

# HOMEWORK 1 SOLUTIONS

## Problem 2

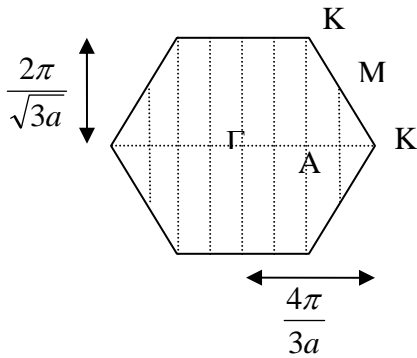
- (a) One can wrap the graphene sheet that constitutes a single walled carbon nanotubes in different ways to form metallic and non-metallic nanotubes. These two forms are distinguished by the coordinates  $(n, m)$  of the  $\mathbf{c}_h$  vector  $(= n\mathbf{a}_1 + m\mathbf{a}_2)$

The general criteria for single walled nanotubes are given in Hamada's paper:

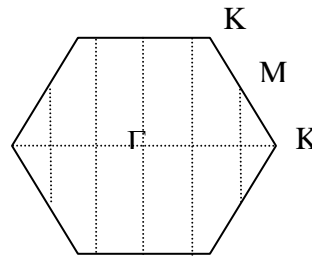
- (1) if  $n=2m$  or  $n-2m$  is a multiple of 3 we get metallic or small band gap nanotubes
- (2) all other nanotubes are semiconducting/insulating.

The physical rationale for these rules comes from examining the Brillouin zone (BZ) of two separate structures that satisfy (1) and (2) – see figure 2 and 4 in Hamada's paper (note also the rotation between the real lattice and the reciprocal lattice, as represented by the BZ in those figures).

Note that there are as many  $\mathbf{k}$ -vectors (dotted vertical lines) in the first BZ as there are lattice points, so in a  $(12, 0)$  nanotubes there are 12  $\mathbf{k}$ -vectors while in a  $(2, 0)$  nanotubes there are 2 distinct  $\mathbf{k}$ -vectors (see figure on the right hand side, the  $\mathbf{k}$  vectors are  $-2, -1, 0, 1, 2$  for the  $(2, 0)$  nanotube).



$(3, 0)$  nanotubes – metallic (no gap present at point  $\mathbf{K}$ )



$(2, 0)$  nanotubes – non metallic (gap present at point  $\mathbf{K}$ )

A nanotubes is metallic if the BZ is filled, i.e., a  $\mathbf{k}$ -vector cuts through point  $\mathbf{K}$ , which is the furthest point in the BZ. This can only happen for a  $(n, 0)$  nanotubes if  $n$  is a multiple of 3 (this is from geometrical considerations: the distance from the center ( $\Gamma$ ) to the point  $\mathbf{A}$  is  $(2p/3a)$  and therefore every third  $\mathbf{k}$ -vector passes through  $\mathbf{K}$ ).

- (b) A carbon nanotube can be considered one-dimensional if its length to diameter ratio is large. So, from these criteria alone, long nanotubes are one dimensional while short nanotubes tend towards a two-dimensional description. From Figure 3a in Saito's paper, there is an evident  $1/E^{1/2}$  dependence characteristic of a 1-Dimensional DOS. However, this is not definitive. For example, looking at Figure 2 in Hamada's paper, the energy levels are seen to be evenly spaced (i.e. more characteristic of a 2-D rather than a 1-D density of states). So in summary, the DOS would be characterized by a mixture of 1-D and 2-D, the relative ratio depending on the structural characteristic of the nanotubes.
- (c) A two-walled carbon nanotubes with an inner metallic wall and an outer insulating wall could be useful as a nano-cable. While the diameter is a good control variable for the design, this alone is not enough, as a larger diameter/outer nanotubes is likely to be more metallic (as the energy gap is inversely proportional to the diameter). As remarked in Saito's paper, by using an initial pentagonal template "armchair" type metallic nanotubes can be grown.

Therefore one idea for the design is:

- (1) use a pentagon template and an appropriate diameter  $d_{CNT}$  for the inner metallic nanotubes (Energy gap of a nanotubes =  $0.9 \text{ eV}/d_{CNT} \text{ (nm)}$ ). A 40 nm nanotubes is metallic at room temperature.
- (2) Use a hexagonal template for the growth of a zig-zag nanotubes, which is semiconducting/insulating.

The template for example could be obtained in a Y-junction, as represented below. The green regions represent the pentagonal defects that are formed when nanotubes are joined together and the blue regions represent hexagons characteristic of a straight nanotubes structure.

