

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

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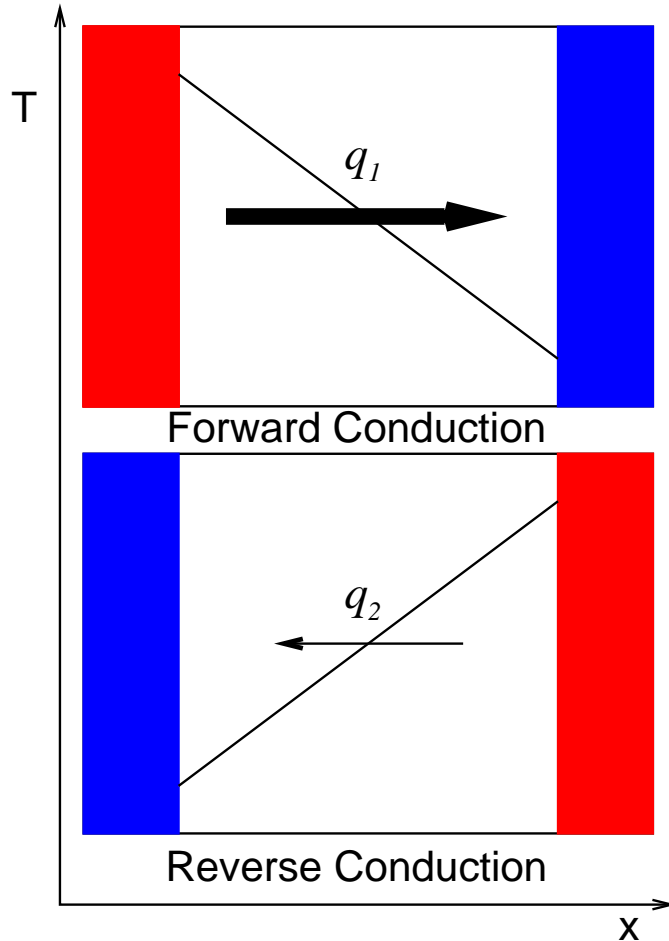
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Thermal rectification is a phenomenon where transport through a device is dependent on direction



