Monte Carlo Study of Thermal Rectification in Nanostructured Asymmetric Boundaries

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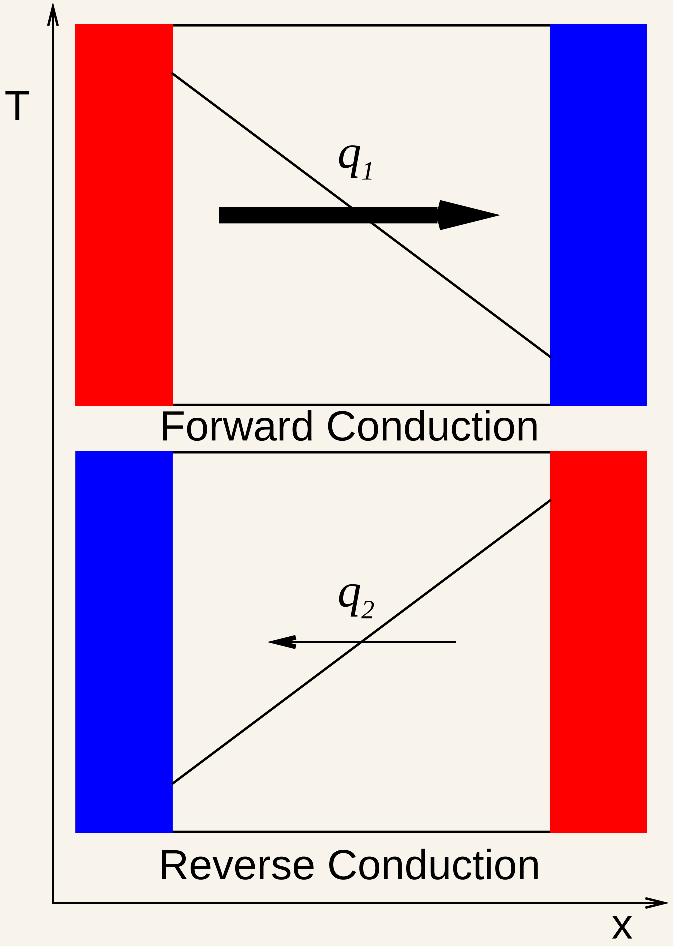
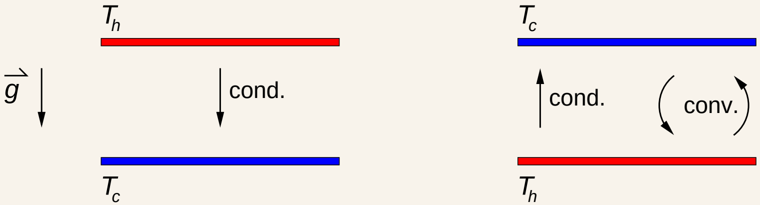
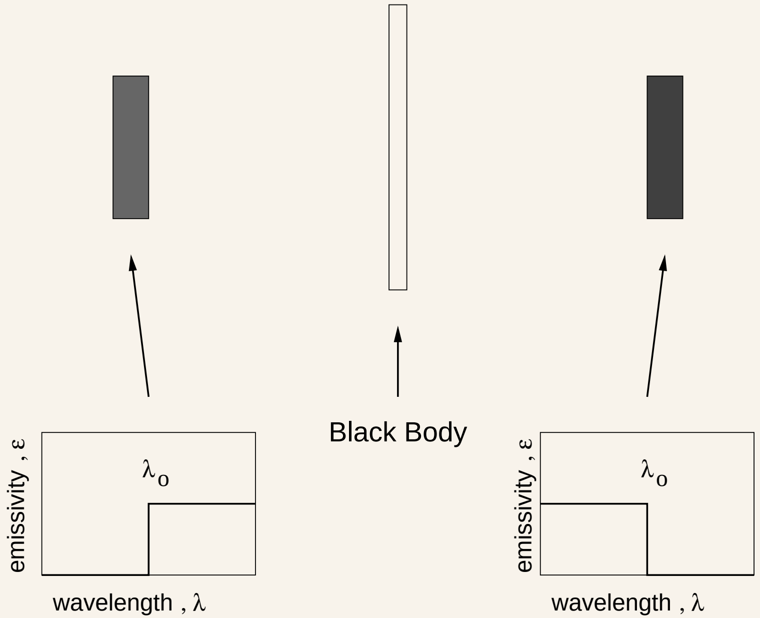
Introduction

