Molecular Dynamics Simulation of Thin Films with Rough and Asymmetric Interfaces

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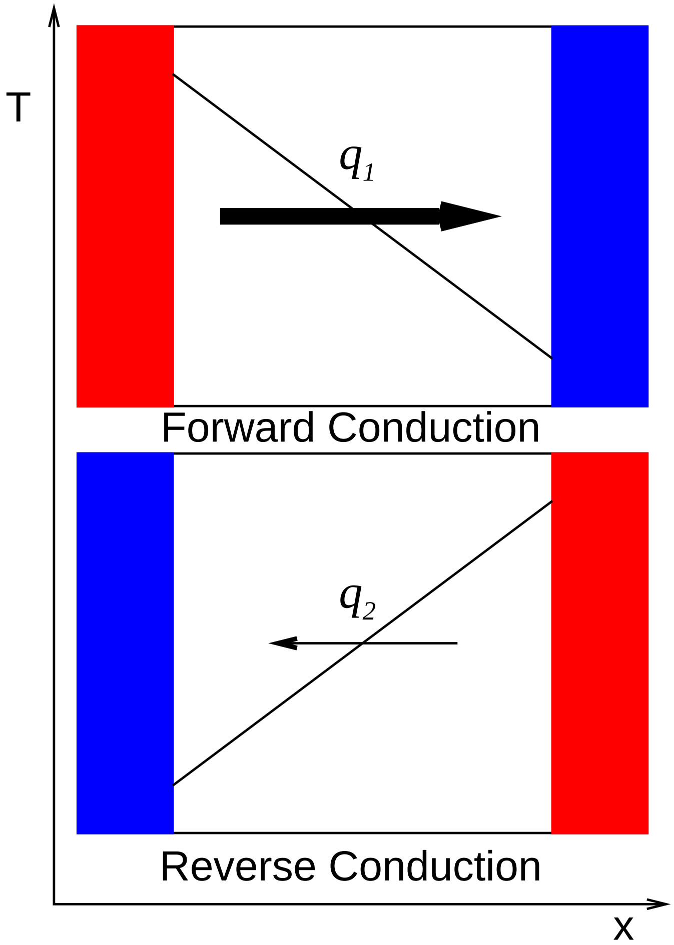
Introduction

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



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

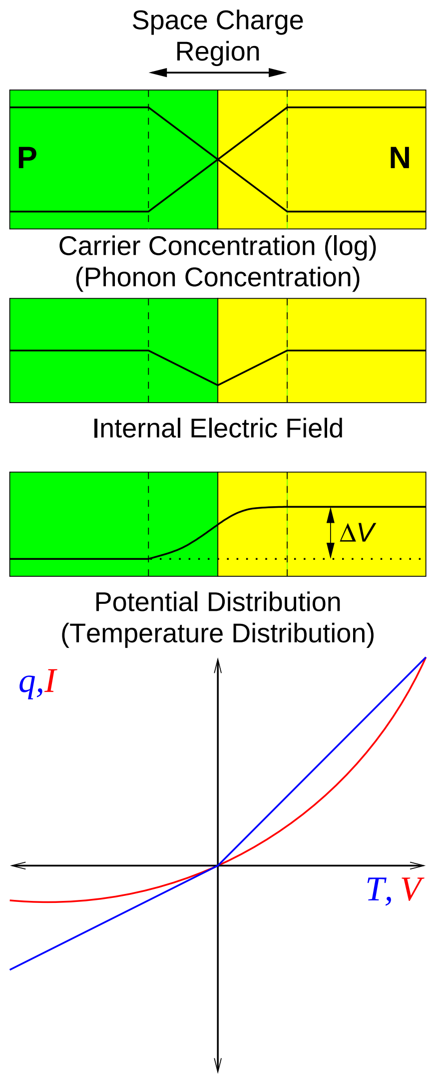
$$q_1 > q_2$$

$$k_1 > k_2$$

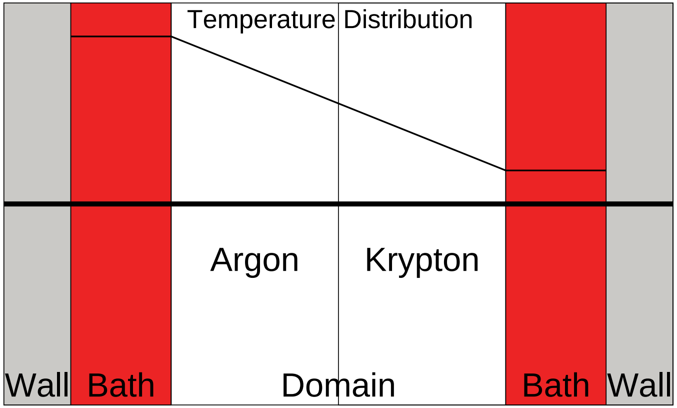
- Widespread applications in thermal management problems
  - Cooling of micro/nano electronics
  - Improvement of macroscale refrigeration and energy saving buildings

