Monte Carlo Study of Thermal Transport of Direction and Frequency Dependent Boundaries in High Kn Systems

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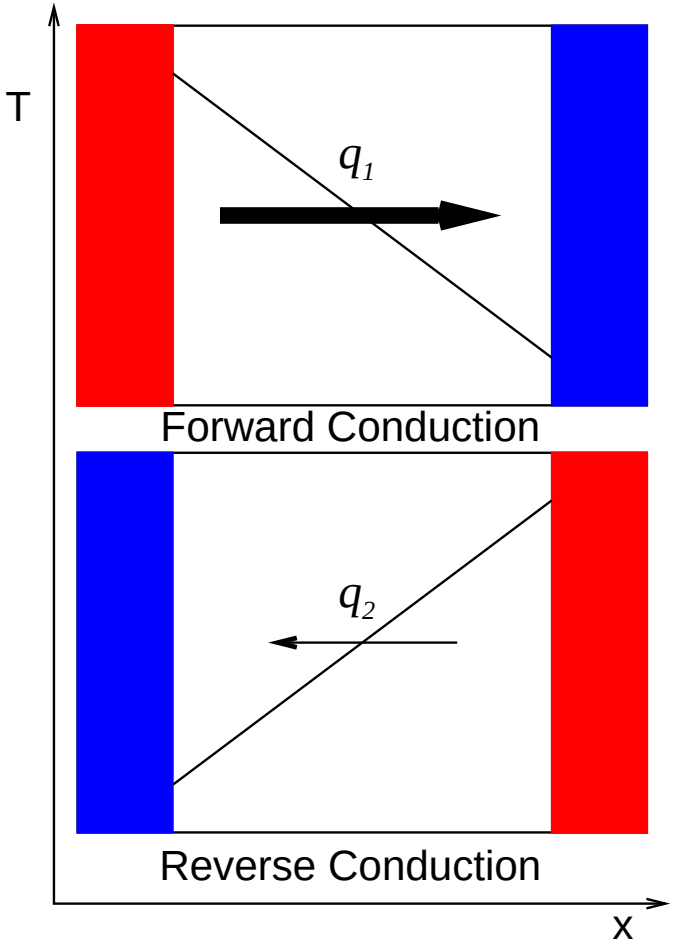
Introduction

Thermal rectification is a phenomenon where transport through a device is dependent on direction



$$q = -kA\frac{dT}{dx}$$

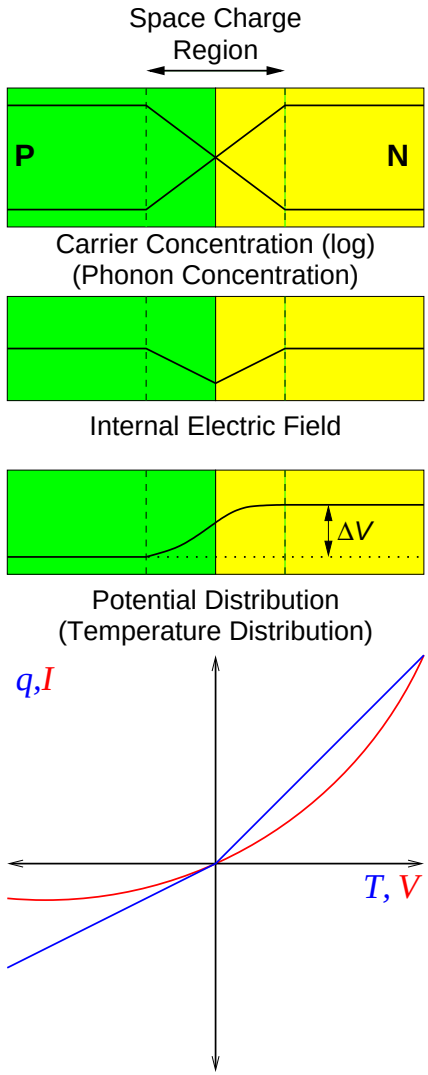
$$q_1 > q_2$$

$$k_1 > k_2$$

- Widespread applications in thermal management problems
  - Cooling of micro/nano electronics
  - Improvement of macroscale refrigeration and energy saving buildings

Analog to pn-junction (Diode)

- In equilibrium electrons diffuse into p-type semiconductor and holes diffuse into n-type semiconductor, this creates the space charge region and built-in potential (voltage)
- A forward bias decreases the potential across the junction which enhances transport
- A reverse bias increases the potential across the junction reduces transport resulting in minimal current flow
- Thermal rectifying behaviour should be observed if a device could be created in which phonon transport can be manipulated

