COMSOL Conference – Lausanne – October 2018

Nanoscale Heat Transport and Phonon Hydrodynamics

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- Motivation
- Nanoscale Heat Transport
- Kinetic Collective Model
- Experimental validation
- Conclusions

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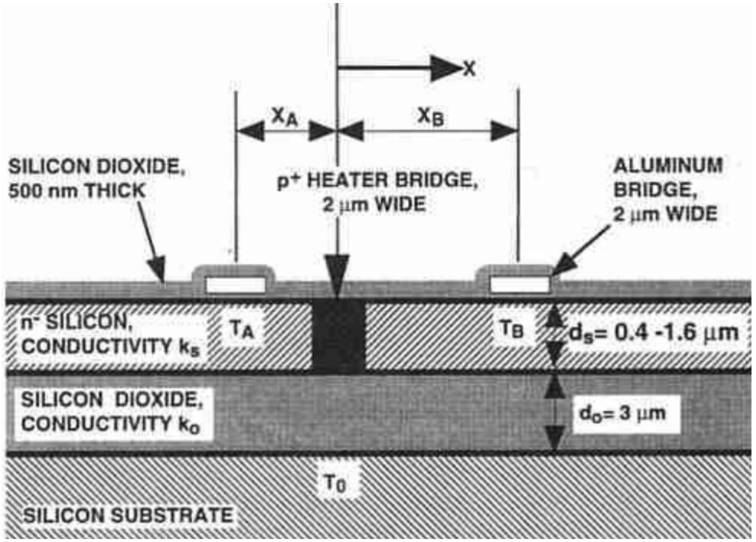
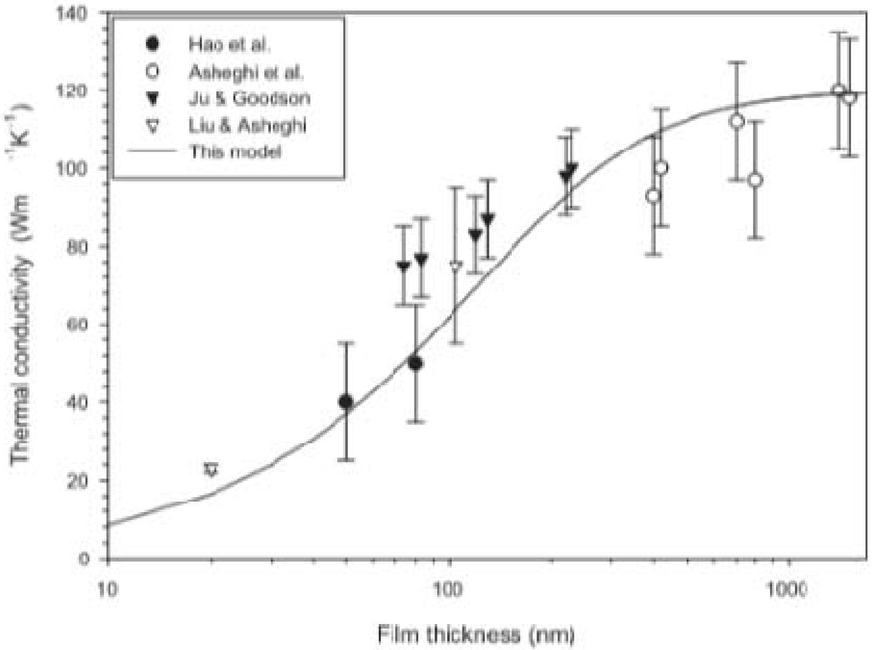
Fourier / Diffusive model