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



Simulation Method



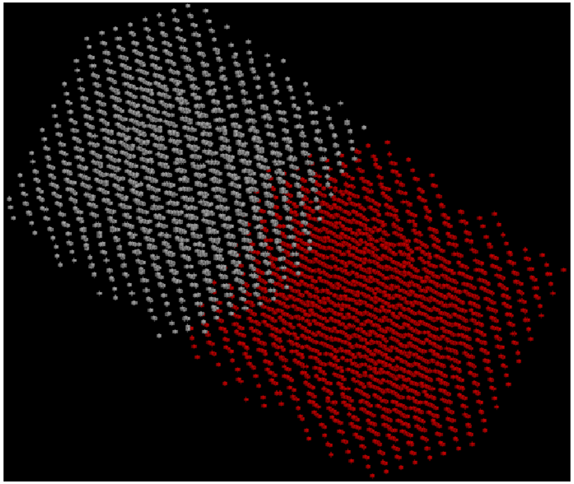
Material	Parameter	Value
Kr	$\epsilon(J)$	2.25×10^{-21}
	$\sigma(m)$	3.65×10^{-10}
	$a(m)$	5.69×10^{-10}
	$m(kg)$	1.35×10^{-25}
Ar	$\epsilon(J)$	1.67×10^{-21}
	$\sigma(m)$	3.40×10^{-10}
	$a(m)$	5.31×10^{-10}
	$m(kg)$	6.63×10^{-26}

- Using XMD, open source molecular dynamics code to calculate thermal conductivity
- Argon/Krypton FCC domain, wall and bath
- Fixed position walls at boundaries orthogonal to transport and periodic boundaries parallel to transport
- Baths are held at a constant temperature
- Records energy added/subtracted from baths each 100 steps

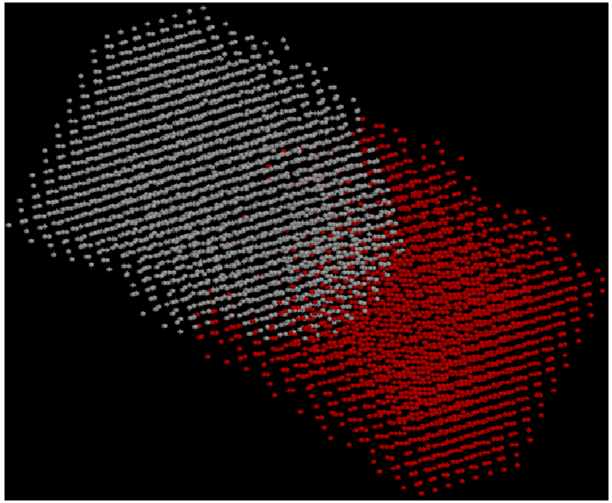
$$U(r_{ij}) = 4\epsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right]$$