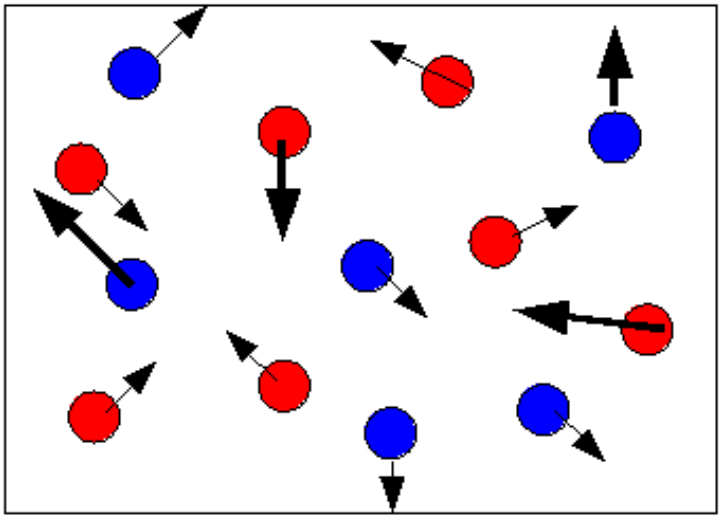


Boltzmann Transport Equation

- Phonons treated as particles with distribution function $f = f(\bar{r}, \bar{p}, t)$

$$\frac{\partial f}{\partial t} + \bar{v} \cdot \nabla_r f + \bar{F} \cdot \nabla_p f = \left(\frac{\partial f}{\partial t}\right)_{scat} \approx \frac{f_0 - f}{\tau_{relax}}$$

- It is very difficult to obtain a closed-form solution
- In the current work we solve it using a probabilistic simulation known as Monte Carlo Method



Simulation Method

- Initialization
  - Number of phonons initially prescribed (1,000,000)
  - Randomly distributed throughout the device
  - Polarization and frequency obtained based on initial temperature
  - Momentum calculated from analytic dispersion relation
- Three-phonon and impurity scattering were not considered to investigate the system in the ballistic regime
- Cross sections of $100 \times 100\,\mathrm{nm}$ to $1000 \times 1000\,\mathrm{nm}$ and lengths of $100\,\mathrm{nm}$ to $1000\,\mathrm{nm}$

Analytic phonon dispersion	$\Rightarrow$	$\omega(k) = \omega_{max,b}\sqrt{\frac{1-\cos ka}{2}}$
3-D Density of States	$\Rightarrow$	$D(k) = \frac{k^2}{2\pi^2 V_g}$
Phonon group velocity	$\Rightarrow$	$V_g = \nabla_k \omega$
Bose-Einstein distribution	$\Rightarrow$	$\langle n \rangle = \frac{1}{\exp\frac{\hbar\omega}{k_B T}-1}$

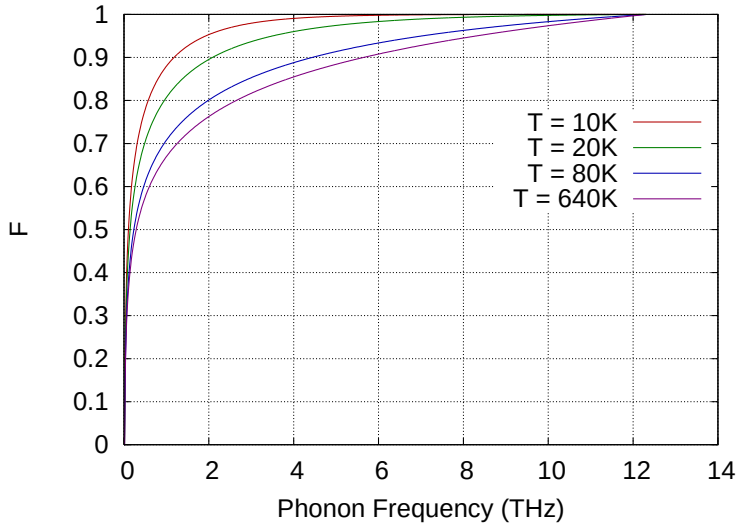
Simulation Method Cont.

