Thermal Transport in Nanowires

- Nanoscale Heat Transfer
- Need for Analytical Methods
- Guyer-Krumhansl Equation
- Higher Order Heat Transport Equation
- Comparison for Nanowires

Nanoscale Heat Transfer

Fourier Law breaks down for microscale and nanoscale systems.

Problem is of increasing relevance -

- Nanofabrication
- Reducing size of semiconductor devices
- Increasing transistor density (Moore's Law)

Complexibility arises due to the existence of **three phonon scattering** mechanisms -

N Processes - Conserve momentum, redistribute energy across the spectrum.

R Processes - Do not conserve momentum.

Need for Analytical Methods

Microscopic Methods
Molecular dynamics simulations are computationally demanding and cannot be scaled.

Mesoscopic Methods
Other methods model phonon behaviour using empirical data from microscopic methods. Variations of the BTE are used in conjunction with modelled phonon behavior.

Macroscopic Methods
Existing analytical generalized heat transport methods rely on approximations where they either neglect certain N processes or R processes.

Guyer-Krumhansl Equation

$$\tau_R \frac{\partial \mathbf{q}}{\partial t} + \mathbf{q} + \lambda \nabla T = l^2 \left[\nabla^2 \mathbf{q} + 2 \nabla (\nabla \cdot \mathbf{q}) \right]$$

A **phenomenological phonon hydrodynamic** model accounts for non-local effects at the wall. (Phonon-Boundary Scattering)

The general form of the transport equation appears to remain the same across derivations.

The coefficient on the RHS, changes depending on the treatment and consideration of phonon scattering mechanisms.

Higher Order Heat Transport Equation

A **generalized heat transport equation** is obtained by analyzing the evolution of **q** using a higher order transport equation developed for rarefied gas flows.

Appropriate simplifications for a solid material are made - variation of pressure, density, stress tensor, and macroscopic velocity are set to zero.

$$\tau_R \frac{\partial \mathbf{q}}{\partial t} + \mathbf{q} + \nabla T = m_1 \mathbf{q} (\nabla \cdot \mathbf{q}) + m_2 (\mathbf{q} \cdot \nabla) \mathbf{q} + m_3 \nabla (\mathbf{q} \cdot \mathbf{q}) + m_4 \nabla^2 \mathbf{q} + m_5 \nabla (\nabla \cdot \mathbf{q}) + m_6 \mathbf{q} (\mathbf{q} \cdot \nabla T) + m_7 (\mathbf{q} \cdot \mathbf{q}) \nabla T$$

Treatment for Nanowires

GK Equation[1]

Assumptions

1. Steady State Conditions
2. Longitudinal Temperature Variation
3. Diffusive Boundary

$$\mathbf{q} + \lambda \nabla T = l^2 \nabla^2 \mathbf{q}$$

Remaining terms eliminated as per assumption 1.

Boundary Conditions for Bulk Component

$$q_b(R) = 0$$

No slip boundary condition at the wall.

$$\left.\frac{\partial q_b}{\partial r}\right|_{r=0} = 0$$

Symmetry condition at the centre.

[1] As proposed in Sellitto et al.

$$q_b(r) = \lambda \left[1 - \frac{J_0(ir/l)}{J_0(iR/l)}\right] \frac{\Delta T}{L}$$

$$q_w(r) = -Cl \left.\frac{\partial q_b}{\partial r}\right|_{r=R} = -\lambda \left(C \left[\frac{iJ_1(iR/l)}{J_0^2(iR/l)}\right] J_0(iR/l) \right) \frac{\Delta T}{L}$$

$$q(r) = q_b(r) + q_w(r)$$

$$\lambda_{eff}(R) = \frac{\int_0^R 2\pi r\, q(r)\, dr}{\pi R^2 |\nabla T|}$$

$$\lambda_{eff}(\mathrm{Kn}) = \lambda \left(1 - 2\mathrm{Kn} \left[\frac{J_1(i/\mathrm{Kn})}{J_0(i/\mathrm{Kn})}\right]^2 \left[\frac{J_0(i/\mathrm{Kn})}{iJ_1(i/\mathrm{Kn})} + C\right]\right)$$

Sellitto splits heat flux term into the bulk and the wall component by arguing that the Knudsen layer extends into the whole wire.

This linear approximation is poor and wholly unnecessary as it implies that the wall contribution is uniform throughout the wire.

Treatment for Nanowires

Higher Order Equation

$$\mathbf{q} + \lambda \nabla T = m^2 l^2 \nabla^2 \mathbf{q}$$

Under steady state assumption.
Non-linear terms neglected for nanostructures.