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



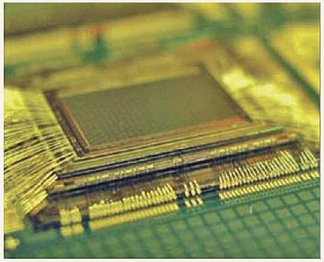




Motivation

Smart Thermal Systems

Chip Technology



directindusty.com

micropower-global.com

Portable Electronics

Thermoelectrics

melcor.com

Thermal Barrier Coatings

siemens.com

Historical Evidence

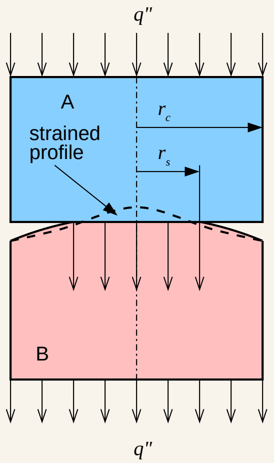
First reported observation was by Starr in 1936

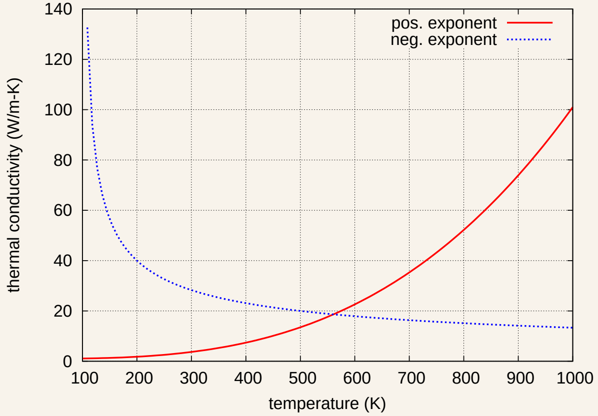
Level of rectification: $\varepsilon = \frac{\kappa^{+} - \kappa^{-}}{\kappa^{+} + \kappa^{-}}$

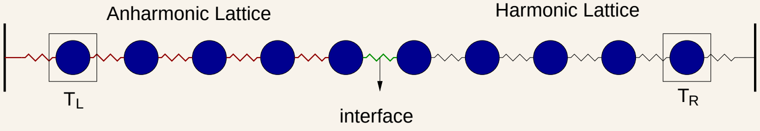
Investigators	System	Mechanism	ε
Starr, 1936	Cu/Cu_2O	electronic	0.39
Barzelay, 1955	Al/SS	thermal warping	0.67
Rogers, 1961	Al/SS	thermal potential barrier	0.1
Powell et al., 1962	Al/SS	thermal warping	0
Clausing, 1966	SS/Al	thermal strain	0.2
Lewis and Perkins, 1968	Al/SS	thermal warping	0.41
O'Callaghan et al., 1970	varied	thermal warping	0.13
Stevenson et al., 1991	varied	thermal warping	0.21
Chang et al., 2006	CNT and BNNT	non-uniform mass loading	0.034

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)