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

$$q_1 > q_2$$

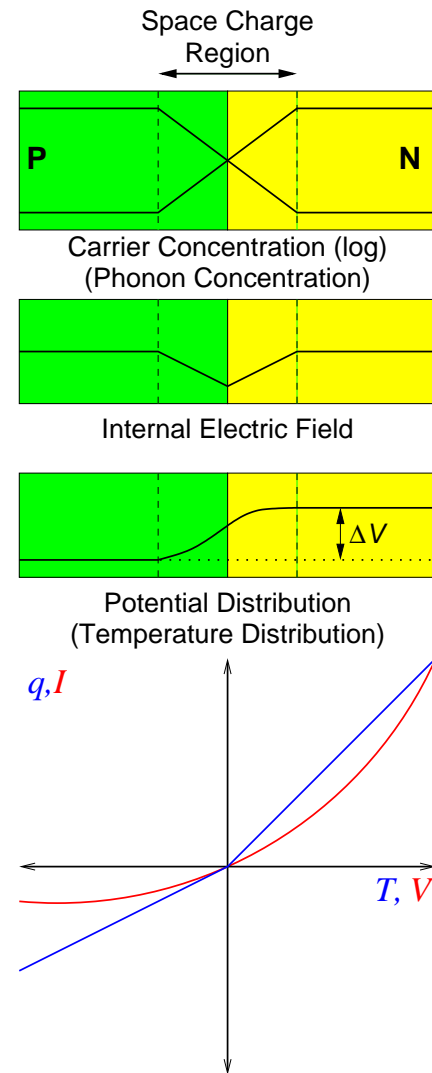
$$k_1 > k_2$$

- 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



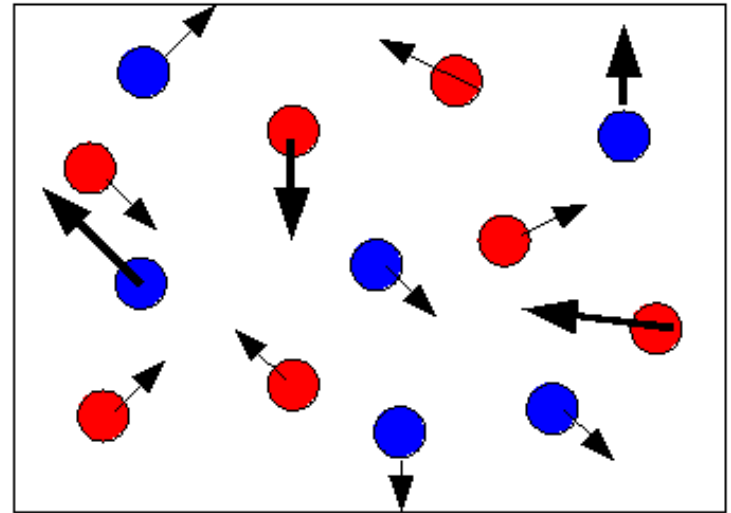
# Boltzmann Transport Equation



- 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





- 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  $100 \times 100$  nm to  $1000 \times 1000$  nm and lengths of 100 nm to 1000 nm

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

# Simulation Method Cont.

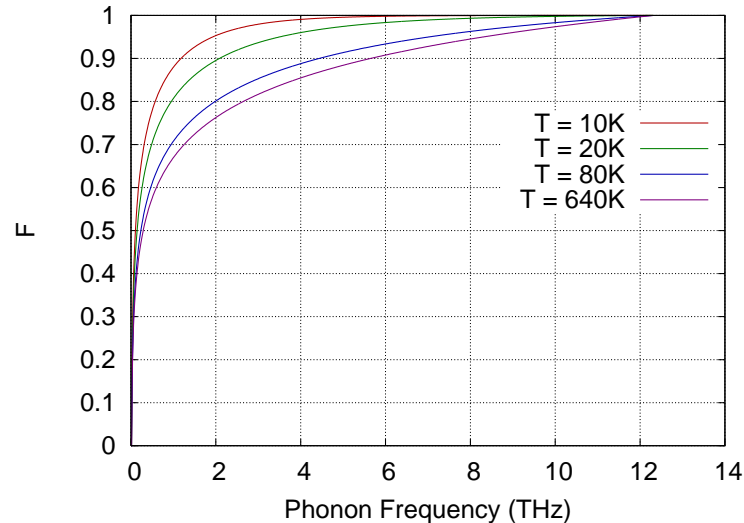


The device is composed of an isotropic material with **Silicon-like properties**

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

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

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

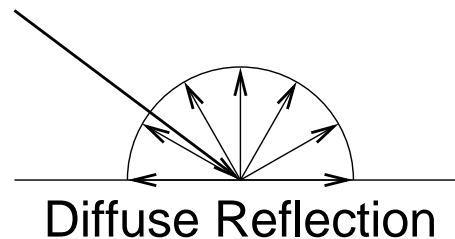
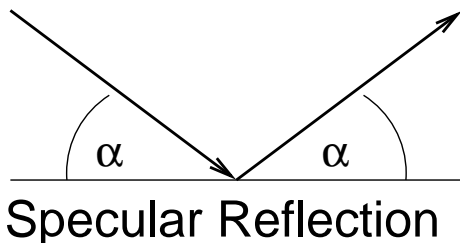


- The normalized density function is a key element in this study by shown the concentration of high frequency (energy) phonons at a specified temperature