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

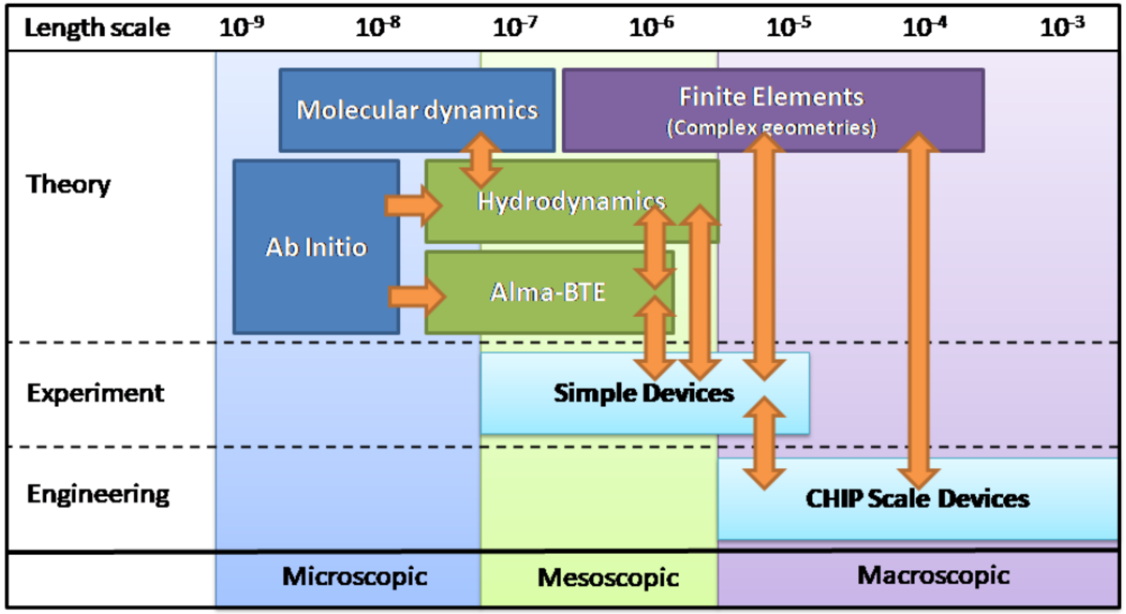
$$q = -\kappa \nabla T$$

Breakdown of Fourier law at reduced length and time scales.



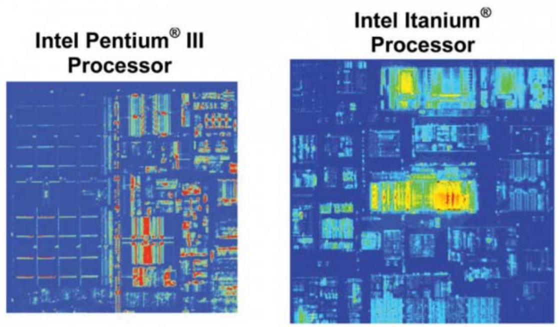


3>> Motivation



* 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.

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Boltzmann Transport Equation
Describes the non equilibrium evolution of the phonons (energy carriers).