First Order Boundary Condition

$$q(R) = -Cl \left.\frac{\partial q}{\partial r}\right|_{r=R}$$

First order slip condition at wall.
C is a boundary coefficient
l is the mean free path.

$$\left.\frac{\partial q}{\partial r}\right|_{r=0} = 0$$

Symmetry condition at the centre.

Second Order Boundary Condition

$$q(R) = -Cl \left.\frac{\partial q}{\partial r}\right|_{r=R} + \alpha l^2 \left.\frac{\partial^2 q}{\partial r^2}\right|_{r=R}$$

α is the second boundary coefficient.
Describes phonon backscattering effect.

First Order Solution

$$q_{FO}(r) = \frac{\lambda \Delta T \left(m J_0\left(\frac{ir}{ml}\right) - m J_0\left(\frac{iR}{ml}\right) + iC J_1\left(\frac{iR}{ml}\right)\right)}{L\left(iC J_1\left(\frac{iR}{ml}\right) - m J_0\left(\frac{iR}{ml}\right)\right)}$$

$$\lambda_{eff\,|\,\mathrm{FO}} = \lambda \frac{m I_0\left(\frac{1}{m\,\mathrm{Kn}}\right) + (C - 2m^2\mathrm{Kn}) I_1\left(\frac{1}{m\,\mathrm{Kn}}\right)}{m I_0\left(\frac{1}{m\,\mathrm{Kn}}\right) + C\, I_1\left(\frac{1}{m\,\mathrm{Kn}}\right)}$$

Second Order Solution

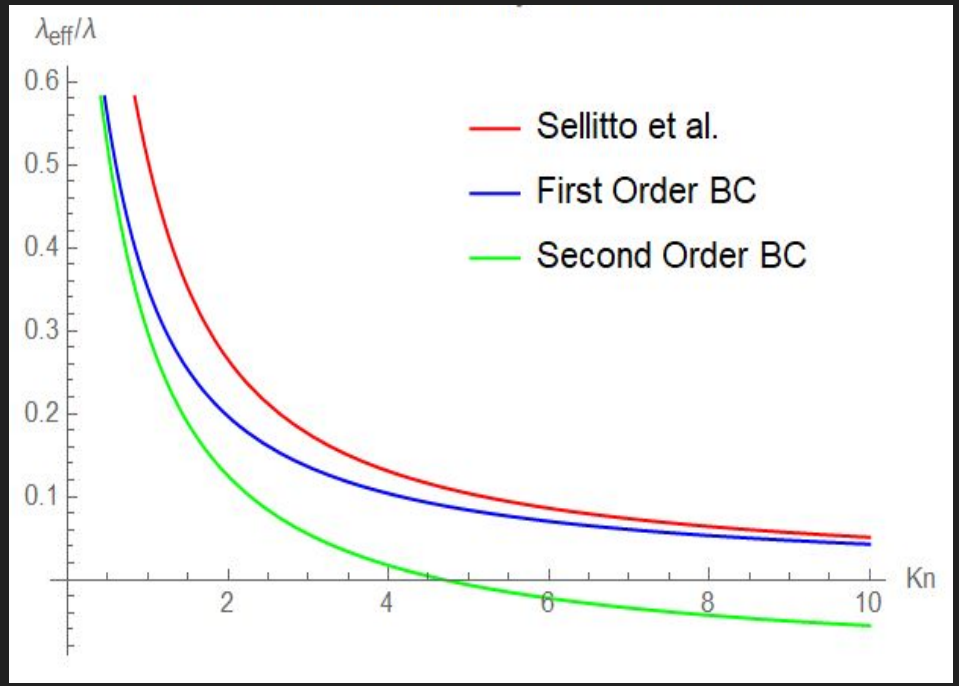
$$q_{SO}(r) = -\frac{\lambda \Delta T}{L} \frac{m^2 R J_0\left(\frac{ir}{ml}\right) + R(\alpha - m^2) J_0\left(\frac{iR}{ml}\right) + im(CR + \alpha l) J_1\left(\frac{iR}{ml}\right)}{R(m^2 - \alpha) J_0\left(\frac{iR}{ml}\right) - im(CR + \alpha l) J_1\left(\frac{iR}{ml}\right)}$$

$$\lambda_{eff\,|\,\mathrm{SO}} = \lambda \frac{(m^2 - \alpha) I_0\left(\frac{1}{m\,\mathrm{Kn}}\right) + m(C + \mathrm{Kn}(\alpha - 2m^2)) I_1\left(\frac{1}{m\,\mathrm{Kn}}\right)}{(m^2 - \alpha) I_0\left(\frac{1}{m\,\mathrm{Kn}}\right) + m(C + \alpha \mathrm{Kn}) I_1\left(\frac{1}{m\,\mathrm{Kn}}\right)}$$

