Simple Model of Thermal Conductivity in Carbon Nanotubes and Nanoscale Materials

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Carbon nanotubes (CNT's) are a novel material with unique physical properties due to their one-dimensional structure. In particular, CNTs are known to have high thermal conductivity which provides for many useful applications in industry including computing and other electrical circuits. The study of thermal conductivity in CNT's (~3500 W/mK) and similar nano scale materials has usually been restricted to elaborate theories which rely on quantum mechanical principles and macroscale energy transfer. In this work, we propose a simple semiclassical model of heat transfer in solids that can provide a thorough explanation of macroscale thermal phenomenon through atomic vibrations. The model is based on a one-dimensional linear chain of atoms connected by springs, which allows us to predict the temperature by considering the energy associated with any single atom. We can then observe thermal behavior by relating temperature, time, and position coordinates to the macroscopic heat equation. In an attempt to validate our simple model, we determine thermal constants and compare the results with some previous theoretical works and experimental data.

Simple Model for Thermal Conductivity in Carbon Nanotubes and Nanoscale Materials

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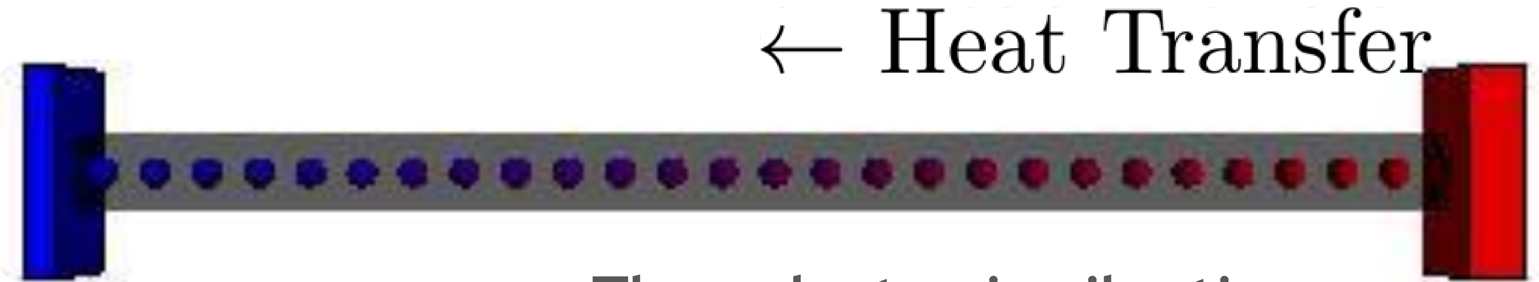
Thermal Conductivity in Single Wall Carbon Nanotubes

Thermal Conductivity

$$\frac{\partial T(x,t)}{\partial t} = \lambda \frac{\partial^2 T(x,t)}{\partial x^2}$$

λ- Thermal Diffusivity

$\leftarrow$ Heat Transfer



Through atomic vibrations

Current Model: *Landauer Energy Flux*

$$\dot{Q}_{ph} = \kappa \Delta T \qquad \dot{Q}_{ph} = \sum_M \int_0^\infty \frac{dq}{2\pi} \hbar\omega_M(q) v_M(q) \times [\eta(\omega_M, T_{hot}) - \eta(\omega_M, T_{cold})]\zeta_m(q)$$

T - Temperature
x - Position
M - Phonon mode
q - Wavenumber of phonon
$\hbar\omega_m(q)$ - Phonon energy
$v_m(q)$ - Phonon group velocity
$\eta(\omega_m, T)$ - Distribution of phonons
$\zeta_m(q)$ - Trasmission probability
$\dot{Q}_{ph}$ - Heat Flux
κ- Thermal Conductivity

- Predict Quantized Conductance
- Approaches unity at low T

$$4\kappa_0 = 4(\pi^2 k_B^2 T/3h)$$

Yamamoto et al., PRL, 075502 (2004)

