Carbon Nanotubes

Materials
Allotropes of Carbon

Diamond, graphite, lonsdalerite, C60, C70, carbon, amorphous carbon, carbon nanotube
Carbon Nanotube (CNT)

SWNT Single Wall is 1 atom thick
MWNT, Multi-walled is more than 1 atom thick
Typical diameter: 1 nm
Shown is zip-zag CNT
Note hemispherical cap
1. Pick an atom (A) on a blue line and draw armchair vector to other blue line.

2. Find the atom on the other edge closest to the armchair intersection. Connect A & B w chiral vector R (red). Wrapping angle is angle between armchair and chiral vectors.

3. Cut tube parallel to axis. The edges correspond to the blue lines.

4. \(a_1\) lines along zig-zag line. \(a_2\) is reflection of \(a_1\) about armchair vector.

5. \(n a_1 + m a_2 = R\)

Origin:
www.pa.msu.edu/cmp/csc/ntproperties/equilibriumstructure.html
CNT Geometry

(n,n) armchair vector  (n,0) zigzag vector
DIAMETER CNT

\[ d = \frac{|C|}{\pi} = \frac{a_{cc}}{\pi} \sqrt{3(m^2 + mn + n^2)} \]

\[ \Theta = \tan^{-1} \left[ \frac{\sqrt{3}n}{2m + n} \right] \]

\( a_{cc} = 0.142 \text{ nm} \)  C-C bond length

\( a = \sqrt{3}a_{cc} = 0.249 \text{ nm} \)  length unit vector
Importance of CNT Chirality

• Effects: conductance, density, lattice structure, and other properties.
• Metallic if \( n - m \) is divisible by three. Otherwise, semiconducting.
• CNT diameter:
  \[
d = (n^2 + m^2 + nm)^{1/2} \approx 0.0783 \text{ nm}
\]
Bandgap CNT

\[ \text{Egap} = 2 \, y_0 \, a_{cc} / d \]

Where:
\[ y_0 = \text{C-C bonding energy} \, [2.7 \, \text{ev}] \]
\[ a_{cc} = \text{nearest neighbor distance} \, [0.142\, \text{nm}] \]
\[ d = \text{CNT diameter} \]
Density of States

Source: http://www.pa.msu.edu/cmp/csc/ntproperties/opticalproperties.html
Metallic vs Semiconductor CNTs

\[ m = n \] metallic
\[ n - m = 3i \] semimetallic
\[ n = m \neq 3i \] semiconducting
CNT Bandgap - Crystalline

Simple formula

\[ E_g (eV) = \frac{0.9}{d (nm)} \]

More accurate

\[ E_g = 2\gamma_0 \frac{a_{cc}}{d} \left[ 1 + (-1)^p 2\beta \frac{a_{cc}}{d} \cos(3\theta) \right] \]

\[ \gamma_0 = 2.53\text{eV} \quad \beta = 0.43 \quad p = n - 2m - 3i \]
Bandgap Amorphous CNT

\[ E_g = \frac{3}{\sqrt{2}} m_C \langle \omega^2 \rangle \frac{a_{CC}}{d} \]

\( m_C = \text{mass of carbon} \ (2 \times 10^{-23} \text{ g}), \)

\( \langle \omega \rangle = \text{average phonon energy} (1600 \text{ cm}^{-1}) \)
Amorphous vs Crystalline

![Graph showing the comparison between Amorphous carbon nanotube and Crystalline carbon nanotube with respect to $E_g$ (eV) and $100/d$ (Å⁻¹).]
- Ballistic conductor
- Resistivity CNT robes $10^{-4} \ \Omega\cdot\text{cm}$
- Max current density $> 10^{13} \ \text{amp/cm}^2$

Source: Stefan Frank, Science 280, 1744 (1988)
Gated pn Junction

Intrinsic conductivity type = p  n-type by vapor exposure
<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value and units</th>
<th>Observations</th>
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</thead>
<tbody>
<tr>
<td>Length of the unit vector</td>
<td>$a = \sqrt{3}a_{C-C} = 2.49,\text{Å}$</td>
<td>$a_{C-C} = 1.44,\text{Å}$ is the carbon bond length</td>
</tr>
<tr>
<td>Current density</td>
<td>$&gt;10^9,\text{A/cm}^2$</td>
<td>-1000 times larger than the current density in copper</td>
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<td></td>
<td></td>
<td>- Measured in MWCNTs</td>
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<tr>
<td>Thermal conductivity</td>
<td>6600 $\text{W/mK}$</td>
<td>More thermally conductive than most crystals</td>
</tr>
<tr>
<td>Young modulus</td>
<td>1 Tpa</td>
<td>Many orders of magnitude stronger than the steel</td>
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<tr>
<td>Mobility</td>
<td>10,000-50,000 $\text{cm}^2\text{V}^{-1}\text{s}^{-1}$</td>
<td>Simulations indicate motilities beyond 100,000 $\text{cm}^2\text{V}^{-1}\text{s}^{-1}$</td>
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<tr>
<td>Mean free path (ballistic transport)</td>
<td>300-700 nm semiconducting CNT</td>
<td>- Measured at room temperature</td>
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<td>1000-3000 nm metallic CNT</td>
<td>- At least three time larger than the best semiconducting heterostructures</td>
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<tr>
<td>Conductance in ballistic transport</td>
<td>$G = 4e^2/h = 155\mu\text{S}$ ;</td>
<td>The electrons are strongly correlated in CNTs</td>
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<tr>
<td>Luttinger parameter</td>
<td>$1/G = 6.5\text{kΩ}$</td>
<td></td>
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<tr>
<td>Orbital magnetic moment</td>
<td>0.7 meV$\text{V}^{-1},d = 2.6,\text{nm}$</td>
<td>The orbital magnetic moment depends on the tube diameter</td>
</tr>
<tr>
<td></td>
<td>1.5 meV$\text{V}^{-1},d = 5,\text{nm}$</td>
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