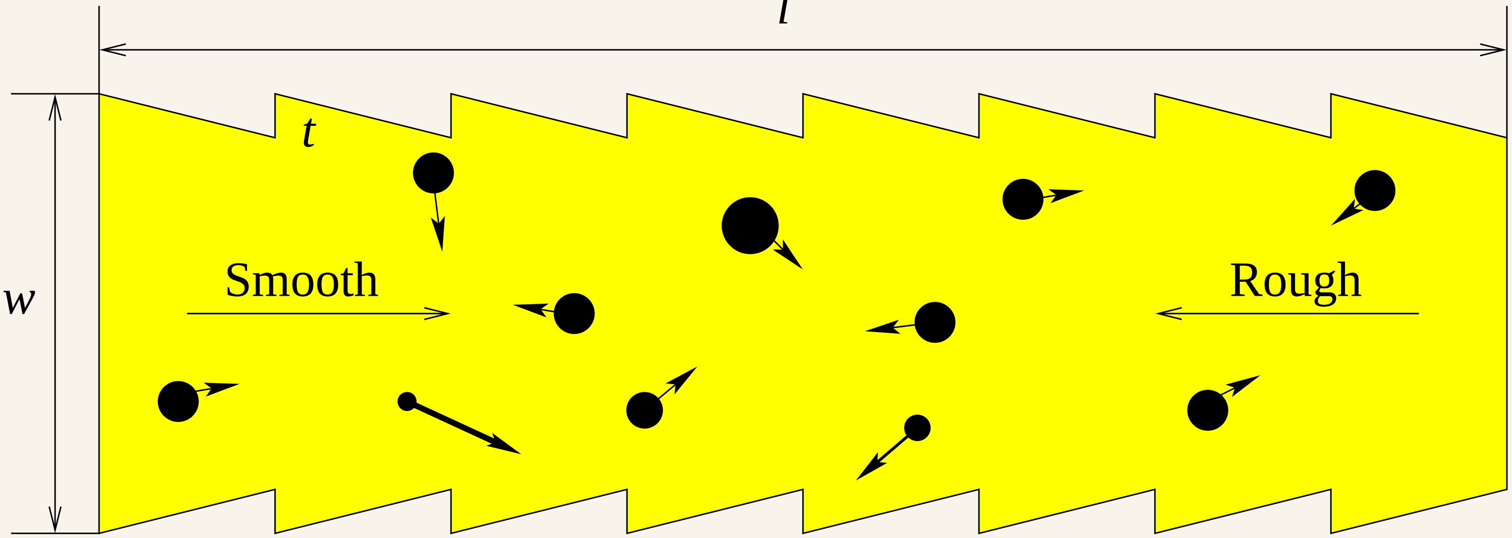




experimental

Nanostructured Boundaries

Simulations using Monte Carlo technique

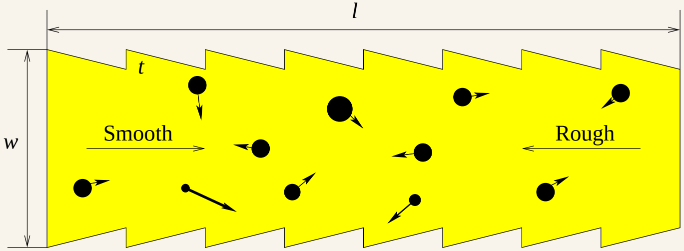


Monte Carlo Simulations

- Initialization
  - Number of phonons initially prescribed ($\geq$ 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 $10 \times 10\,\mathrm{nm}$ to $1000 \times 1000\,\mathrm{nm}$ and lengths of $10\,\mathrm{nm}$ to $1000\,\mathrm{nm}$

Analytic phonon dispersion	$\Rightarrow$	$\omega(k) = \omega_{max,b}\sqrt{\frac{1-\cos ka}{2}}$
Max. TA and LA frequencies	$\Rightarrow$	$1.23 \times 10^{13}\,\mathrm{Hz},\ 4.5 \times 10^{12}\,\mathrm{Hz}$
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	$\Rightarrow$	$\langle n \rangle = \frac{1}{\exp\frac{\hbar\omega}{k_B T} - 1}$

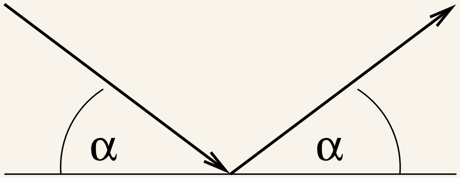
Direction- and Frequency-Dependent Boundaries



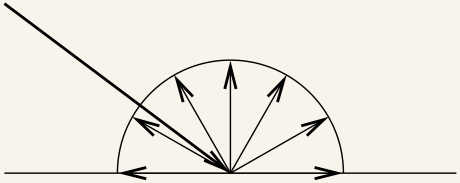
- Boundaries parallel to x-axis have direction and frequency dependence
- If a phonon with negative x-momentum strikes a boundary parallel to the x-axis a parameter, $p(\omega,\eta)$, is calculated based on the phonon frequency and characteristic roughness
- If $p \ll 1$, the phonon has a high probability 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