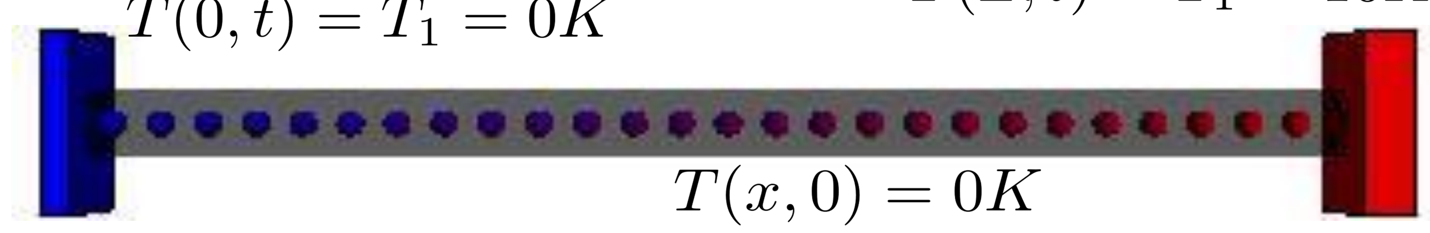
Purpose:
Create a simple semi-classical model to describe thermal conduction in carbon nanotubes

How Do We Obtain Best Fit?

Heat Equation predicts temperature distribution

$$\frac{\partial T(x,t)}{\partial t} = \lambda \frac{\partial^2 T(x,t)}{\partial x^2}$$

$T(0,t) = T_1 = 0K$ $\qquad$ $T(L,t) = T_1 = 10K$



$T(x,0) = 0K$

Initial and Steady State Conditions

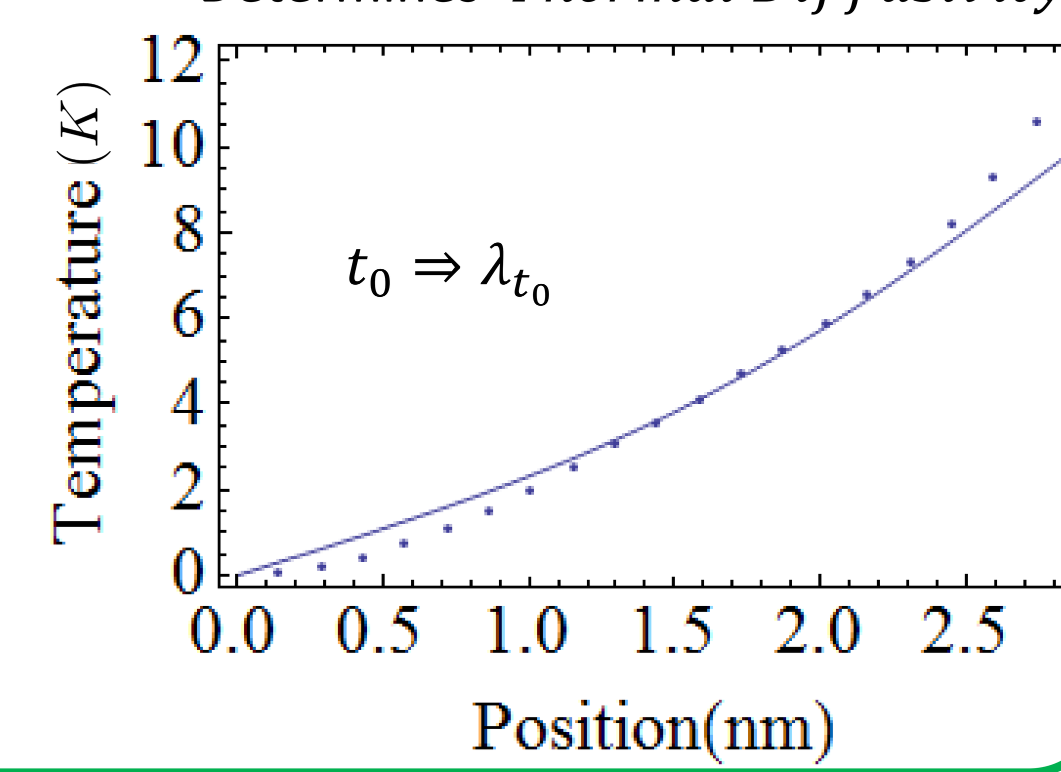
- Solid and left wall at $T = 0$K
- Right wall at $T = 10$K

$$\lim_{t\to\infty} T(x,t) = T_{eq}(x) \qquad T_{eq}(0) = T_1 \qquad C_1 = \frac{T_2 - T_1}{L}$$

$$T_{eq}(x) = C_1 x + T_1 \qquad T_{eq}(L) = T_2$$

Best Fit points to solution

- Determines *Thermal Diffusivity*



General Solution by Separation of Variables

$$T(x,t) = T_{eq}(x) + \sum_n^l C_n e^{-(\frac{n\pi}{L})^2 \lambda t} \sin(\frac{n\pi x}{L})$$