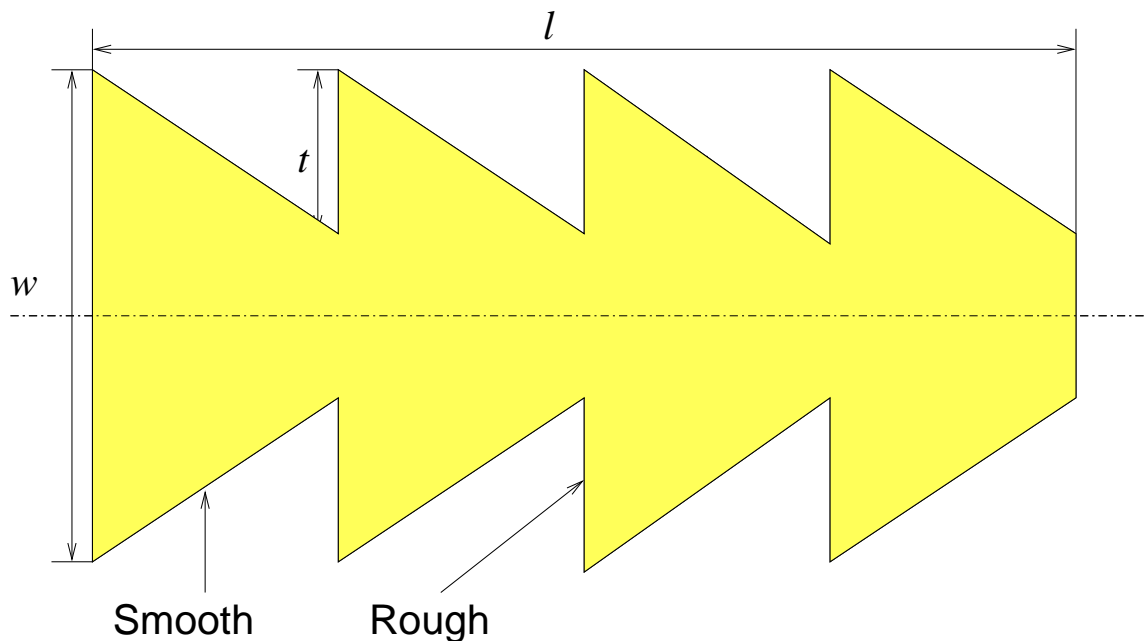
# Definition of Direction and Frequency Dependent Boundaries



- 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
- $p(\omega) = \exp \left[ -\frac{64\pi^5 \eta^2 \omega^2}{V_g^2} \right]$

