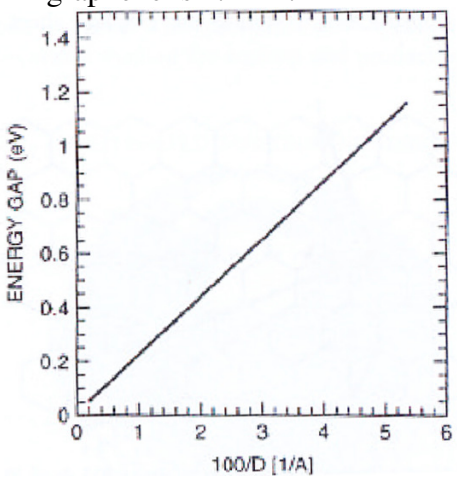
Problem:

1. Calculate the length of the chiral vector, and the chiral angle of a (7, 3) nanotube. What's the diameter of it? Is it metallic of semiconducting? If it is semiconducting, what's the bandgap? You can use the following graph. The bond length of the 2D graphene is 1.42 A.



2. Repeat the same procedure for a (10, 0) nanotube.
3. (Optional) Go to http://www.jcrystal.com/products/wincnt/index.htm and download a free nanotube program, the "nanotube modeler". You can create a 3D model of a nanotube, or bucky ball.
4. (Optional) You can use the tools in http://www.nanohub.org/tools/cntbands-ext/ to calculate the band structure of a nanotube.

Answers

1. Length of the unit vector: $a = |a_1| = |a_2| = \sqrt{3}a_{C-C} = 1.732 \times 1.42 = 2.46A$,

$|C_h| = a\sqrt{n^2 + m^2 + nm} = 2.46 \times 8.89 = 21.9A$

$$\cos\theta = \frac{C_h \cdot a_1}{|C_h||a_1|} = \frac{n + m/2}{\sqrt{n^2 + m^2 + nm}} = 0.956$$

$\theta = 17.03^0$

Diameter $D = \frac{|C_h|}{\pi} = 6.97A$

Since 2n+m=17 is not divisible by 3, it is a semiconducting nanotube.
100/D=14.3 (1/A), so it is beyond the scope of the graph. However we can extrapolate the bandgap using the linearity of the curve. The slope of this curve is 1.05/5=0.21 eV A, so the bandgap is 14.3 X 0.21=3.0 eV.

$$| C_h | = a\sqrt{10^2 + 0^2 + 0} = 2.46 \times 10 = 24.6A$$

$$\cos\theta = \frac{C_h \cdot a_1}{| C_h || a_1 |} = \frac{n}{\sqrt{n^2 + m^2 + nm}} = 1$$

$$\theta = 0$$

Diameter $D = \frac{| C_h |}{\pi} = 7.83A$

Since 2n+m=20 is not divisible by 3, it is a semiconducting nanotube.
100/D=12.8 (1/A), the bandgap is 12.8 X 0.21=2.68 eV.