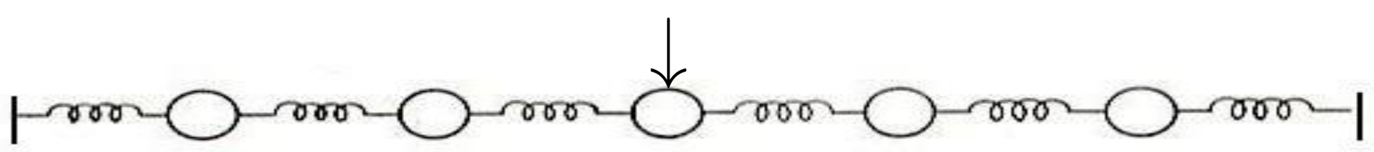
Where

$$C_n = \frac{2}{L}\int_0^L (T(x,0) - T_{eq}(x)) \sin\left(\frac{n\pi x}{L}\right) dx$$

On the Atomic Scale

Atomic scale model

u_n- Displacement of n^{th} atom



$$m\ddot{u}_n = -2ku_n - \gamma\dot{u}_n + ku_{n-1} + ku_{n+1}$$

Amplitude of Motion Relates to Energy

$$\langle A(t)^2 \rangle = \frac{1}{P}\int_{t-P/2}^{t+P/2} u_n(t')^2 dt'$$

$$E = k_B T = \frac{1}{2}k\langle A(t)^2 \rangle$$

m - Mass of Carbon Atom
k - Spring constant
γ - Damping Factor
A - Amplitude of Motion
P- Period of Oscillation
n - 20 Atoms

Boundary Conditions: The Simple Case

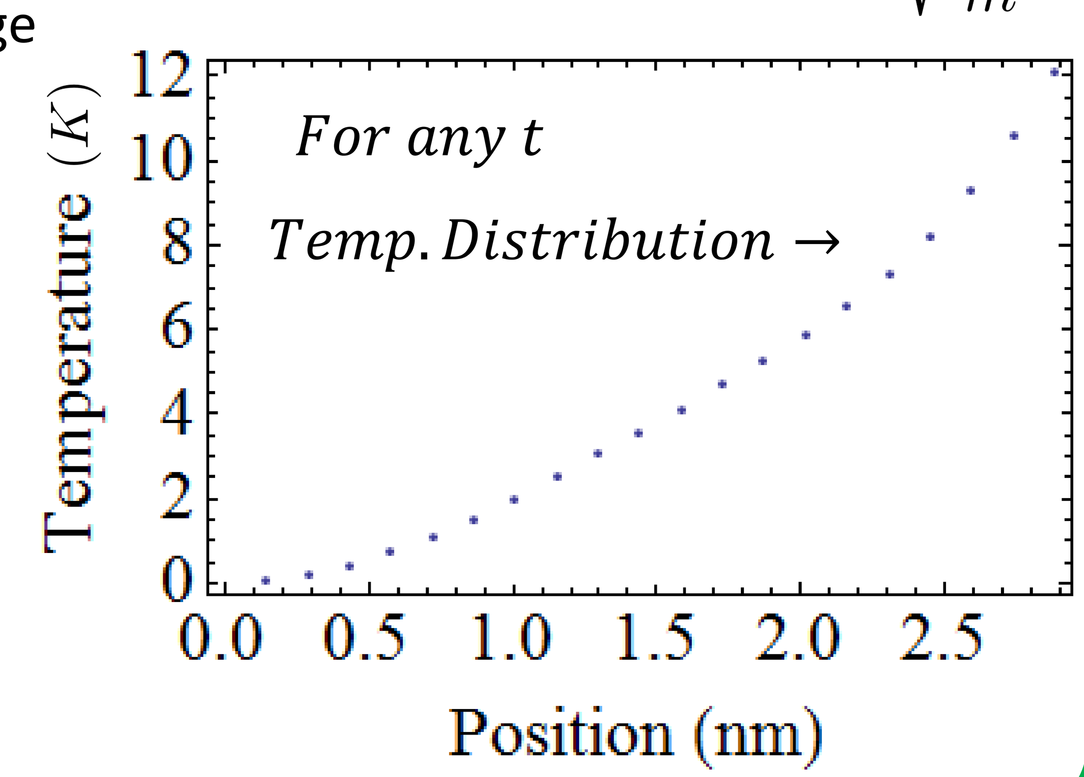
- Solid at $T = 0$K $\Rightarrow$ No Initial Motion

$$u_n(0) = 0 \qquad u'_n(0) = 0$$

- Right wall at $T = 10$K $\Rightarrow$ Fixed Vibration

$$F_T(t) = kA_T \cos(\omega t) \qquad \omega = \sqrt{\frac{k}{m}}$$

- Monitor Energy change through vibration amplitude
- Used Mathematica to numerically solve for 20 atoms
- Obtain temperature distribution along 1D solid