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

↓

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

↓

Grad/Chapman-Enskog equations
Guyer-Krumhansl equations

→ Thermodynamic output
Heat Flux $\mathbf{q}$
Temperature T

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Hydrodynamic Equations

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

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

Relaxation Time

Bulk Thermal conductivity

Non Local Length

Slip Boundary Conditions

$$\mathbf{q}_t = -C\ell \; \nabla \mathbf{q}_t \cdot \mathbf{n}$$

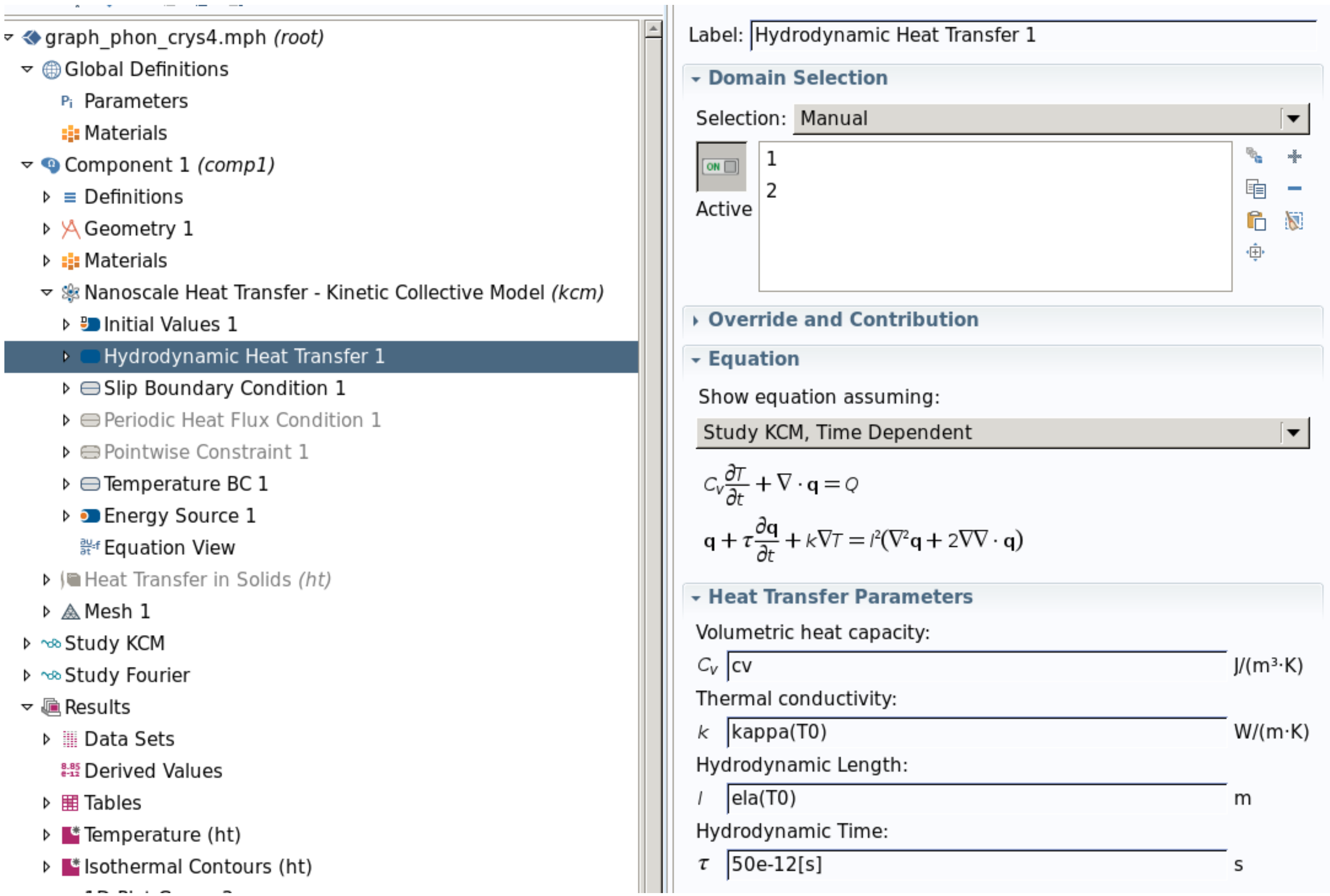
$$\mathbf{q} \cdot \mathbf{n} = 0$$

Surface specularity

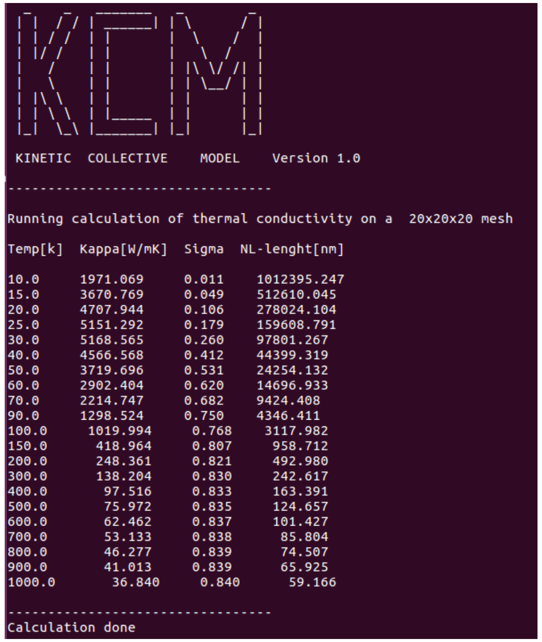
- Calculated from first principles.
- Material properties.
- Only depend on temperature.

6>> Kinetic Collective Model

COMSOL interface for solving thermal transport in complex geometries.