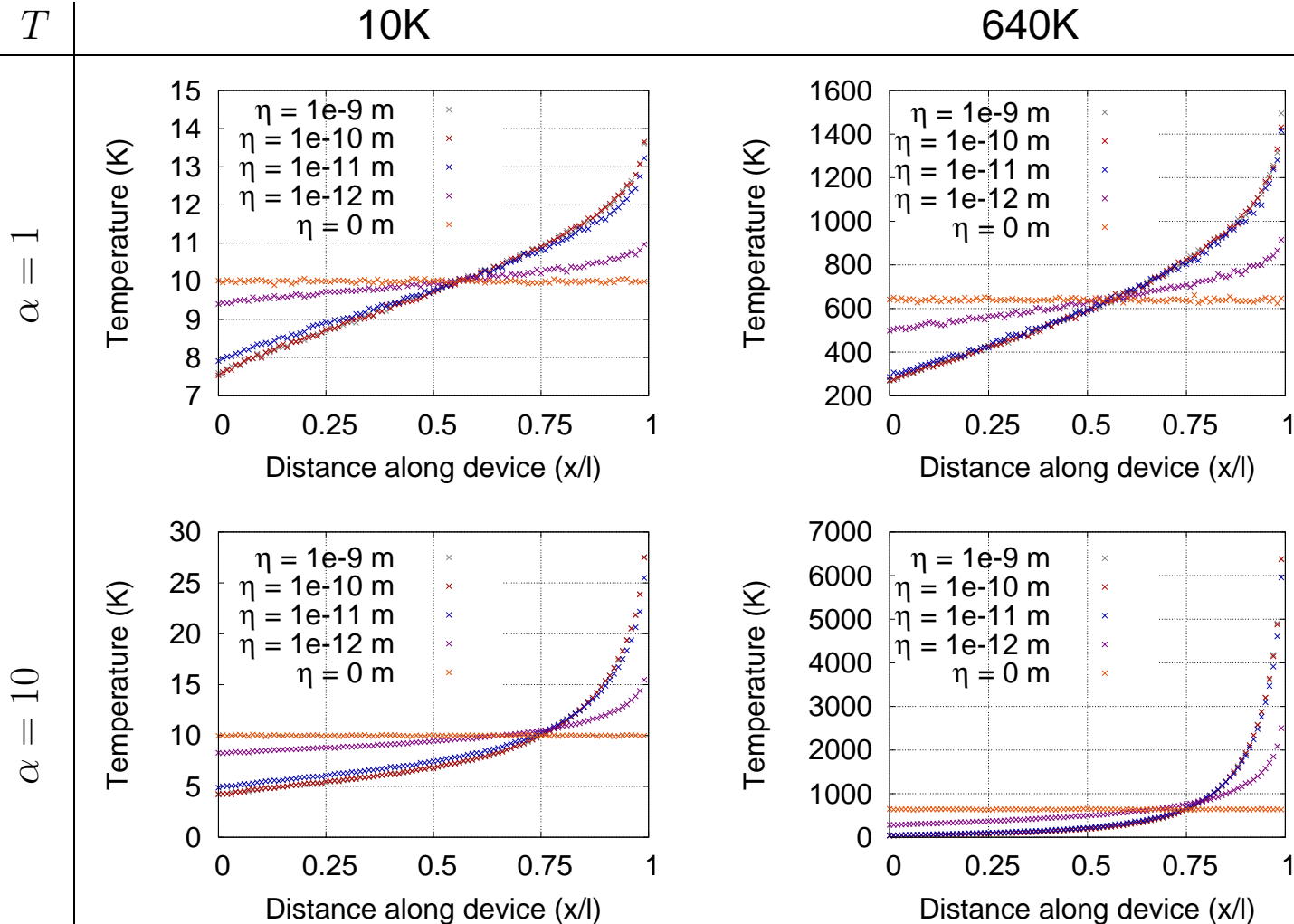


# Definition of Direction and Frequency Dependent Boundaries Cont.

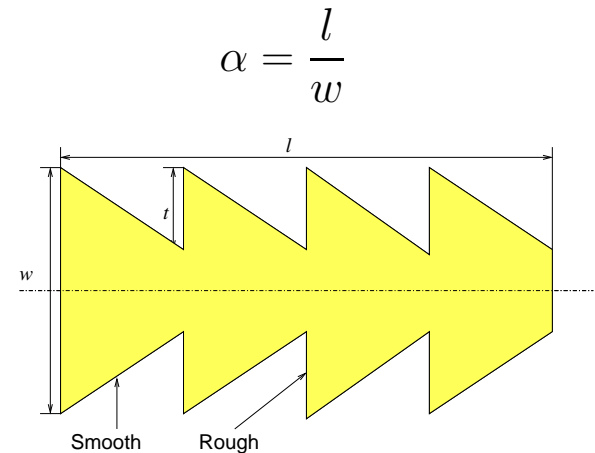
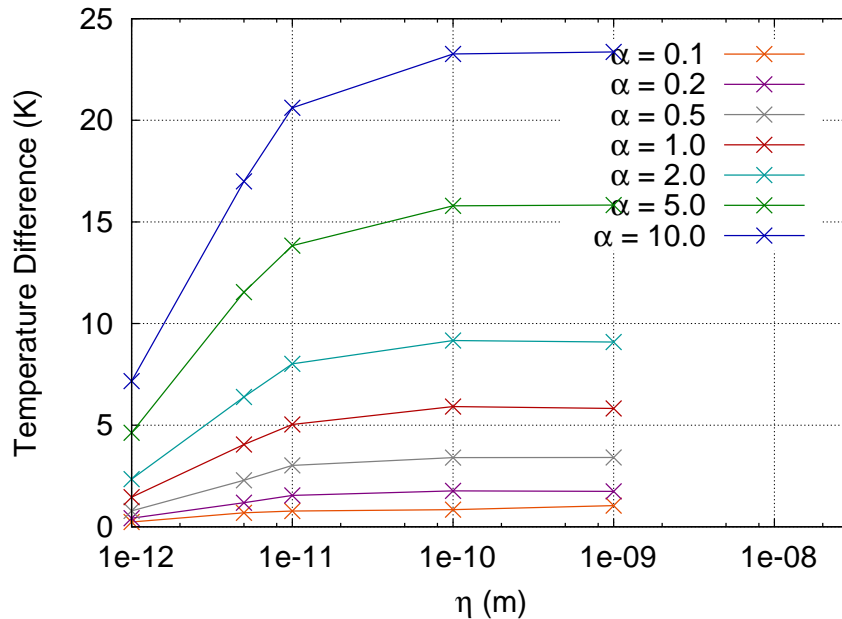