Predicted Results

From Previous Model:

$$\kappa \approx 4(\pi^2 k_B^2 T/3h) \approx 0.0001 \frac{eV}{K\ ps}$$

Since:

$$\lambda \equiv \frac{\kappa}{C_V\ \rho}$$

$$\rho = 23.94 \frac{eV\ ps^2}{nm^5} \qquad C_V \approx 10^{-6} \frac{nm^2}{K\ ps}$$

For a (10,0) semiconducting nanotube

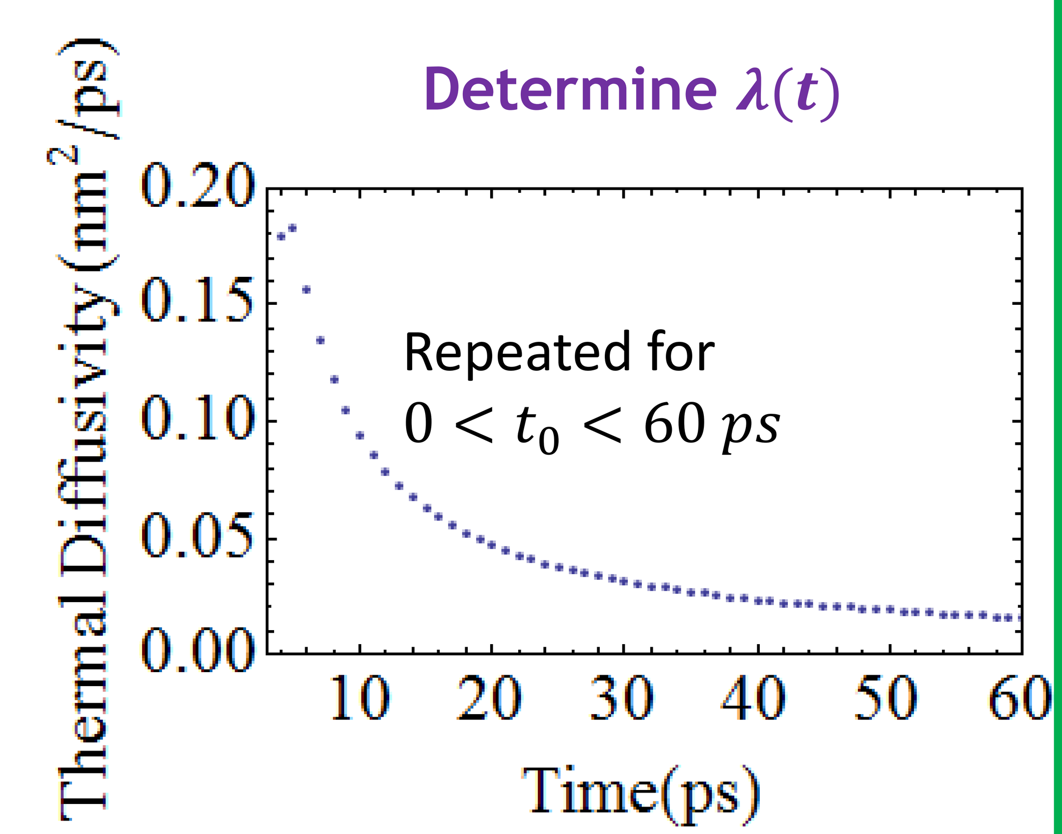
Hone et al., Marcel Dekker,Inc, 606 (2004)

$$\lambda \approx 4.18 \frac{nm^2}{ps}$$

Our model: $0.05 < \lambda < 0.2$

- Manageable considering over simplification

Determine $\lambda(t)$



Summary and Future Work

- Used a **simple spring model** to model thermal conductivity
- Dynamic **Thermal Diffusivity** with reasonable error considering simplification
- Expand model to explain **phonon transport**

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