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 \( f = f(\vec{r}, \vec{p}, t) \)

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

- 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 $100 \times 100 \text{ nm}$ to $1000 \times 1000 \text{ nm}$ and lengths of $100 \text{ nm}$ to $1000 \text{ nm}$

\[
\omega(k) = \omega_{\text{max},b} \sqrt{\frac{1 - \cos ka}{2}}
\]

\[
D(k) = \frac{k^2}{2\pi^2 V_g}
\]

\[
V_g = \nabla_k \omega
\]

\[
\langle n \rangle = \frac{1}{\exp \left(\frac{\hbar \omega}{k_B T}\right) - 1}
\]
The device is composed of an isotropic material with Silicon-like properties

Max. longitudinal acoustic phonon frequency \( \Rightarrow \) \( 1.23 \times 10^{13} \text{ Hz} \)
Max. transverse acoustic phonon frequency \( \Rightarrow \) \( 4.5 \times 10^{12} \text{ Hz} \)

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

- The normalized density function is a key element in this study by showing 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 different 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.
- $p(\omega) = \exp \left[ -\frac{64\pi^5 \eta^2 \omega^2}{V_g^2} \right]$
• $l$ and $w$ are length and width of the device, respectively
• $t$ is the sawtooth depth (of order or smaller than dominate phon on wavelength)
• phonons moving to the right see “smooth” surfaces, phonons moving to the left see “rough” surfaces
## Simulation Results - Temperature distribution

<table>
<thead>
<tr>
<th>$T$</th>
<th>10K</th>
<th>640K</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\alpha = 1$</td>
<td><img src="image1.png" alt="Graph 1" /></td>
<td><img src="image2.png" alt="Graph 2" /></td>
</tr>
<tr>
<td>$\eta = 1 \times 10^{-9}$ m</td>
<td><img src="image3.png" alt="Graph 3" /></td>
<td><img src="image4.png" alt="Graph 4" /></td>
</tr>
<tr>
<td>$\eta = 1 \times 10^{-10}$ m</td>
<td><img src="image5.png" alt="Graph 5" /></td>
<td><img src="image6.png" alt="Graph 6" /></td>
</tr>
<tr>
<td>$\eta = 1 \times 10^{-11}$ m</td>
<td><img src="image7.png" alt="Graph 7" /></td>
<td><img src="image8.png" alt="Graph 8" /></td>
</tr>
<tr>
<td>$\eta = 1 \times 10^{-12}$ m</td>
<td><img src="image9.png" alt="Graph 9" /></td>
<td><img src="image10.png" alt="Graph 10" /></td>
</tr>
<tr>
<td>$\eta = 0$ m</td>
<td><img src="image11.png" alt="Graph 11" /></td>
<td><img src="image12.png" alt="Graph 12" /></td>
</tr>
</tbody>
</table>
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 $\eta = 5 \times 10^{-12} \text{ m}$

- 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 $\eta \approx 0.5a$