Nanoscale Heat Transport and Phonon Hydrodynamics

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- Motivation

- Nanoscale Heat Transport

- Kinetic Collective Model

- Experimental validation

- Conclusions
Fourier / Diffusive model

\[
c \frac{dT}{dt} = -\nabla \cdot q
\]

\[q = -\kappa \nabla T\]

Breakdown of Fourier law at reduced length and time scales.
**Motivation**

- Obtain an improved equation of transport derived from the **microscopic description of the phonons dynamics**.

- Improve the thermal management in nano scale semiconductor devices.

- Predict the appearance of hot spots.
Boltzmann Transport Equation
Describes the non equilibrium evolution of the phonons (energy carriers).

Moment description
\( M_i(x, t) = \int \kappa \cdots \kappa f(\kappa, x, t) \)

Grad/Chapman-Enskog equations
Guyer-Krumhansl equations

BTE output
Phonon distribution function \( f(\kappa, x, t) \)

Thermodynamic output
Heat Flux \( q \)
Temperature \( T \)
Hydrodynamic Equations

\[ c \frac{dT}{dt} + \nabla \cdot \mathbf{q} = 0 \]

\[ \frac{\tau \partial \mathbf{q}}{\partial t} + \mathbf{q} + \kappa \nabla T = \ell^2 (\nabla^2 \mathbf{q} + 2 \nabla \nabla \cdot \mathbf{q}) \]

- Relaxation Time
- Bulk Thermal conductivity
- Non Local Length

Slip Boundary Conditions

\[ q_t = -C' \ell \ \nabla \mathbf{q}_t \cdot \mathbf{n} \]

\[ \mathbf{q} \cdot \mathbf{n} = 0 \]

- Calculated from first principles.
- Material properties.
- Only depend on temperature.

Surface specularity
COMSOL interface for solving thermal transport in complex geometries.

- Discontinuous Galerkin implementation of the boundary conditions.
- Stabilization.
- Multiphysics coupling with Fourier domains (metal domains).

First principles calculation of $\kappa, \ell, \tau$
We obtain a thermal map of the surface of the sample using the optical setup. Heater line and thermometer are also obtained using electrical measurements.

Ziabari et al., Nat. Commun. 9, 255 (2018)
Fourier’s law cannot describe thermal transport in this setup. New equation is needed.

Ziabari et al., Nat. Commun. 9, 255 (2018)
Kinetic Collective Model performs better to experimental data

\[ q = -\kappa \nabla T + \ell^2 \nabla^2 q \]

Ziabari et al., Nat. Commun. 9, 255 (2018)
- At large sizes we recover Fourier model.
- The smaller the size, the larger the effect.
- At extremely small sizes, the model fails due to ballistic effects.

Ziabari et al., Nat. Commun. 9, 255 (2018)
Experimental validation

ANISOTROPIC BEHAVIOUR

Temperature gradient and heat flux are not parallel because of the contribution of the new hydrodynamic term. This is interpretable as a vorticity appearing.


The effective thermal conductivity is lower than the Fourier prediction due to an effect analogous to viscosity in fluids.

Boundary conditions produce a non local reduction of the heat flux.
Silicon Phononic Crystals

Phonic crystal A: \[ a = 4\mu m, d = 2.8\mu m, w = 4.49\mu m \]
Phononic crystal B: \[ a = 20\mu m, d = 11.4\mu m, w = 4.84\mu m \]

Beardo et al. submitted
**Suspended Silicon Structures**

Low thermal conductivity is predicted in the narrower constriction.

Experimental validation in progress by the Eindhoven University of Technology.
- Fourier law breaks down when describing thermal transport at reduced length and time scales.

- Phonon hydrodynamics is a generalization of Fourier law obtained from the microscopic description of the phonon population.

- Phonon vorticity and viscosity appear as phenomenological explanations for the thermal behavior of nano scale devices.

- Numerical implementation of the equations in a COMSOL interface allows to predict heat transport in nanoscale complex geometries.
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