$$q = -kA\frac{\Delta T}{L}$$

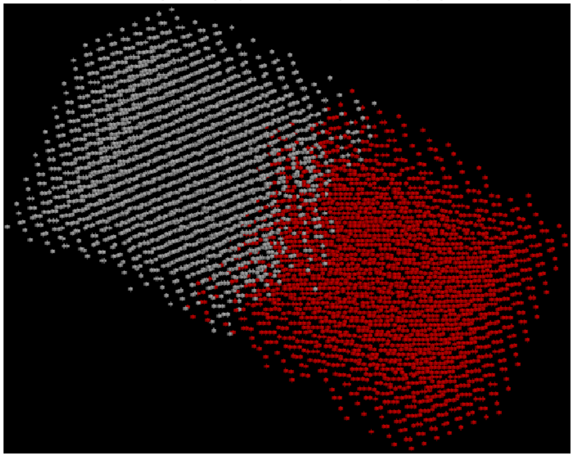
Device Simulations



Perfect Interface



Asymmetrical Interface



Diffuse Interface

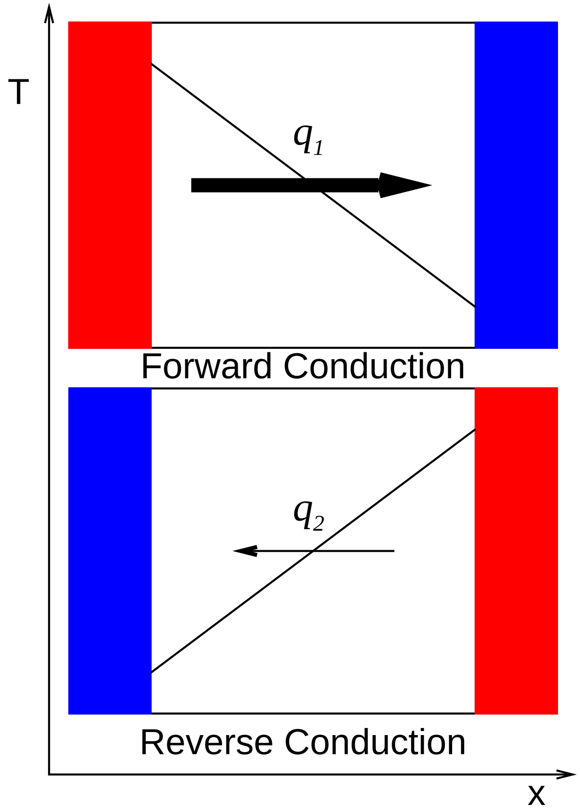
- $8 \times 8\,\mathrm{UC}^2$ FCC domain cross-sections
- $8 - 96\,\mathrm{UC}$ lengths
- Equal amounts of Argon and Krypton
  - Argon - Gray
  - Krypton - Red

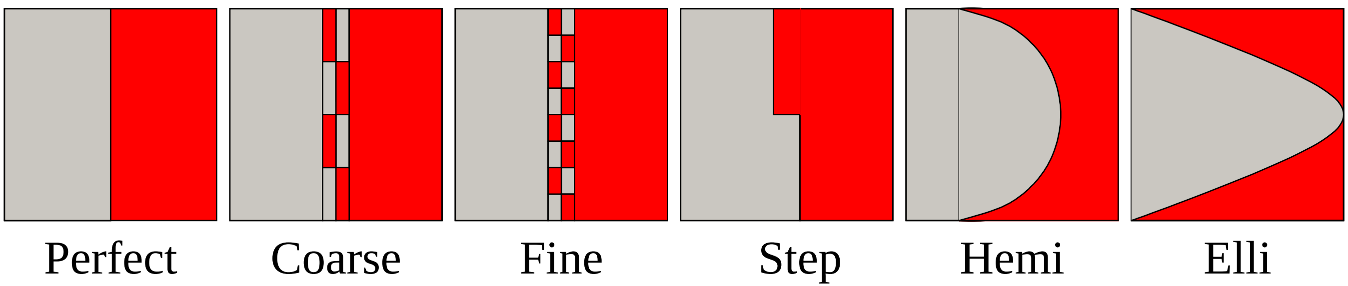
Determination of Thermal Rectification

- Apply temperature gradient and allow simulation to run to steady-state, calculate thermal conductivity
- Reverse temperature gradient and allow simulation to run, calculate thermal conductivity