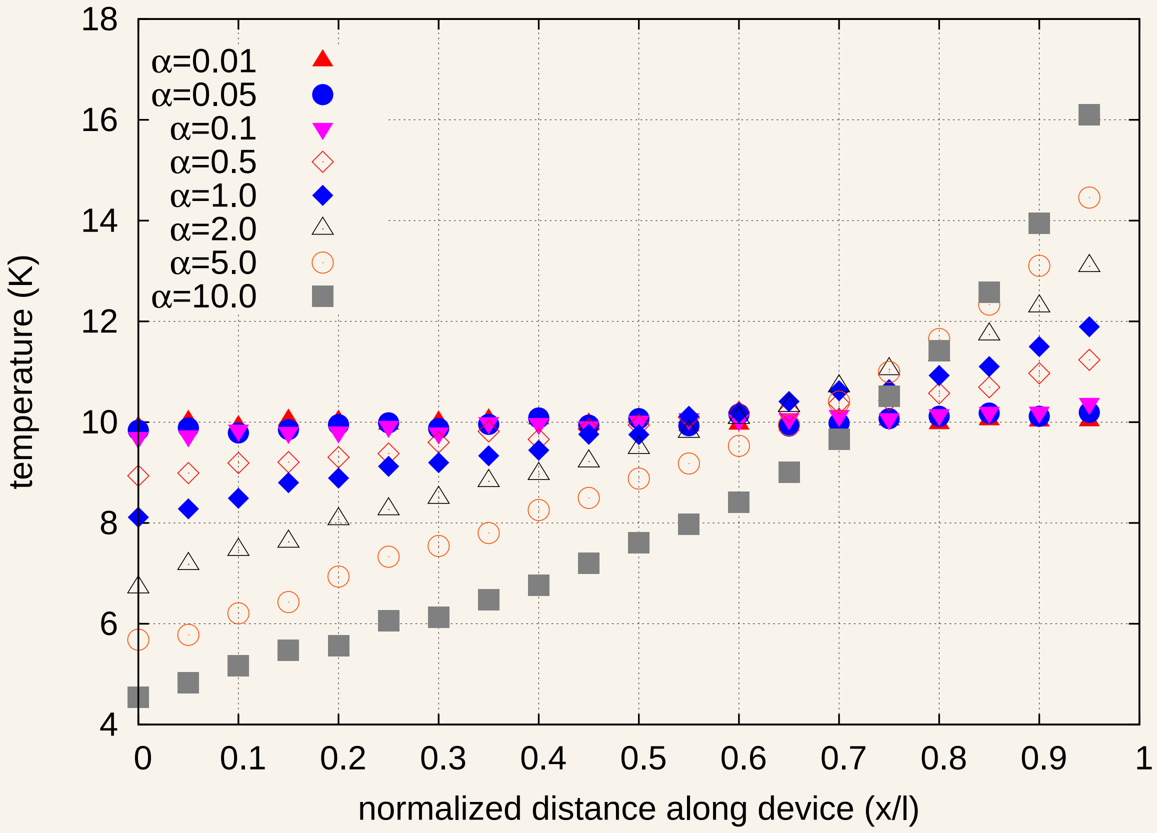


Specular Reflection



Diffuse Reflection

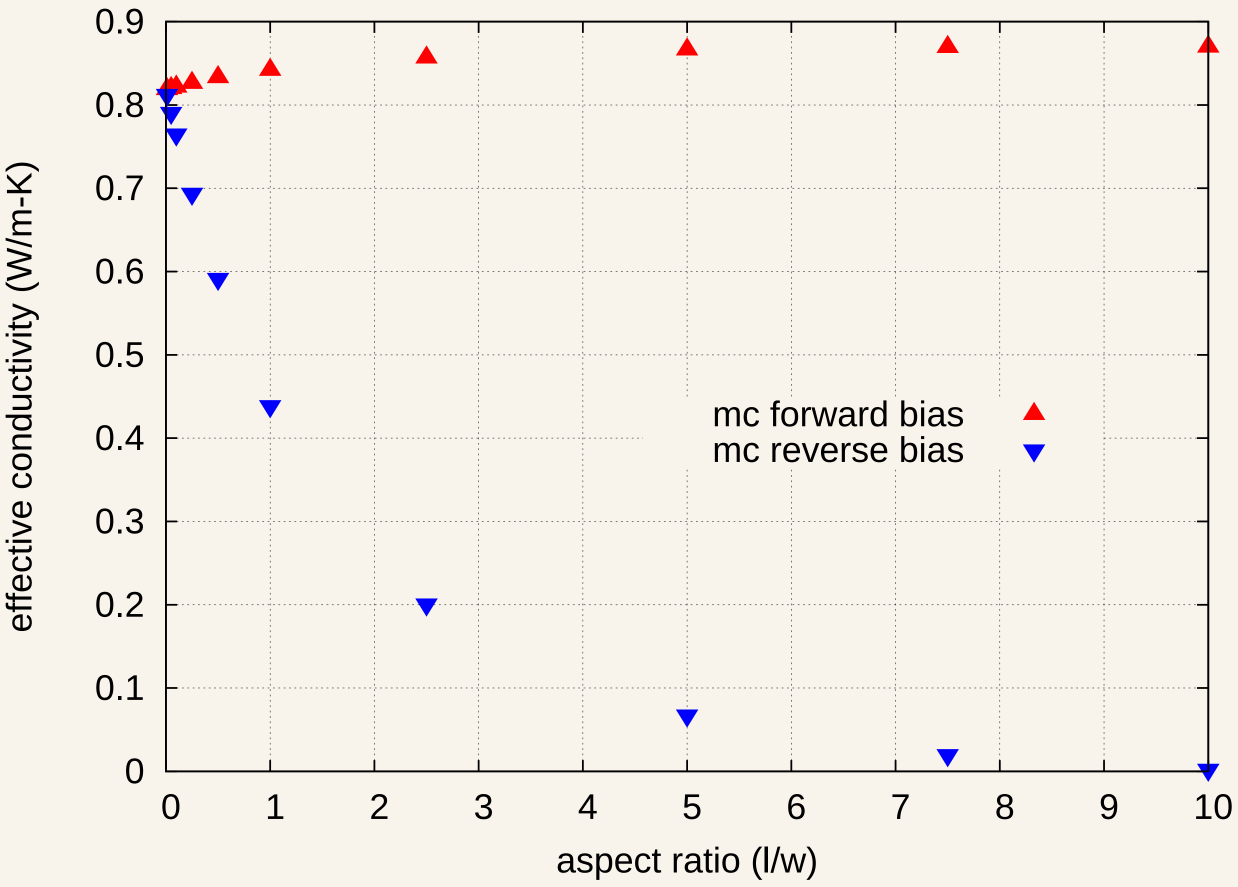
MC Results - Device Aspect Ratio