$\alpha = 2/9$ $\quad m^2 = 18/5\pi$

Comparison of Results

Ratio of Effective and Bulk Conductivity vs. Knudsen Number

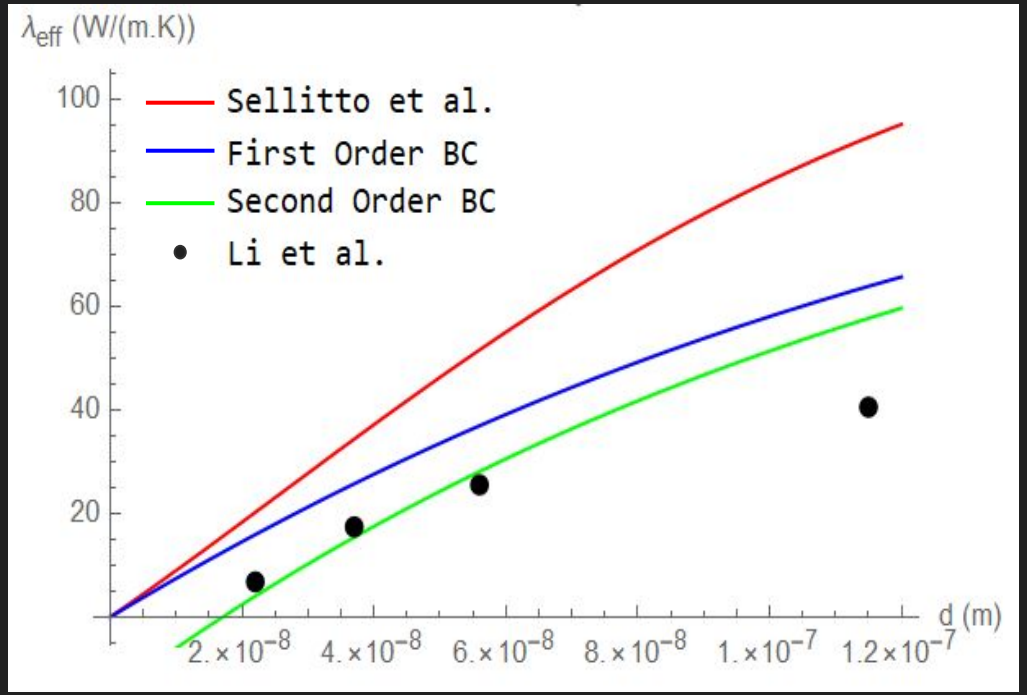


Comments

- Second order BC solution shows the insulator-conductor transition at higher Knudsen numbers.
- Both First Order and Second Order BC show a marked difference from the equation proposed by Sellitto, implying the inadequacy of a additive boundary contribution.

