Electro-Thermal Transport in Metallic Single-Wall Carbon Nanotubes

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Carbon Nanotubes for Electronics

- Great **electrical** & **thermal** conductors
  - Semiconducting → transistors
  - Metallic → interconnects

- (Some) open questions:
  - Thermal conductivity of single-walled carbon nanotubes (SWNTs)
  - Great thermal conductivity, poor thermal conductance (small $d$)
  - Transport issues
Properties of Metallic SWNTs

(what we know so far)

• Electrical properties (on insulating substrates)
  – Yao (PRL’00), Javey (PRL’04), Park (NL’04)
  – Current saturation near 20 µA for tubes longer than 1 µm
  – Larger currents (up to 100 µA) for short ~10 nm tubes

• Thermal properties
  – Yu (NL’05), Mingo (NL’05), Pop (PRL ’05)
  – Thermal conductivity dominated by phonon transport
  – 3500 Wm⁻¹K⁻¹ around 300 K, decreases as 1/T above
Summary of This Talk

• Metallic single-wall nanotubes
  – On insulating substrate (silicon nitride or oxide)

• Coupled electrical and thermal transport
  – Essential for predicting breakdown voltage of SWNTs on substrates exposed to air (oxygen)
  – Use breakdown voltage scaling to find heat loss coefficient

• Unified electro-thermal model
  – Must include optical phonon absorption (usually neglected) to explain “upkick” in low-bias resistance vs. $T$
Back-of-Envelope Estimate (Suspended)


• Thermal conductivity \( k \sim 3000 \text{ W/m/K} \)

• Typical \( L \sim 1 \mu\text{m}, d \sim 1 \text{ nm} \) suspended nanotube:
  – Thermal conductance \( \sim 25 \text{ nW/K} \)
  – Thermal resistance \( \sim 40 \text{ K/\mu W} \)

• Moderate power \( \sim 10 \mu\text{W} \) (10 \( \mu\text{A} @ 1 \text{ V} \)) \( \implies \Delta T = 400 \text{ K} \!\)
Back-of-Envelope Estimate (On-Substrate)

- SWNT on insulating solid substrate
- Heat dissipated into substrate rather than along tube length
- What is the heat loss coefficient $g$?
- [A: need some gauge of the tube temperature]
Nanotube Temperature Gauge
• Doesn’t exist
• But… oxidation (burning) temperature is known
Breakdown of SWNTs in Air (Oxygen)

- Thermogravimetric (TGA) data shows SWNTs exposed to air breakdown by oxidation at $500 < T_{BD} < 700 \, ^\circ\text{C} (800–1000 \, \text{K})$
- Joule breakdown voltage data shows $V_{BD}$ scales with $L$ in air
- Supports cooling mechanism along the length, into the substrate

**Breakdown of SWNTs: Analysis**

\[ A \nabla (k \nabla T) + p' - g(T - T_0) = 0 \]

At breakdown: \[ p' = I_{BD} V_{BD} / L \]

\[ V_{BD} = gL(T_{BD} - T_0) / I_{BD} \]

- **Empirically note that:**
  - \( V_{BD} \) vs. \( L \) in air scales approx. 5 V/\( \mu m \)
  - Breakdown currents for \( L > 1 \ \mu m \) always about \( I_{BD} \approx 20 \ \mu A \)

- **Analytic solution of heat conduction equation**
  - Heat loss per unit length: \( g \approx 0.14 - 0.2 \ \text{WK}^{-1}\text{m}^{-1} \) given range of \( T_{BD} \)

- **No** assumption was made about electrical transport model
Back-of-Envelope Estimate (Revisit)

- Using $g \approx 0.15 \text{WK}^{-1}\text{m}^{-1} \rightarrow 1/g \approx 6 \text{K}\mu\text{m}/\mu\text{W}$
- Consistent with typical solid-solid thermal interface resistance values, given the SWNT-substrate contact area ($\sim Lx d$)
- At moderate power per length $p' \approx 10 \text{µW}/\mu\text{m} \rightarrow \Delta T \approx 60 \text{K}$
Combined Electro-Thermal Model

