NanoIntegris

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 1.4nm

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

- $E_{M11}=6\gamma_o a_{cc}/d$
- $E_{M22}=12\gamma_o a_{cc}/d$
- $E_{M33}=18\gamma_o a_{cc}/d$

Semiconducting

- $E_{S11}=2\gamma_o a_{cc}/d$
- $E_{S22}=4\gamma_o a_{cc}/d$
- $E_{S33}=8\gamma_o a_{cc}/d$

Simple Tight Binding Predictions

Using $a_{cc} \sim 0.143$ nm, $\gamma_o \sim 2.9$ eV and $d \sim 1.2\text{-}1.7$ nm, we can obtain rough estimates for E_{ii} 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 ovelap between E_{S22} and E_{M11}
- UV-Vis-NIR absorbance can be used to confirm predictions

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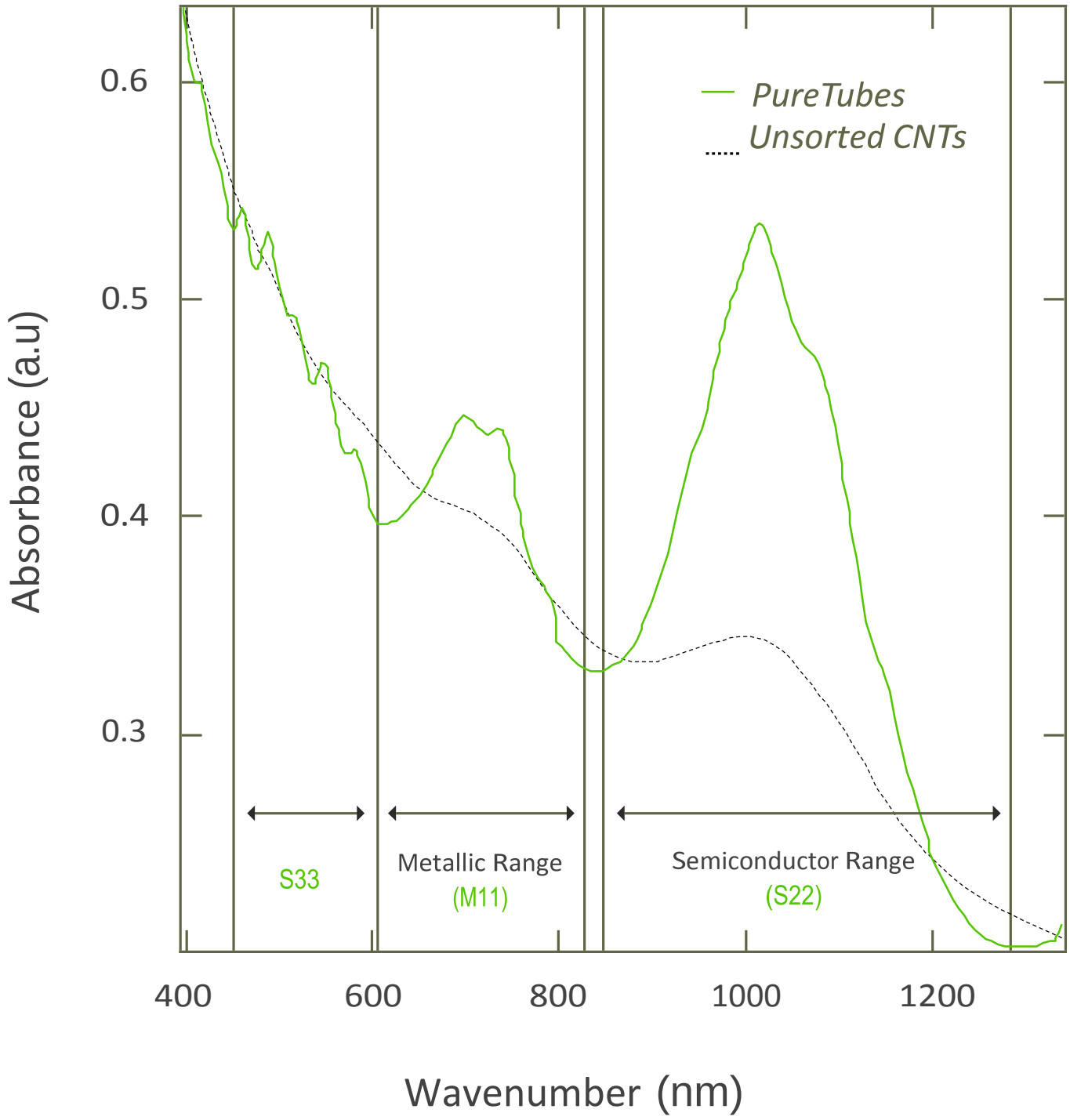

UV-Vis-NIR: PureTubes

Clear peaks detected for both metallic and semiconducting nanotubes: M11, S22, S33

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Absorbance of Unseparated 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

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 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

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

- 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 : ~10^3
- High On-Current : I_{ON} > 1mA at V_{sd} ~ 2V