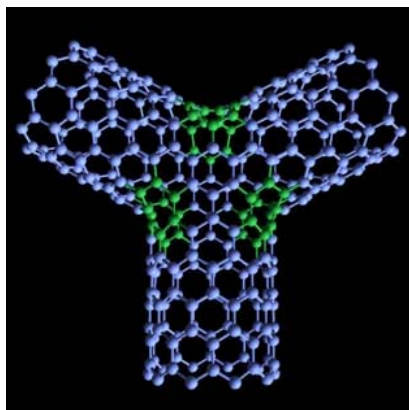


Figure taken from:

<http://www.staff.uni-mainz.de/banhart/c-nanostructures/nanostructures-page.htm>

By equation given in class: 
$$v = \frac{k_s h_G}{k_s + h_G} \frac{C_T}{N} Y = \frac{1}{(1/h_G + 1/k_s)} \frac{C_T}{N} Y$$

$h_G = 0.5 \text{ cm s}^{-1}$

$k_s = 4 \times 10^6 \exp(-1.45 \text{ eV}/kT) \text{ cm s}^{-1}$

Partial pressure of incorporating species = 1 torr

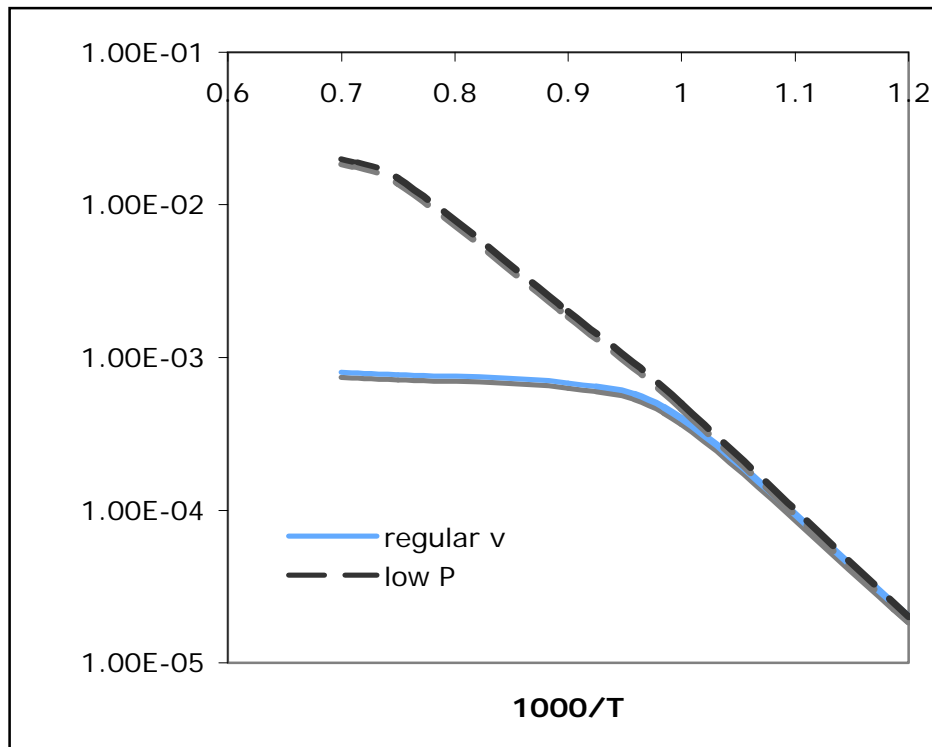
Total pressure = 1 atm

$C_T/N = 1/10,000$

$Y = P_g/P_{\text{total}} = 1 \text{ torr}/760 \text{ torr}$

For the low pressure case, only  $h_G$  changes (increases by 100 times).  $\frac{C_T}{N} \cdot \frac{P_g}{P_{\text{total}}}$  remains

constant. The plot of  $v$  for each case vs.  $1/T$  is shown below. For the 1 atm total pressure case, curve  $v$ , the transition between surface reaction controlled and diffusion controlled regimes is at  $\sim 800^\circ\text{C}$ , while for the low pressure case the transition occurs above  $1200^\circ\text{C}$ .



Problem 4.

- (a) In positive tone patterning, the radiative energy breaks bonds in the polymer, making it more soluble. The etchant then dissolves away the regions which have been exposed. In negative tone patterning, the radiative energy forms crosslinks between polymer chains, making the polymer stronger and less soluble. The etchant then dissolves away the regions which were *not* exposed.
- (b) E-beam lithography can produce extremely fine features since the beam can be focused down to near the very small electron wavelengths. For polymers whose

cross-linking can be initiated by charge, this can also set off a chain reaction, in which one cross-linking reaction charges the neighboring chain, initiating another cross-linking reaction, etc. The required energy/unit area is thus much smaller for certain polymers (PGMA, for example). On the other hand, the beam must travel over a very complex path in order to “write” the patterns into the photoresist polymer, which can take a very long time, which scales roughly as the number of features. Far-UV lithography exposes the whole die or wafer at once, regardless of the complexity of the features.