The device is composed of an isotropic material with Silicon-like properties

Max. longitudinal acoustic phonon frequency $\Rightarrow$ $1.23 \times 10^{13}\,\mathrm{Hz}$

Max. transverse acoustic phonon frequency $\Rightarrow$ $4.5 \times 10^{12}\,\mathrm{Hz}$

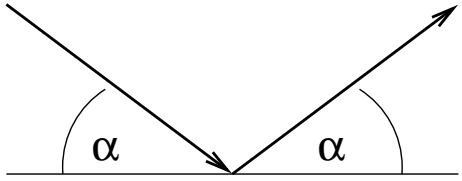
Normalized density function $\Rightarrow$ $F(\omega) = \sum_b \frac{\int_0^{\omega} \langle n \rangle D(\omega) d\omega}{\int_0^{\omega_{max,b}} \langle n \rangle D(\omega) d\omega}$



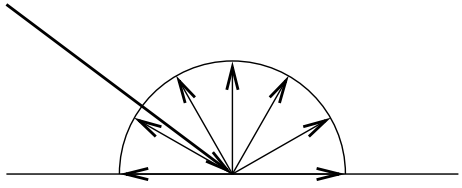
- The normalized density function is a key element in this study by shown the concentration of high frequency (energy) phonons at a specified temperature

Definition of Direction and Frequency Dependent Boundaries

- Boundaries parallel to x-axis have direction and frequency dependence
  - Boundaries are flat in simulation
  - Directional dependence comes from asymmetric sawtooth geometry
  - Frequency dependence comes from specified surface roughness
  - Both dependencies come from difference roughnesses of the surfaces
- If a phonon with negative x-momentum strikes a boundary parallel to the x-axis a parameter, $p(\omega, \eta)$, is calculated based on the phonon frequency and characteristic roughness
- if $p \ll 1$, the phonon has a high probability of a diffuse reflection
- $p(\omega) = \exp\left[-\frac{64\pi^5\eta^2\omega^2}{V_g^2}\right]$