First principles calculation of κ, ℓ, τ



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

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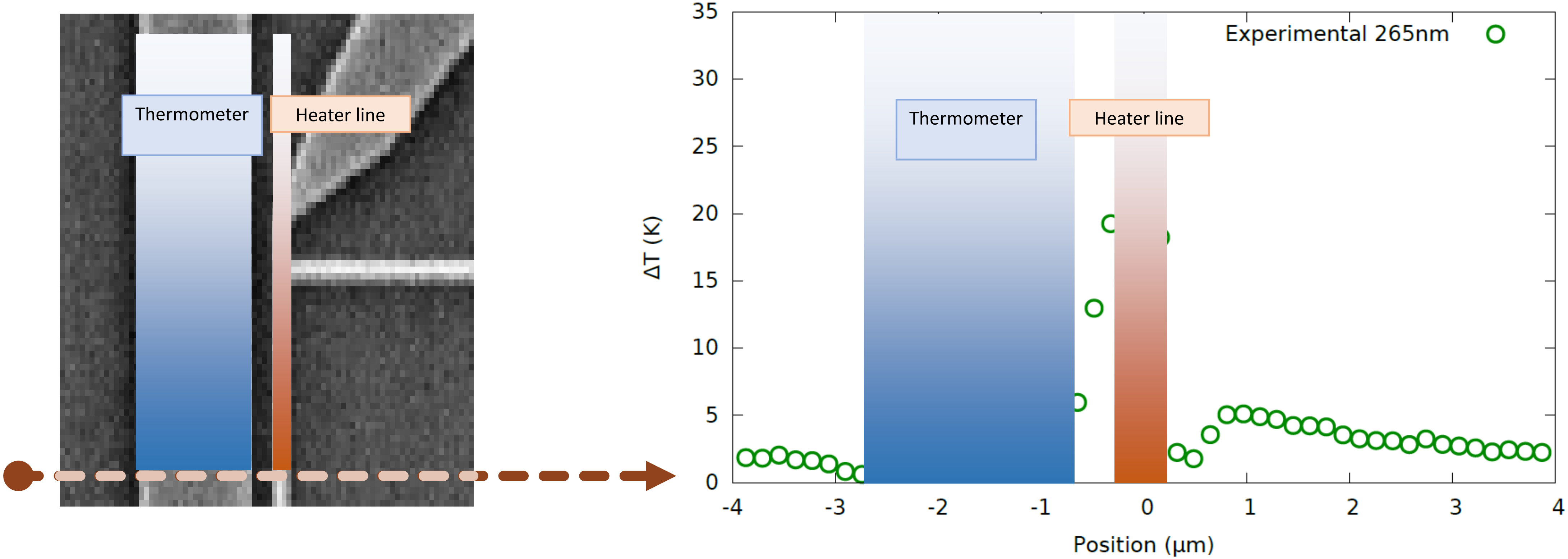
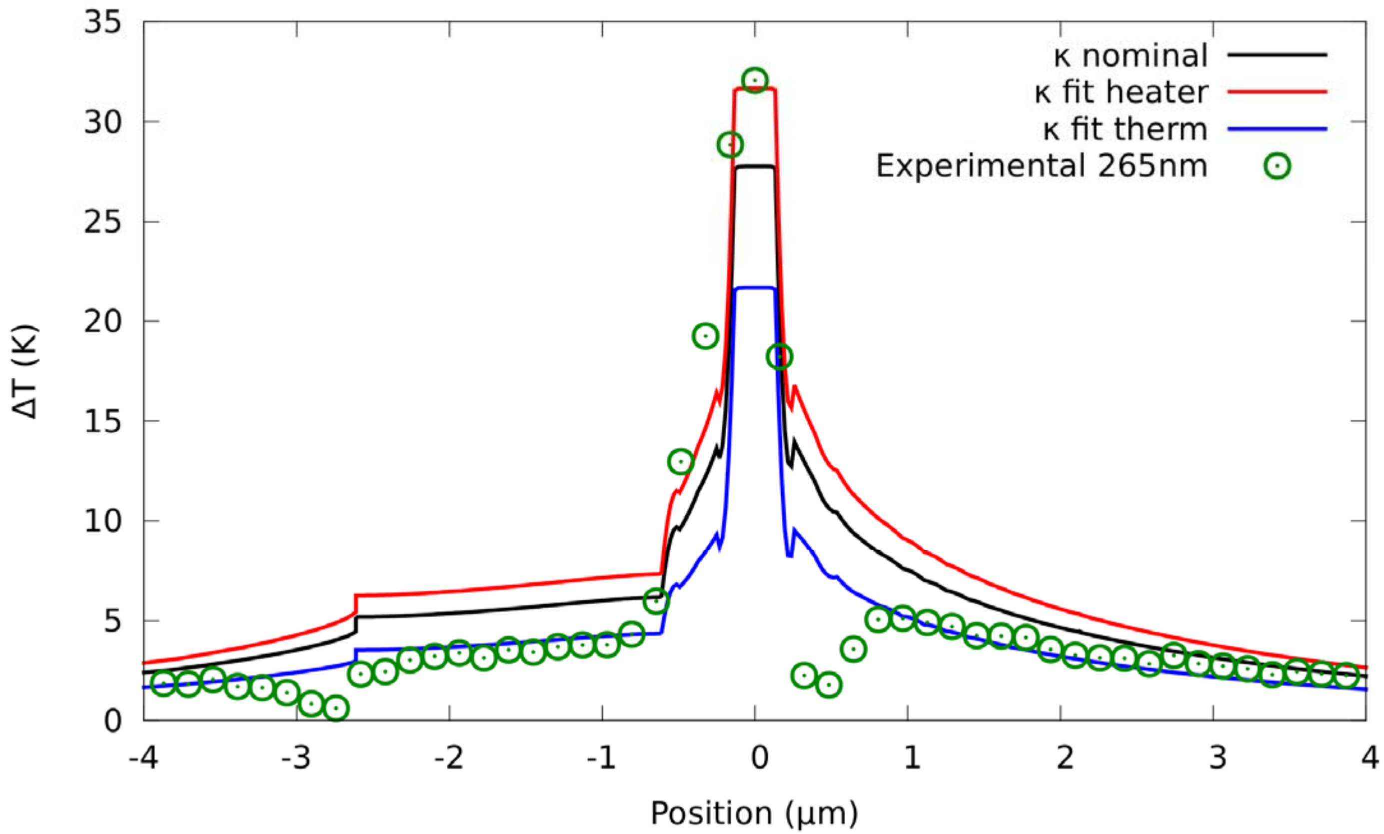
Heater on InGaAs substrate.



