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Notes on NanoInteris Purity Calculations

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

NanoInteris 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 1.4nm

Simple Tight Binding Predictions

Largely from *Acc. Chem. Res. 35*, 1018 (2002)

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

Formulas for E_{ii} energies:

Metallic

- ${}^{M}E_{11} = 6\gamma_o a_{cc}/d$
- ${}^{M}E_{22} = 12\gamma_o a_{cc}/d$
- ${}^{M}E_{33} = 18\gamma_o a_{cc}/d$

Semiconducting

- ${}^{S}E_{11} = 2\gamma_o a_{cc}/d$
- ${}^{S}E_{22} = 4\gamma_o a_{cc}/d$
- ${}^{S}E_{33} = 8\gamma_o a_{cc}/d$

Simple Tight Binding Predictions

Using a_{cc} ~ 0.143 nm, γ_o ~ 2.9 eV and d ~ 1.2-1.7 nm, we can obtain rough estimates for E_{ii} ranges:

→ ${}^{S}E_{22}$ transitions should lie between ~ 900-1270 nm

→ ${}^{M}E_{11}$ transitions should lie between ~ 600-850 nm

→ ${}^{S}E_{33}$ transitions should lie between ~ 450-630 nm

→ ${}^{M}E_{22}$ transitions should lie between ~ 300-420 nm

- Minimal overlap between ${}^{M}E_{11}$ and ${}^{S}E_{22}$
- UV-Vis-NIR absorbance can be used to confirm predictions

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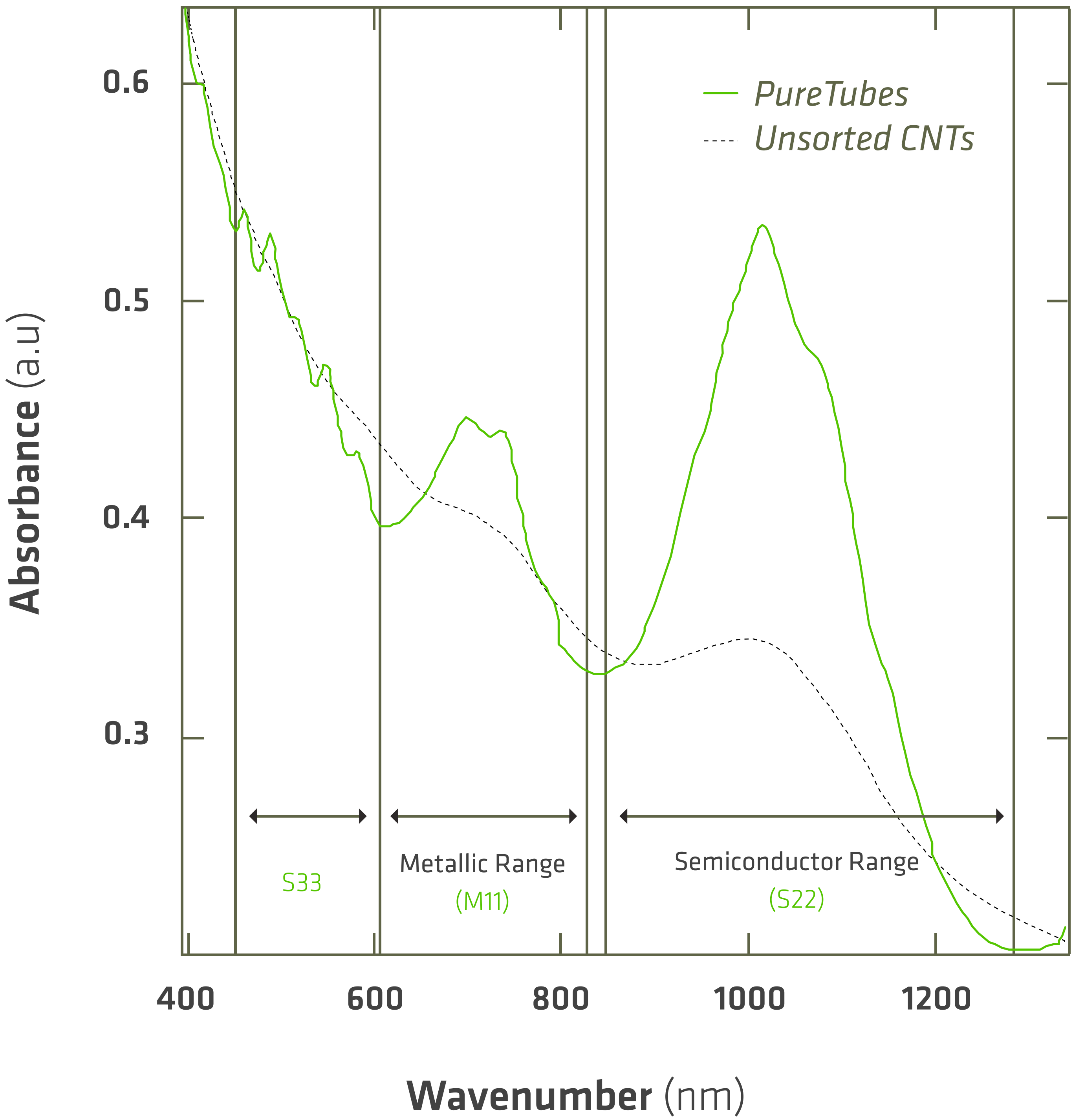

UV-Vis-NIR: PureTubes
Clear peaks detected for both metallic and semiconducting nanotubes: M11, S22, S33

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Absorbance of Unseparated SWNTs

- 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

From Arnold *et al*, *Nature Nano* **1**, 60 (2006)

- Enriched samples **(ratio of M11 to S22)** used to make thin film transistors
- Tubes with absorbance from 900-1200 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

From Avouris & Hersam, *ACS Nano* **2**, 2445 (2008)

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