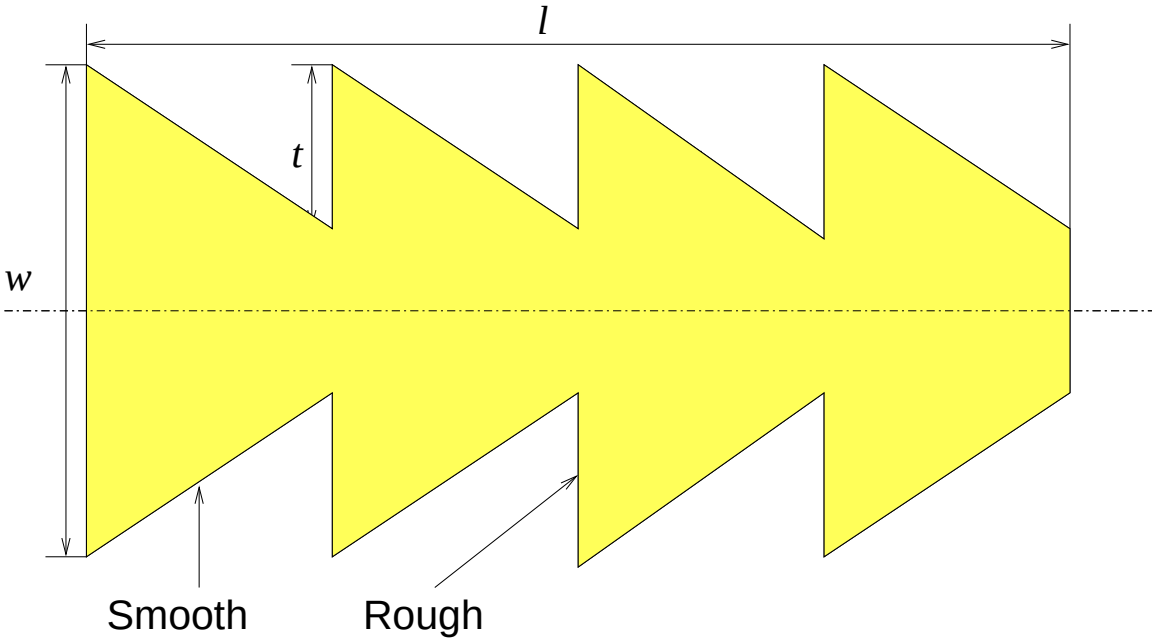


Specular Reflection



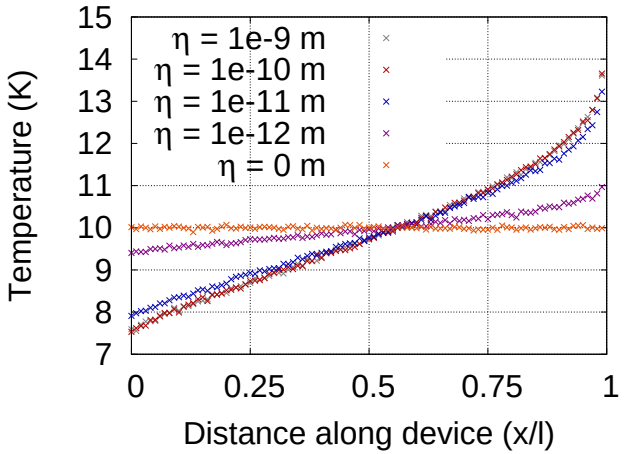
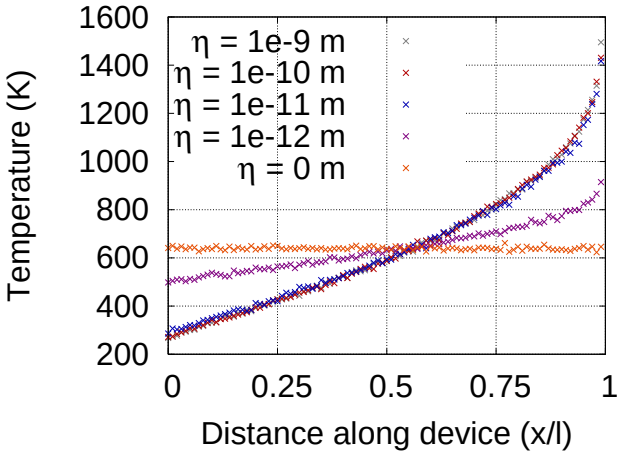
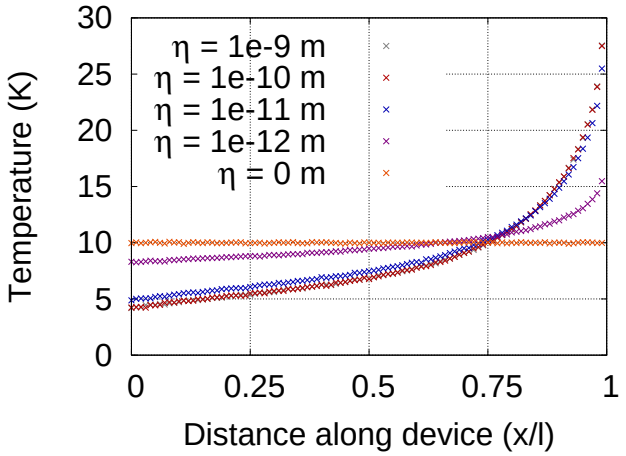
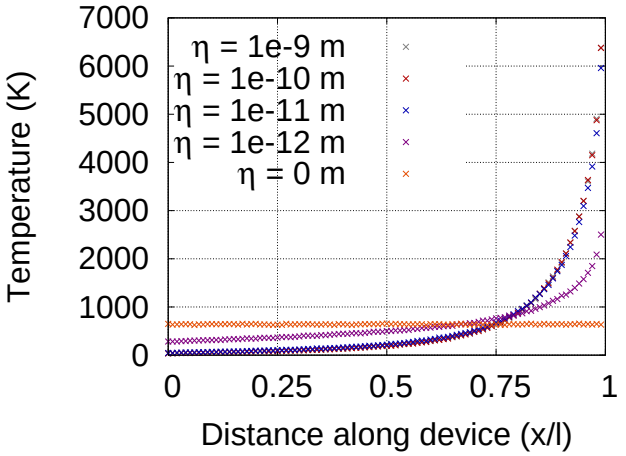
Diffuse Reflection

Definition of Direction and Frequency Dependent Boundaries Cont.