- Landauer-type electrical resistance
- Include Joule heating, couple with heat conduction equation
- Self-consistent solution
- Need temperature-dependent mean free paths (MFPs)

\[ R(V, T) = R_C + \frac{h}{4q^2} \left[ \frac{L + \lambda_{\text{eff}}(V, T)}{\lambda_{\text{eff}}(V, T)} \right] \]

\[ A\nabla(k\nabla T) + p' - g(T - T_0) = 0 \]

where

\[ p' = I^2(R - R_C)/L \]

\[ k(T) = 3500(300/T) \]
Combined Electro-Thermal Model

- Landauer-type electrical resistance
- Include Joule heating, couple with heat conduction equation
- Self-consistent solution
- Need temperature-dependent mean free paths (MFPs)
Temperature Dependence of MFPs

\[ \lambda_{\text{eff}} = \left( \lambda_{AC}^{-1} + \lambda_{OP,ems}^{-1} + \lambda_{OP,abs}^{-1} \right)^{-1} \]

\[ \lambda_{AC} = \lambda_{AC,300} \left( \frac{300}{T} \right) \]

\[ \lambda_{OP,abs}(T) = \lambda_{OP,300} \frac{N_{OP}(300) + 1}{N_{OP}(T)} \]

- Include scattering by optical phonon (OP) absorption
- Note OP emission may occur after:
  - (1) A carrier gains enough energy (\( \hbar \omega_{OP} \sim 0.18 \) eV) from E-field
  - (2) An OP absorption event
- OP absorption is a strong function of \( T \) via \( N_{OP} = \left[ \exp(\hbar \omega_{OP} / k_B T) - 1 \right]^{-1} \)
Role of Optical Phonon Absorption

- **Low-bias** resistance of metallic SWNTs
- Subtle effect in the “up-kick” of SWNT low-bias resistance near room temperature $T$
- Important for temperature coefficient of resistivity (TCR) of SWNT interconnects: $\sim 0.0026 \text{ K}^{-1}$, comparable to 40 nm Cu vias
**Electro-Thermal Modeling of SWNTs**

- *Long tubes heat up less*: better heat-sinking, lower power density
- Model suggests current saturates near 20 µA due to self-heating
- Self-heating may be neglected when $p' < 5 \text{ µW/µm}$ (design goal?)
- Current enhancement (> 20 µA) in shortest (< 1 µm) SWNTs very likely aided by Joule heating shifting towards the contacts
Metallic SWNT Resistance Components

\[ k \approx 3500 \text{ Wm}^{-1}\text{K}^{-1} \]
\[ L_{\text{tube}} \approx 2 \mu\text{m}, \ d \approx 2 \text{ nm} \]
\[ L_{\text{contact}} \approx 2 \mu\text{m} \]

<table>
<thead>
<tr>
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<tbody>
<tr>
<td>Tube</td>
<td>(3 \times 10^8) K/W</td>
<td>(2 \times 10^9) K/W</td>
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<tr>
<td>Contacts</td>
<td>(6 \times 10^6) K/W</td>
<td>(2 \times 10^9) K/W</td>
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- \(R_{\text{elec.}} \sim 10 \times R_{\text{phon.}} \rightarrow \text{phonons dominate heat conduction}\)
- \(R_{\text{contact}} < 0.1 \times R_{\text{tube}}\) as long as \(L_{\text{contact}} > 0.8/L_{\text{tube}}\) (\(\mu\text{m}\))
Conclusions

• High-bias breakdown in air (oxidation)
  – Extract thermal conductance to substrate along SWNT length
  – $g \approx 0.15 \text{ Wm}^{-1}\text{K}^{-1}$, limited by nanotube-substrate interface

• Electro-thermal model for transport in metallic SWNTs
  – Estimate MFPs(T) and include optical phonon absorption
  – Relevant in long (> 1 $\mu$m) SWNTs even at low bias ($T > 300$ K)
  – Can we break the 20 $\mu$A current saturation “limit” for long metallic SWNTs by engineering (increasing) $g$?

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