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)

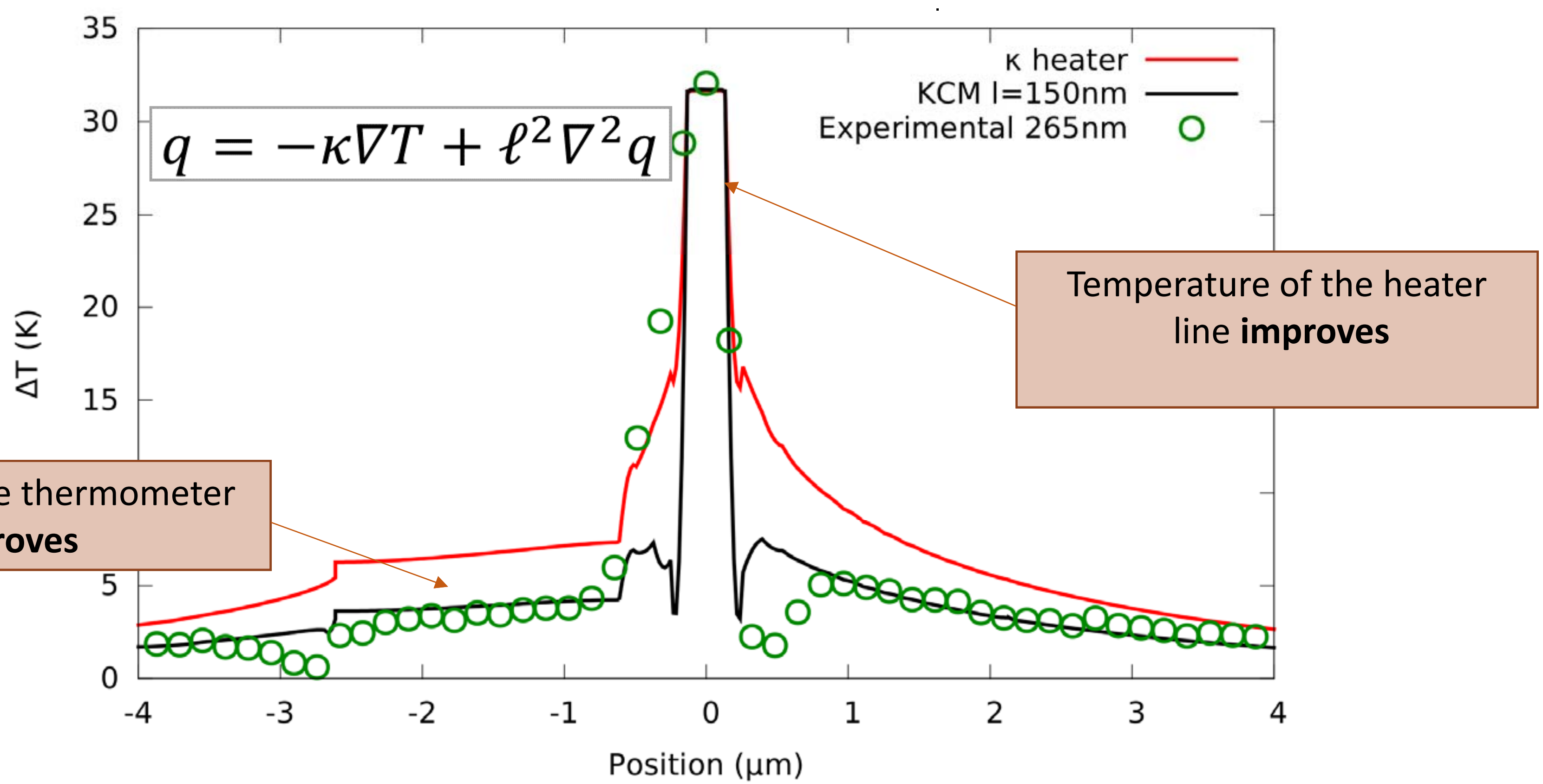
8>> Experimental validation



Fourier's law cannot describe thermal transport in this setup. New equation is needed.

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

9>> Experimental validation



Kinetic Collective Model performs better to experimental data

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