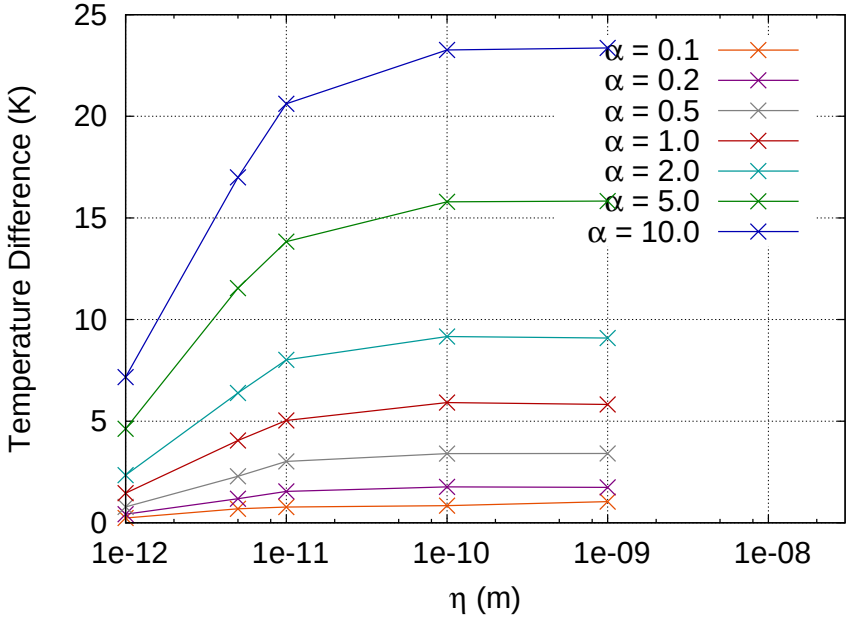


- l and w are length and width of the device, respectively
- t is the sawtooth depth (of order or smaller than dominate phonon wavelength)
- phonons moving to the right see “smooth” surfaces, phonons moving to the left see “rough” surfaces

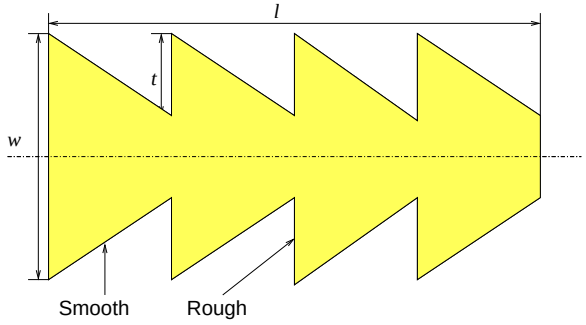
Simulation Results - Temperature distribution

T	10K	640K
$\alpha = 1$		
$\alpha = 10$		

Simulation Results - Temperature difference at $T = 10\,\mathrm{K}$

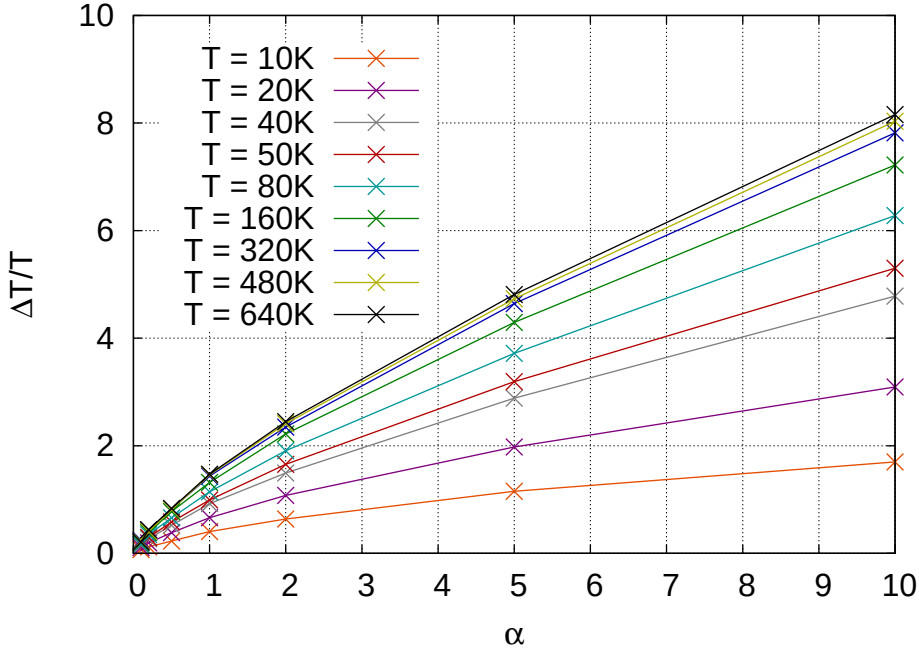


$$\alpha = \frac{l}{w}$$



- Increased biasing with increased surface roughness of “rough” surface
- Increased biasing with increased aspect ratio (greater percentage of direction and frequency dependent surface area)

Simulation Results - Normalized temperature difference for $\eta = 5 \times 10^{-12}\,\mathrm{m}$



- Normalized temperature difference increases with increasing temperature and aspect ratio
- This increase with temperature is explained by the normalized density function

Conclusions

- Self-biasing devices can be achieved with the use of asymmetric geometries and surface roughnesses (anisotropic behavior in an isotropic material)
- With the addition of thermalizing boundaries we should see thermal rectification in the ballistic transport regime
- The impact of the boundaries will be reduced at higher temperatures when scattering is included and when the device surface area to volume ratio is decreased
- Fabrication
  - Atomically smooth $\eta = 0$
  - One unit cell variation $\eta \approx 0.5a$