 4**. Semiconductor-metal transitions for selected double-walled carbon nanotubes