- $l$  and  $w$  are length and width of the device, respectively
- $t$  is the sawtooth depth (of order or smaller than dominate phonon wavelength)
- phonons moving to the right see “smooth” surfaces, phonons moving to the left see “rough” surfaces

## Simulation Results - Temperature distribution

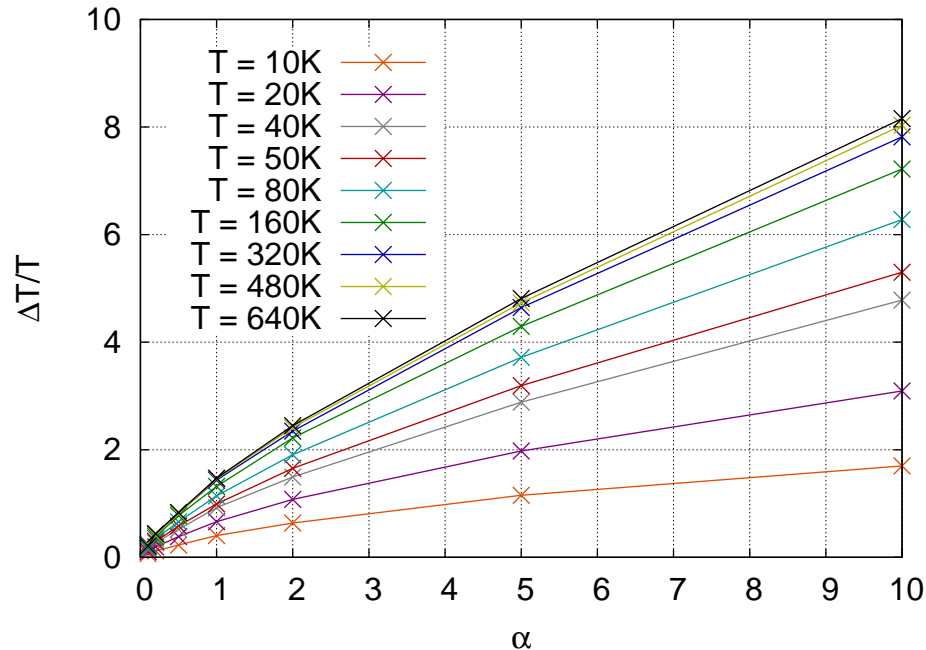


# Simulation Results - Temperature difference at $T = 10\text{ K}$



- 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 $\eta = 5 \times 10^{-12}$ m



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



- 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  $\eta \approx 0.5a$