$$\alpha = l/w$$

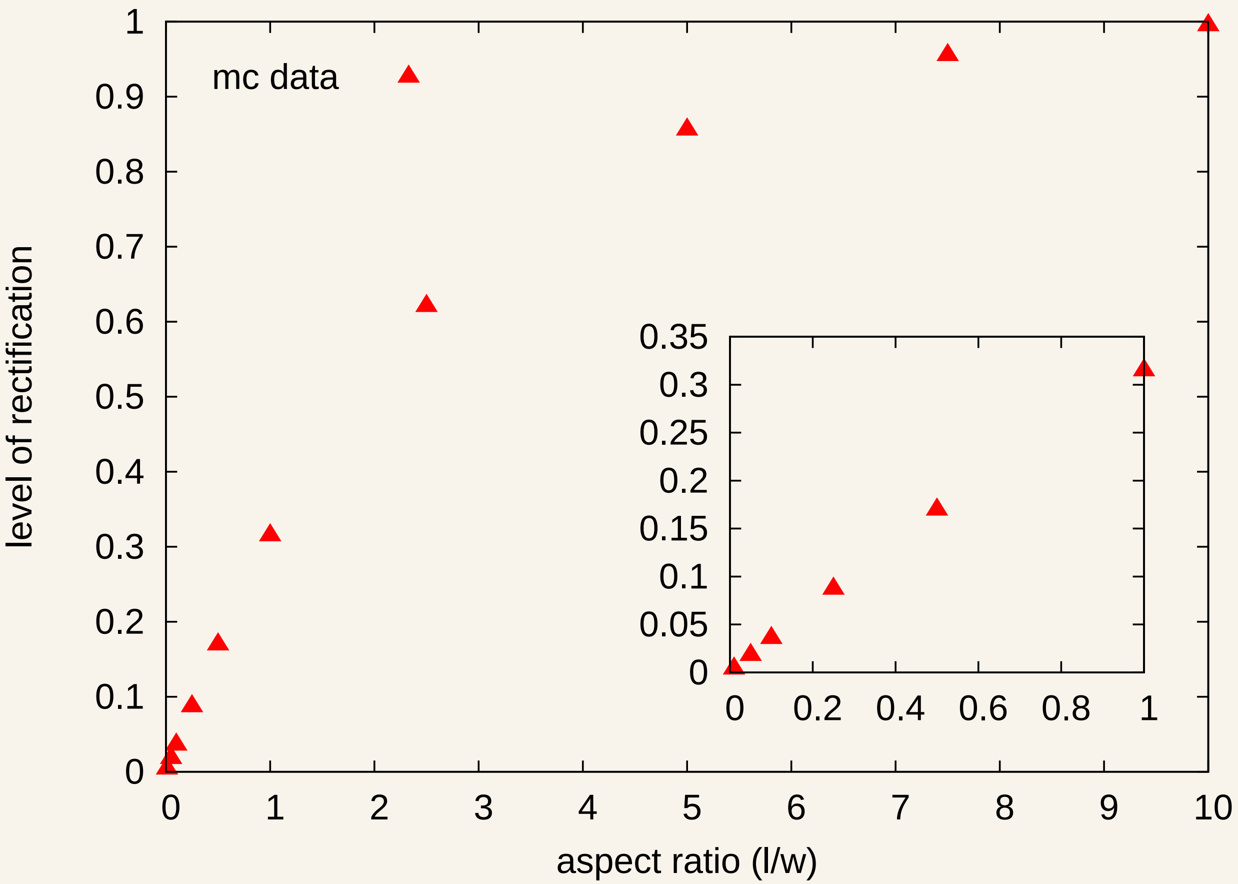
- Boundaries are insulated, so the device is self-biasing.

MC Results - Device Aspect Ratio



