Notes on NanoIntegris Purity

The following describes our method for quantifying the relative metallic and semiconducting enrichment of our nanotube products. In short, we determine the metallic/semiconducting transition-energy peaks of the CNT species in our material using simple tight-binding calculations. We then measure these peaks via optical absorbance, and scale them by empirically determined extinction coefficients. Read on for more information.

Starting Material and Predictions

NanoIntegris Process:
• We start with electric-arc discharge SWNTs having a fairly narrow diameter distribution.

Manufacturer Claims:
• Manufacturer claims: tight diameter distribution between 1.2-1.7 nm (with majority between 1.25-1.55 nm), peaked at 1.4 nm

Simple Tight Binding Predictions

Rough values for transition energies can be calculated from simple tight binding calculations.

Formulas for $E_{ii}$ energies:

<table>
<thead>
<tr>
<th>Metallic</th>
<th>Semiconducting</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E_{M11}=6\gamma_o a_{cc}/d$</td>
<td>$E_{S11}=2\gamma_o a_{cc}/d$</td>
</tr>
<tr>
<td>$E_{M22}=12\gamma_o a_{cc}/d$</td>
<td>$E_{S22}=4\gamma_o a_{cc}/d$</td>
</tr>
<tr>
<td>$E_{M33}=18\gamma_o a_{cc}/d$</td>
<td>$E_{S33}=8\gamma_o a_{cc}/d$</td>
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Using $a_{cc}$ ~ 0.143 nm, $\gamma_o$ ~ 2.9 eV and $d$ ~ 1.2-1.7 nm, we can obtain rough estimates for $E_s$ ranges:

• $E_{S22}$ transitions should lie between ~900-1270 nm
• $E_{M11}$ transitions should lie between ~600-850 nm
• $E_{S33}$ transitions should lie between ~450-630 nm
• $E_{M22}$ transitions should lie between ~300-420 nm
• Minimal overlap between $E_{S22}$ and $E_{M11}$
• UV-Vis-NIR absorbance can be used to confirm predictions
Notes on Nanointegris Purity

UV-Vis-NIR: PureTubes
Clear peaks detected for both metallic and semiconducting nanotubes: M11, S22, S33
Notes on NanoIntegris Purity

Absorbance of Unseparated SWCNT

- Broad peak at 900-1270 nm > S22
- Broad peak at 600-850 nm > M11
- Several small peaks from 400-600 nm > S33
  - We see peaks where we would expect them
  - We estimate our purities based on ratios of the M11 and S22 peak areas after linear background subtraction
  - The individual peak areas are scaled by empirically-determined values for the M11 and S22 extinction coefficients to determine metal-semiconductor purities

Experimental Confirmation of Metal vs. SC Character

- Enriched samples (ratio of M11 to S22) used to make thin film transistors
- Tubes with absorbance from 900 to 1200 nm behaved like semiconductors (conductivity varied dramatically with gate bias)
- Tubes with absorbance from 600-800 nm behaved like metals (~constant conductivity vs. gate bias)

Additional Confirmation of Metal vs. SC Character

- 83 single nanotube transistors fabricated from ~99% SC material -> 82 displayed semiconducting behavior
- TFTs made from ~99% pure material displayed a combination of high on/off ratios and high on-currents
  - High On/Off Ratio : \( \sim 10^3 \)
  - High On-Current : \( I_{ON} > 1\)mA at \( V_{sd} \sim 2\)V