Nanotube
Boron Nitride Nanotubes (BNNTs) vs Carbon Nanotubes (CNTs)

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Physics 141A

Image: nasa
Outline

1. Crystal structures of Nanotubes (NTs)
2. Physics Properties: BNNTs vs CNTs
3. What make BNNTs special?
   3.1 Neutron Absorption: BNNTs
   3.2 Giant Stark Effect (GSE): BNNT
4. Future
0. What’s wrong with CNTs ???

Expensive

Nobel Prize 1996

Nobel Prize 1954

Nobel Prize 2010
1. Crystal Structures

Wikipedia/CNTs
BNNT (boron nitride nanotube)
Blue=boron
Grey=nitrogen

CNT (carbon nanotube)
Grey=carbon

images: www.computenano.com
Rules?

\( n = m \): metallic

\( n - m \) is a multiple of 3: semiconducting with a very small band gap

Otherwise: moderate semiconductor

Exception?

Source: wikipedia/CNT

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**CNT Band Structures**

**BNNT Band Structures**

Insulator (Wide band gap semiconductor)

\( Eg = 5.5 \text{ eV} \)

Source: Physics Today
Band Gap Tuning 1

Possible Combinations of $B_xC_yN_z$

S. Azevedo and R. de Paiva 2006 Europhys. Lett. 75 126
Band Gap Tuning 1

Possible Combinations of $B_xC_yN_z$

- (a) island-like $BC_2N$
  - 1.37 eV = 906 nm

- (b) island-like $BC_2N$
  - 0.96 eV = 1292 nm

- (c) stripe-like $BC_2N$
  - 1.57 eV = 790 nm

- (g) BCN
  - 0 eV

- (h) BCN
  - 0 eV

- (i) $BC_3$
  - 0 eV

- (d) stripe-like $BC_2N$
  - 1.07 eV = 1116 nm

- (e) $B_3N_2C_2$
  - 1.69 eV = 735 nm

- (f) $B_3N_2C_2$
  - 2.45 eV = 506 nm

- (j) $NC_3$
  - 0 eV

Calculated band gaps

S. Azevedo and R. de Paiva 2006 Europhys. Lett. 75 126
2. Physical Properties

DOS (E) is proportional to $E^{-1/2}$

Source: Wikipedia/CNTs
Metallic SWNT

$v_1 \rightarrow c_1$ corresponds to the “first van Hove” optical transition

Semiconducting SWNT

$v_2 \rightarrow c_2$ corresponds to the “second van Hove” optical transition

Source: Wikipedia/CNTs
The Yin-Yang of Nanotubes

Sp2 bond, Strength, Stiffness, Aspect Ratio, Thermal Conductivity,

White, High temperature, Electrical Insulator

BNNT

Black, Lower temperature, Electrical Conductor

CNT

Source: NASA Langley Research
### Comparison of Material Properties, CNT v BNNT

<table>
<thead>
<tr>
<th>Property</th>
<th>Carbon nanotubes</th>
<th>Boron nitride nanotubes</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Electrical properties</strong></td>
<td>Metallic or semiconducting</td>
<td>Always semiconducting (about 5.5 eV band gap)</td>
</tr>
<tr>
<td><strong>Mechanical properties (Young’s modulus)</strong></td>
<td>1.33 TPa</td>
<td>1.18 TPa</td>
</tr>
<tr>
<td><strong>Thermal conductivity</strong></td>
<td>60 – 40,000 W/mK</td>
<td>~ 3000 W/mK (Cu = 400 W/mK)</td>
</tr>
<tr>
<td><strong>Thermal oxidation resistance</strong></td>
<td>Stable up to 300–400°C in air</td>
<td>Stable up to 800°C in air</td>
</tr>
<tr>
<td><strong>Neutron scattering cross-section</strong></td>
<td>C = 0.0035</td>
<td>B = 767 (B$^{10}$ ~ 3800) N = 1.9 Excellent radiation shielding</td>
</tr>
<tr>
<td><strong>Polarity</strong></td>
<td>Covalent bond (No dipole)</td>
<td>Permanent dipole <strong>Piezoelectric</strong> (0.25–0.4 C/m$^2$)</td>
</tr>
<tr>
<td><strong>Surface morphology</strong></td>
<td>Smooth</td>
<td>Corrugated</td>
</tr>
<tr>
<td><strong>Color</strong></td>
<td>Black</td>
<td>Gray</td>
</tr>
<tr>
<td><strong>Coefficient of Thermal Expansion</strong></td>
<td>-1 x 10^{-6}</td>
<td>-1 x 10^{-6}</td>
</tr>
</tbody>
</table>
3. What make BNNTs ideal materials for space applications?
Very strong and light materials
Neutron (and UV) absorption: protect the crew and equipment
Neutron (and UV) absorption: protect the crew and equipment

<table>
<thead>
<tr>
<th>Material</th>
<th>Atomic mass</th>
<th>Density (g/cm³)</th>
<th>Neutron Scatter Cross Sections</th>
<th>Neutron Absorption Cross-sections (barns)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Hydrogen</td>
<td>1.01</td>
<td>gas</td>
<td>82.02</td>
<td>0.33</td>
</tr>
<tr>
<td>Boron</td>
<td>10.81</td>
<td>Boron nitride (&quot;BN&quot;) (2.27); BNNT (1.37)</td>
<td>5.24</td>
<td>710 (¹⁰⁵B: 3835)</td>
</tr>
<tr>
<td>Carbon</td>
<td>12.01</td>
<td>1.8–3.5</td>
<td>5.55</td>
<td>0.0035</td>
</tr>
<tr>
<td>Nitrogen</td>
<td>14.01</td>
<td>gas</td>
<td>11.51</td>
<td>1.9</td>
</tr>
<tr>
<td>Oxygen</td>
<td>16.00</td>
<td>gas</td>
<td>4.23</td>
<td>0.00019</td>
</tr>
<tr>
<td>Aluminum</td>
<td>26.98</td>
<td>2.7</td>
<td>1.50</td>
<td>0.231</td>
</tr>
<tr>
<td>Titanium</td>
<td>47.87</td>
<td>4.54</td>
<td>4.35</td>
<td>5.0</td>
</tr>
<tr>
<td>Lead</td>
<td>207.2</td>
<td>11.34</td>
<td>11.12</td>
<td>0.17</td>
</tr>
</tbody>
</table>

Source: NIST
Giant Stark Effect (GSE): BNNTs

Band Gap Tuning 2! → Photovoltaics
Mechanical Properties Revised at high T

At 700°C

Specific Modulus
GPa/(g/cm³)

Specific Strength, GPa/(g/cm³)

- Baseline Materials
- 5 - 10 years (TRL = 4 - 6)
- 10 - 20 years + (TRL = 1 - 3)

BNNT

TiAl

SiC/Be

Highest published

Wei, et al., Tensile Tests on Individual Multi-Wall Boron Nitride Nanotubes, Advanced Materials, V 22, 43, p 4895© 2010
“...(the nanotube is) the strongest fiber that you can make out of anything, ever.”

~ (the late) Prof. Richard Smalley
Nobel Prize, Chemistry, 1996
Conclusion

• 1D nanostructures
• Metal, semiconductors, band gap tuning
• High (Young) modulus, thermal oxidation temperature, neutron absorption
• Promising materials for aerospace
• What’s wrong with CNTs and BNNTs
  ➔ structure control, mass production
Thank you for your attention!

Q & A