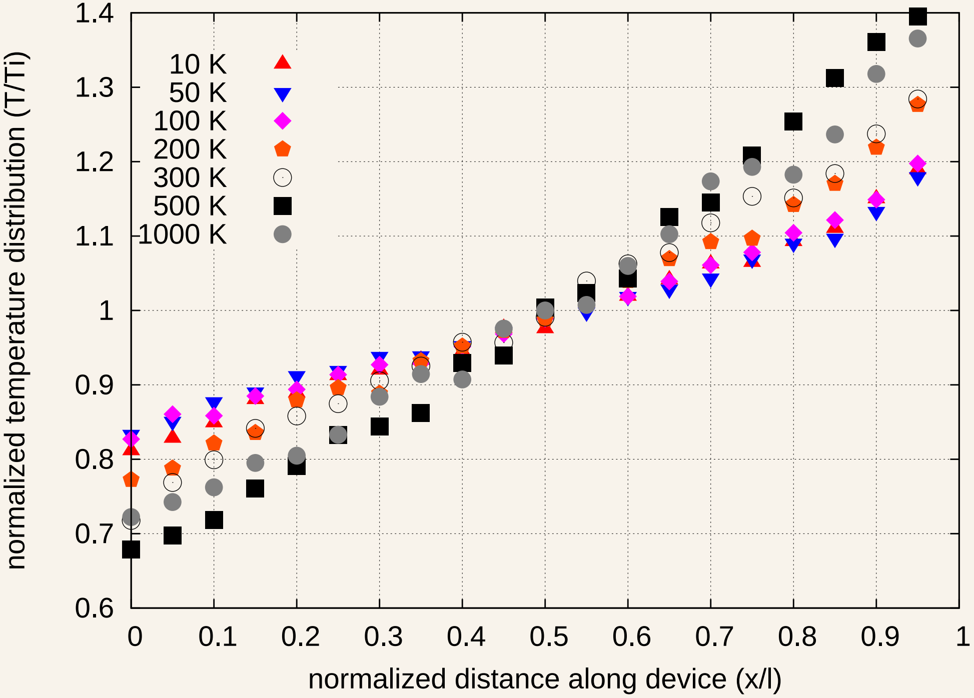
- For a biased device, the amount of transport is calcuated so thermal conductivity can be deduced.