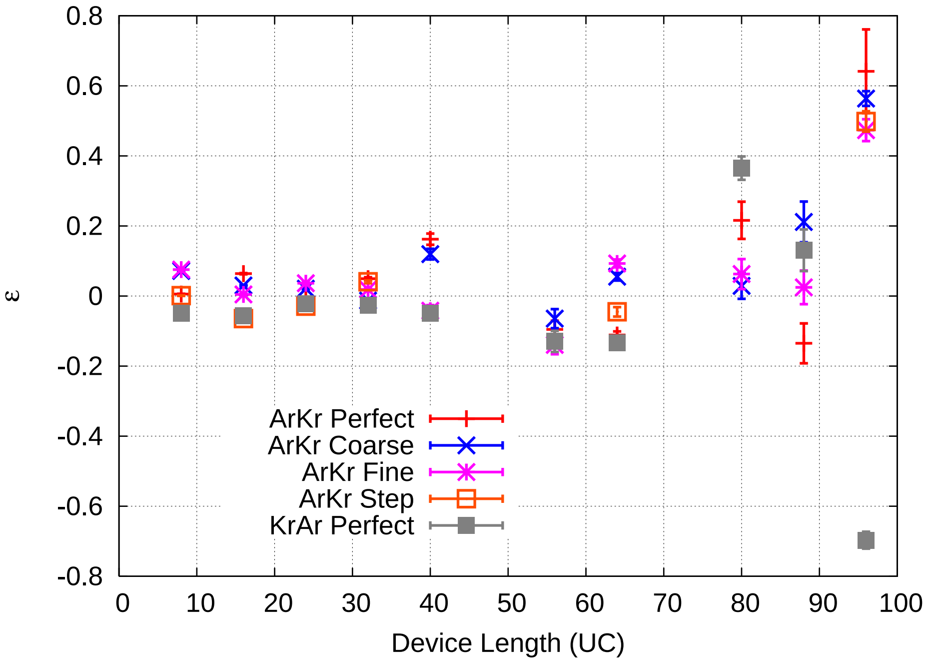
$$\epsilon = \frac{k^+ - k^-}{k^-}$$

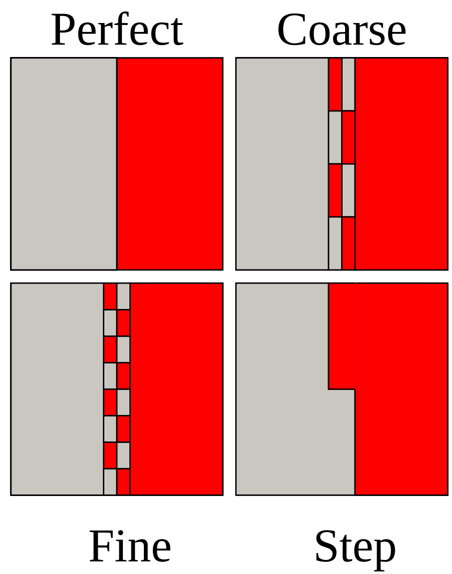
- Simulations were run up to $4.8\,\mathrm{ns}$ to obtain averaged values of thermal conductivity.





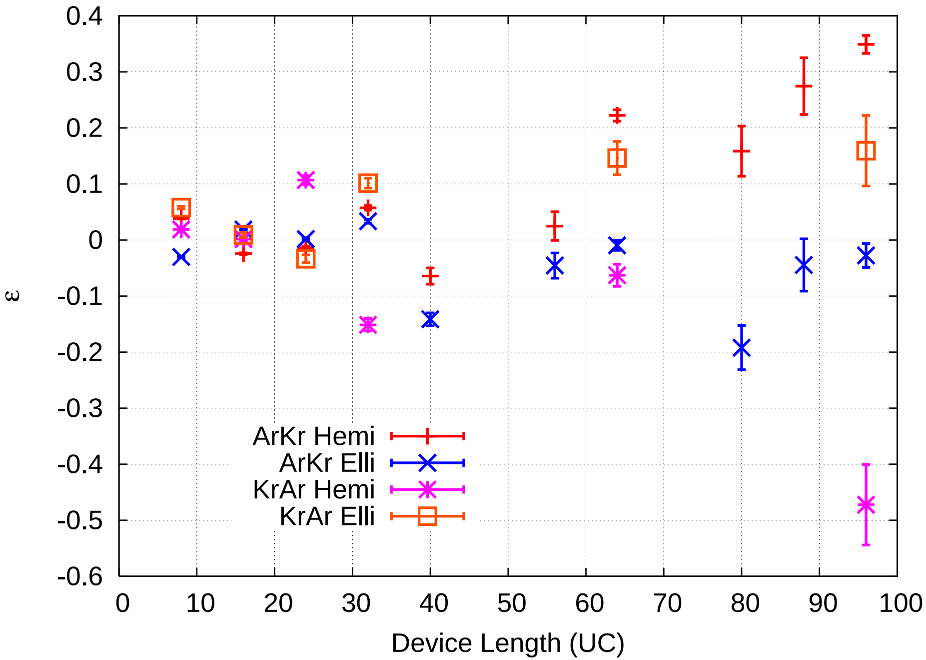
Simulation Results - Interface Rectification

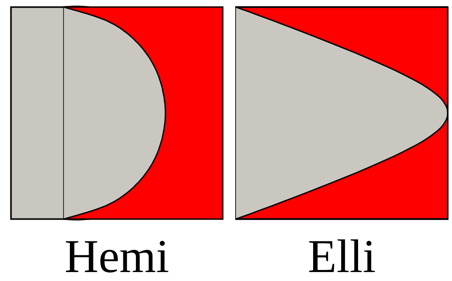




- Rectification occurs in longer devices
- Transport preferred from argon to krypton (soft, light material to stiff, heavy material)
- No noticable difference in rectifying behavior between different interfaces

Simulation Results - Asymmetric Rectification





- Rectification occurs in longer hemispherical devices
- Transport preferred from argon to krypton (soft, light material to stiff, heavy material)
- Ellipsoidal interface results in very little rectification (very poor rectifying interface)

Conclusions

- Greatest rectification in perfect and imperfect interfaces (no difference between them)
- Transport preferred from argon (soft and light) to krypton (stiff and heavy) due to the difference in frequency content
- Asymmetry is a form of interface degradation
- Rectification due to interfaces should be present in devices with materials with different frequency content when the interface is designed to selectively scatter specific phonon frequencies