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.
Thermal Conductivity in Single Wall Carbon Nanotubes

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

Heat Equation predicts temperature distribution

\[
T(0, t) = T_1 = 0K \quad T(L, t) = T_1 = 10K
\]

Initial and Steady State Conditions

- Solid and left wall at \( T = 0K \)
- Right wall at \( T = 10K \)

\[
limit_{t \to \infty} T(x, t) = T_{eq}(x)
\]

\[
T_{eq}(0) = T_1 \quad C_1 = \frac{T_2 - T_1}{L}
\]

General Solution by Separation of Variables

\[
T(x, t) = T_{eq}(x) + \sum_{n} C_{n} e^{-\left(\frac{n\pi x}{L}\right)^2 \lambda t} \sin \left(\frac{n\pi x}{L}\right)
\]

Where

\[
C_{n} = \frac{2}{L} \int_{0}^{L} \left( T(x, 0) - T_{eq}(x) \right) \sin \left(\frac{n\pi x}{L}\right) dx
\]

Purpose:

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

On the Atomic Scale

Atomic scale model

\[
u_{n} - Displacement of n^{th} atom
\]

\[
m\ddot{u}_{n} = -2k\dot{u}_{n} - \gamma \dot{u}_{n} + ku_{n-1} + ku_{n+1}
\]

Amplitude of Motion Relates to Energy

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

\[
E = k_BT = \frac{1}{2} k\langle A(t)^2 \rangle
\]

\( m - Mass \) of Carbon \( k - Spring \) constant \( \gamma - Damping \) Factor \( A - Amplitude \) of Motion \( P - Period \) of Oscillation

Boundary Conditions: The Simple Case

- Solid at \( T = 0K \) ⇒ No Initial Motion
  \( u_n(0) = 0 \quad u_n'(0) = 0 \)
- Right wall at \( T = 10K \) ⇒ Fixed Vibration
  \( F_T(t) = k A_T \cos(\omega t) \)
  \( \omega = \sqrt{\frac{k}{m}} \)

Obtain temperature distribution along 1D solid

For any \( t \)

Temp. Distribution

Summary and Future Work

- Predicted Results

Determine \( \lambda(t) \)

Repeated for \( 0 < t_0 < 60 \) ps

\[ \rho = 23.94 \text{ eV ps}^2 \text{ nm}^{-2} \]

For a (10,0) semiconducting nanotube

\[ \lambda \approx 4.18 \text{ nm}^2 \text{ ps}^{-1} \]

Our model: \( 0.05 < \lambda < 0.2 \)

- Dynamic Thermal Diffusivity with reasonable error considering simplification
- Expand model to explain phonon transport

How Do We Obtain Best Fit?

Best Fit points to solution

Determine Thermal Diffusivity

Thermal Conductivity Current Model: Landauer Energy Flux

\[
\dot{Q}_{ph} = \kappa \Delta T \quad \dot{Q}_{ph} = M \int_{0}^{\infty} \frac{dq}{2\pi} h\omega_M(q)\nu_M(q) \times [\eta(\omega_M, T_{hot}) - \eta(\omega_M, T_{cold})] \zeta_M(q)
\]

- Predict Quantized Conductance
- Approaches unity at low \( T \)

\[ 4\kappa_0 = 4(\pi^2 k_B T/3h) \quad \text{Yamamoto et al., PRL, 075502 (2004)} \]

General Solution by Separation of Variables

From Previous Model:

\[ \kappa \approx 4(\pi^2 k_B^2 T/3h) \approx 0.0001 \text{ eV K ps}^{-1} \]

Since:

\[ \lambda \equiv \frac{\kappa}{C_V \rho} \]

\[ C_V \approx 10^{-6} \text{ nm}^2 \text{ ps}^{-1} \]

Hone et al., Marcel Dekker,Inc, 605 (2004)

Our model: \( 0.05 < \lambda < 0.2 \)

- Manageable considering over simplification

Simple Model for Thermal Conductivity in Carbon Nanotubes and Nanoscale Materials

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