Comparison of Results

Effective Thermal Conductivity vs. Wire Diameter



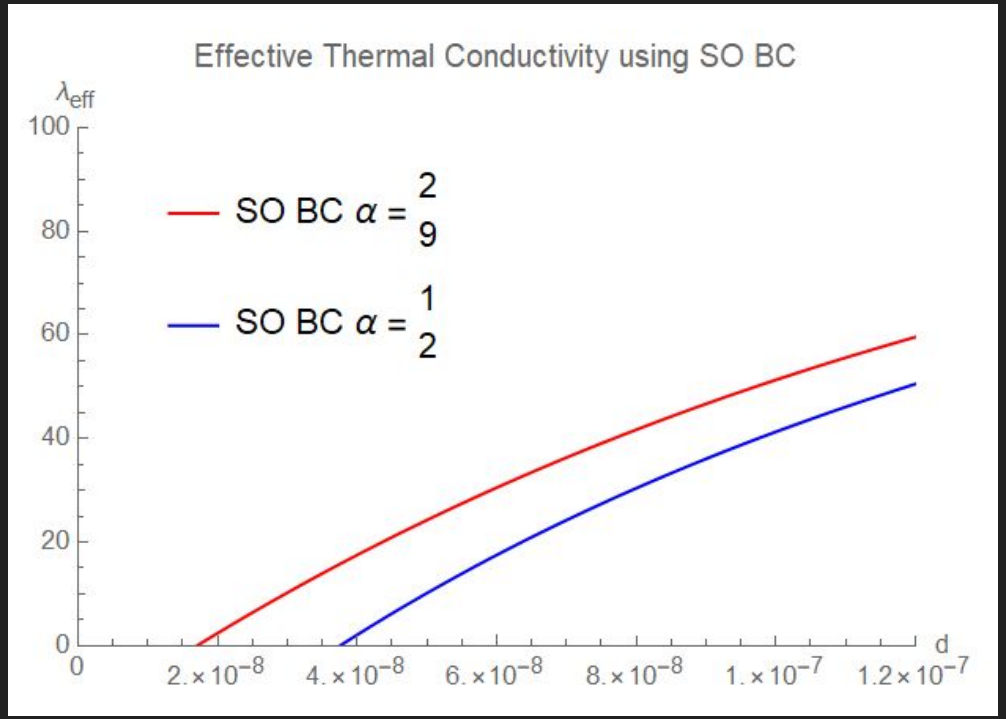
Comments

- All plots shown for C = 1, and second order slip coefficient α = 2/9.
- Second Order BC gives a better correlation to the experimental data (Li et al.) than the equation provided by Sellitto et al.
- Sellitto et al. only performs better at lower values of slip coefficient (C = 0.3).

Diameter @ 90% of Bulk Thermal Conductivity	
Sellitto et al.	0.79 um
Second Order BC	8.83 um

Comparison of Results

Critical Diameter (Vanishing Heat Flux)



Comments

- ❖ Vanishing thermal conductivity below certain radii imply a resistance to heat flow imposed by scale.

1. Metal-Insulator Anderson Transition (Analog)
2. Quantum Localization Effects

α	Critical Radius (in nm)	
	Sellitto et al.	Second Order BC
1/2	17.98	18.77
2/9	8.4	8.52

Potential Discrepancy in Sellitto et al.

Sellitto et al.:

$$\lambda_{eff}(\mathrm{Kn}) = \lambda\left(1 - 2\mathrm{Kn}\left[\frac{J_1(i/\mathrm{Kn})}{J_0(i/\mathrm{Kn})}\right]^2\left[\frac{J_0(i/\mathrm{Kn})}{iJ_1(i/\mathrm{Kn})} + C\right]\right)$$

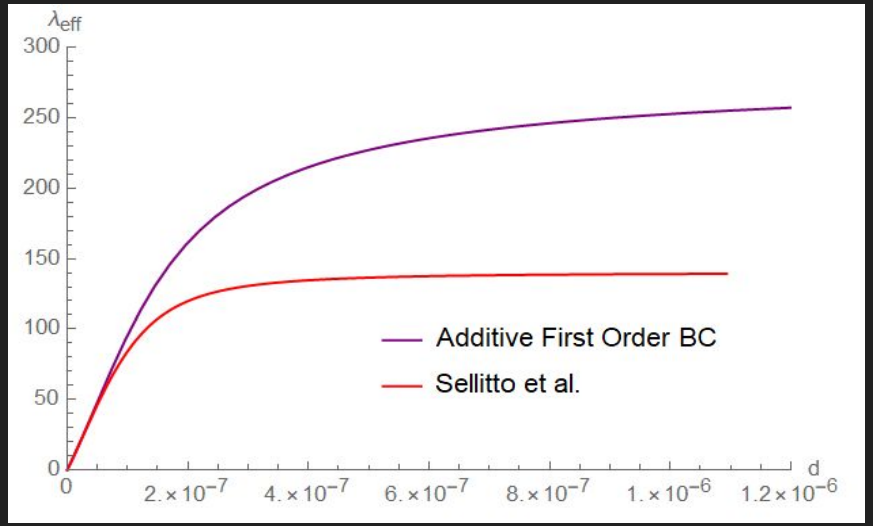
Solved on Mathematica:

$$\lambda_{eff}(\mathrm{Kn}) = \lambda\left[1 + \frac{(C - 2\mathrm{Kn})I_1\left(\frac{1}{\mathrm{Kn}}\right)}{I_0\left(\frac{1}{\mathrm{Kn}}\right)}\right]$$

Comments

- Despite deriving from the same proposed method, the equation on Sellitto et al. appears to have an imposed upper limit at the bulk thermal conductivity value.

Comparison of Thermal Conductivity Saturation Values



- Upper limit is reached at all values of C in Sellitto et al.
  Not the case for the derived Additive BC condition.