MC Results - Device Aspect Ratio

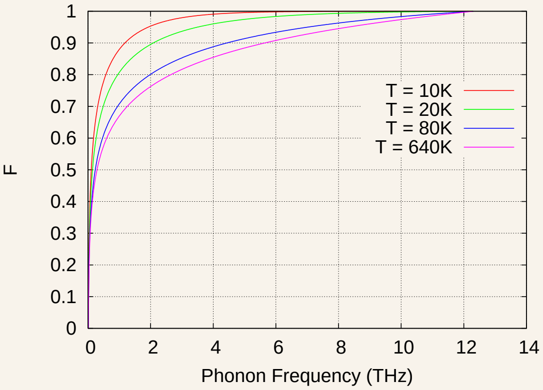


- boundary dominated devices show large amounts of rectification
- $\varepsilon = 1$ means no transport in unfavorable direction

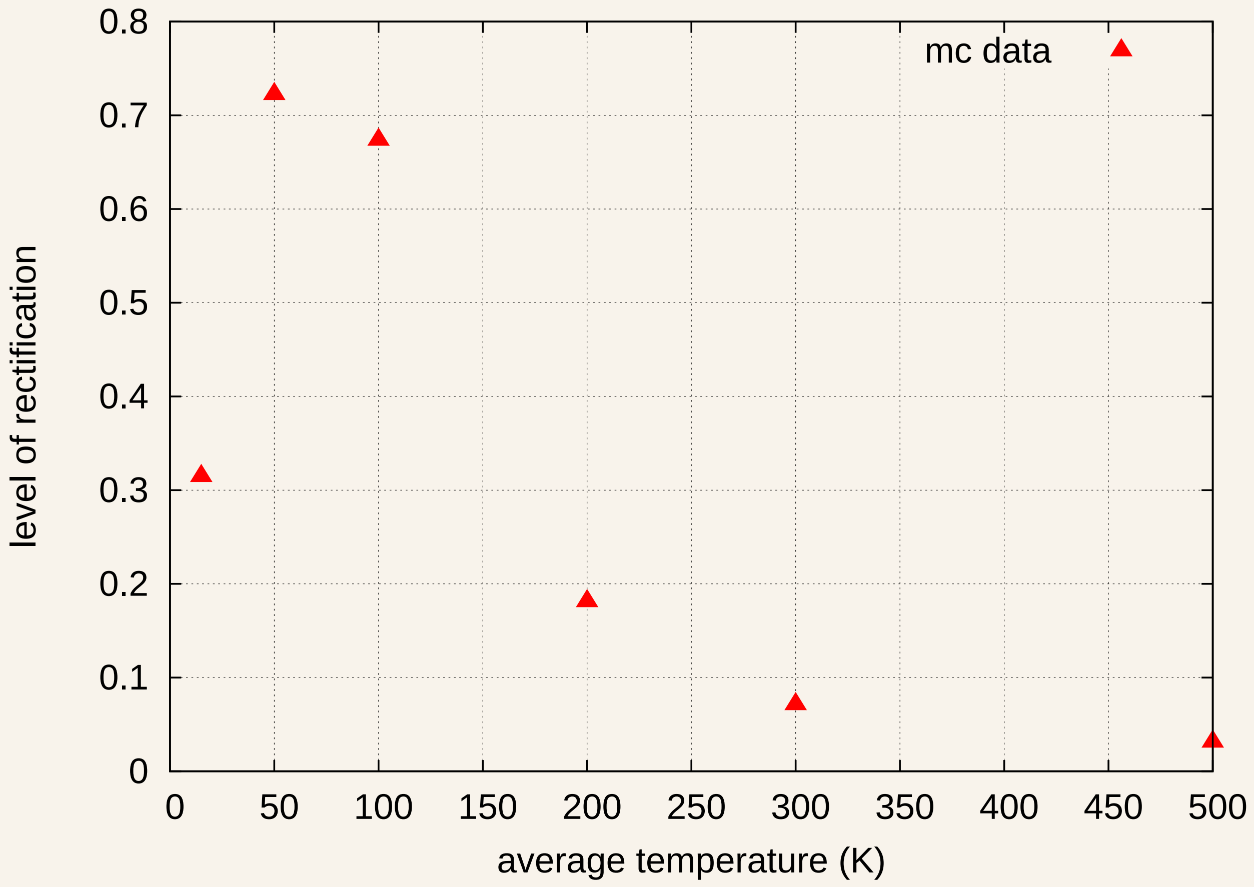
MC Results - Device Temperature



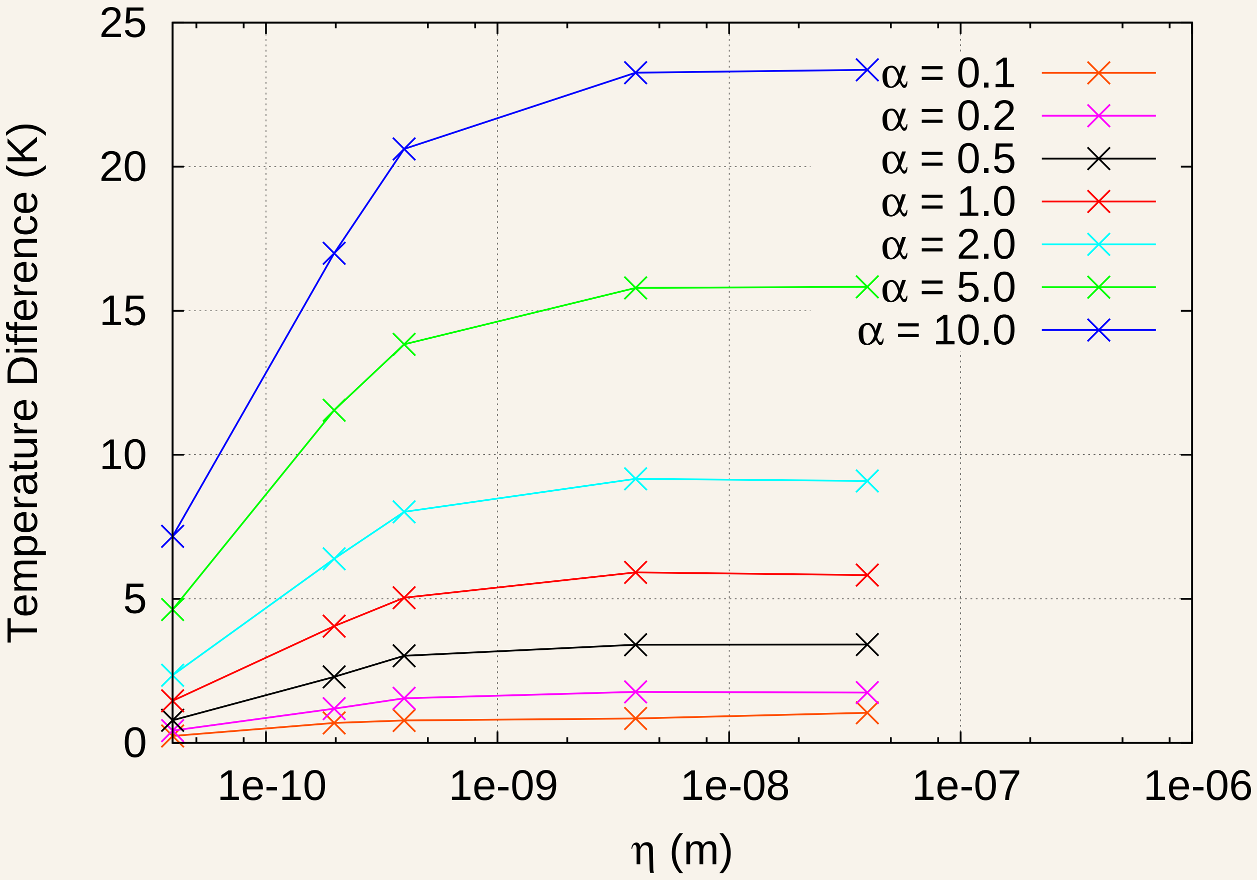
$$F(\omega) = \sum_b \frac{\int_0^{\omega} \langle n \rangle D(\omega)\, d\omega}{\int_0^{\omega_{\max,b}} \langle n \rangle D(\omega)\, d\omega}$$



MC Results - Device Temperature



MC Results - Rough Boundary Roughness



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 rougness that is of the order of the dominant phonon wavelength
- Fabrication is extremely difficult due to boundary requirements