Monte Carlo Study of Thermal Rectification in Nanostructured Asymmetric Boundaries

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

Smart Thermal Systems

Chip Technology

directindustry.com
micropower-global.com

Portable Electronics

Thermoelectrics

melcor.com

Thermal Barrier Coatings

siemens.com
Historical Evidence

First reported observation was by Starr in 1936

Level of rectification: \( \varepsilon = \frac{k^+ - k^-}{k^+ + k^-} \)

<table>
<thead>
<tr>
<th>Investigators</th>
<th>System</th>
<th>Mechanism</th>
<th>( \varepsilon )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Starr, 1936</td>
<td>Cu/Cu(_2)O</td>
<td>electronic</td>
<td>0.39</td>
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<tr>
<td>Barzelay, 1955</td>
<td>Al/SS</td>
<td>thermal warping</td>
<td>0.67</td>
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<tr>
<td>Rogers, 1961</td>
<td>Al/SS</td>
<td>thermal potential barrier</td>
<td>0.1</td>
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<tr>
<td>Powell et al., 1962</td>
<td>Al/SS</td>
<td>thermal warping</td>
<td>0</td>
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<tr>
<td>Clausing, 1966</td>
<td>SS/Al</td>
<td>thermal strain</td>
<td>0.2</td>
</tr>
<tr>
<td>Lewis and Perkins, 1968</td>
<td>Al/SS</td>
<td>thermal warping</td>
<td>0.41</td>
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<tr>
<td>O’Callaghan et al., 1970</td>
<td>varied</td>
<td>thermal warping</td>
<td>0.13</td>
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<tr>
<td>Stevenson et al., 1991</td>
<td>varied</td>
<td>thermal warping</td>
<td>0.21</td>
</tr>
<tr>
<td>Chang et al., 2006</td>
<td>CNT and BNNT</td>
<td>non-uniform mass loading</td>
<td>0.034</td>
</tr>
</tbody>
</table>
Thermal Rectifying Mechanisms

- Contact resistance change due to thermal expansion
  - Rogers (1961)
  - Clausing (1966)
  - O’Callaghan (1970)

- Temperature dependence of thermal conductivity
  - Sun et al. (2001)
  - Hu et al. (2006)
  - Dames (2009)

- Nonlinear lattice/potential
  - Terraneo et al. (2002)
  - Li et al. (2004)
  - Segal and Nitzan (2005)
  - Casati (2005)
Nanostructured Boundaries

Simulations using Monte Carlo technique

- Smooth
- Rough

Dimensions:
- L
- T
- W
Monte Carlo Simulations

- Initialization
  - Number of phonons initially prescribed (≥ 100,000)
  - Randomly distributed throughout the device
  - Polarization and frequency obtained based on initial temperature
  - Momentum calculated from analytic dispersion relation

- Three-phonon scattering is used based on the model and rates from Holland, *Physical Review*, 1963

- Cross sections of $10 \times 10 \text{nm}$ to $1000 \times 1000 \text{nm}$ and lengths of $10 \text{nm}$ to $1000 \text{nm}$

Analytic phonon dispersion $\Rightarrow \quad \omega(k) = \omega_{\text{max},b} \sqrt{\frac{1-\cos ka}{2}}$

Max. TA and LA frequencies $\Rightarrow \quad 1.23 \times 10^{13} \text{Hz}, 4.5 \times 10^{12} \text{Hz}$

3-D Density of States $\Rightarrow \quad D(k) = \frac{k^2}{2\pi^2V_g}$

Phonon group velocity $\Rightarrow \quad V_g = \nabla_k \omega$

Bose-Einstein distribution $\Rightarrow \quad \langle n \rangle = \frac{1}{\exp \frac{\hbar \omega}{k_BT} - 1}$
• Boundaries parallel to x-axis have direction and frequency dependence

• 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

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

Ziman, Electrons and Phonons, 1960

Specular Reflection

Diffuse Reflection
MC Results - Device Aspect Ratio

\[ \alpha = \frac{l}{w} \]

- Boundaries are insulated, so the device is self-biasing.
For a biased device, the amount of transport is calculated so thermal conductivity can be deduced.
MC Results - Device Aspect Ratio

- boundary dominated devices show large amounts of rectification
- $\varepsilon = 1$ means no transport in unfavorable direction
MC Results - Device Temperature

\[ F(\omega) = \sum_b \frac{\int_0^{\omega} \langle n \rangle D(\omega) d\omega}{\int_0^{\omega_{\text{max},b}} \langle n \rangle D(\omega) d\omega} \]
MC Results - Rough Boundary Roughness

![Graph showing temperature difference vs. roughness parameter α. The x-axis represents roughness parameter in meters (m), and the y-axis represents temperature difference in Kelvin (K). Curves are labeled for different values of α: 0.1, 0.2, 0.5, 1.0, 2.0, 5.0, and 10.0.]}
Conclusions

- Rectification can be increased by
  - large aspect ratio devices
  - selecting a temperature that gives a distribution of phonons, but does not introduce too much scattering
  - designing a roughness that is of the order of the dominant phonon wavelength

- Fabrication is extremely difficult due to boundary requirements