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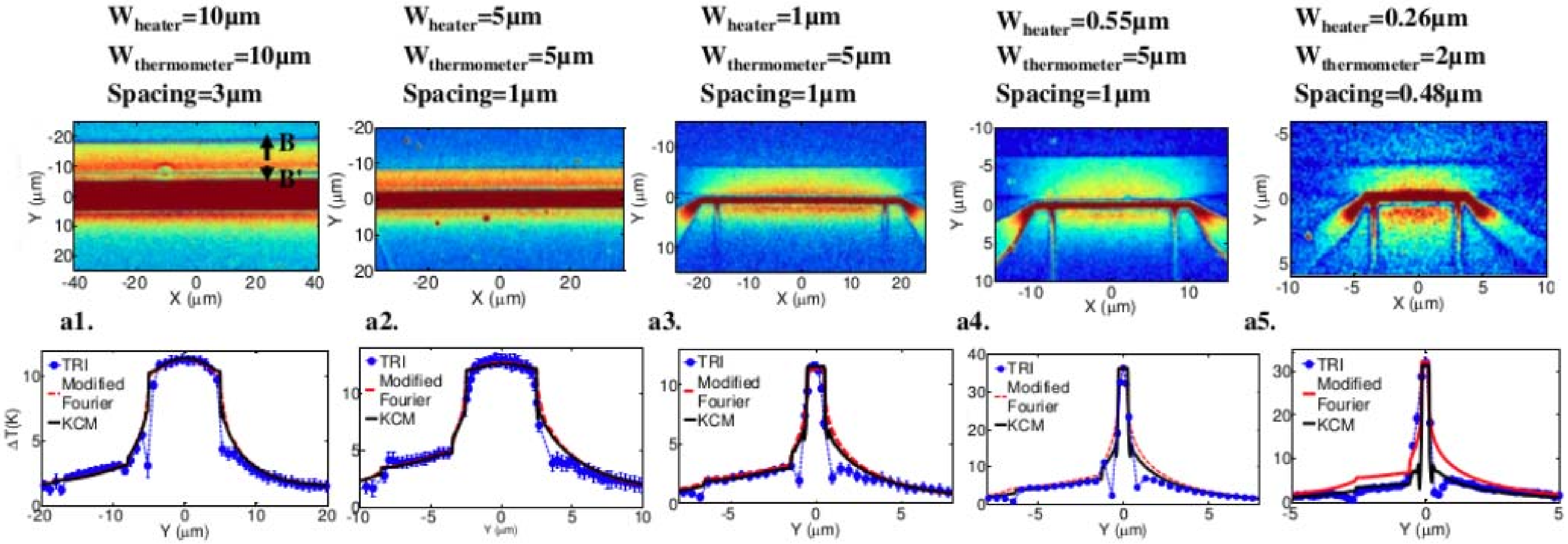
- At large sizes we recover Fourier model.
    - The smaller the size, the larger the effect.
- At extremely small sizes, the model fails due ballistic effects.



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

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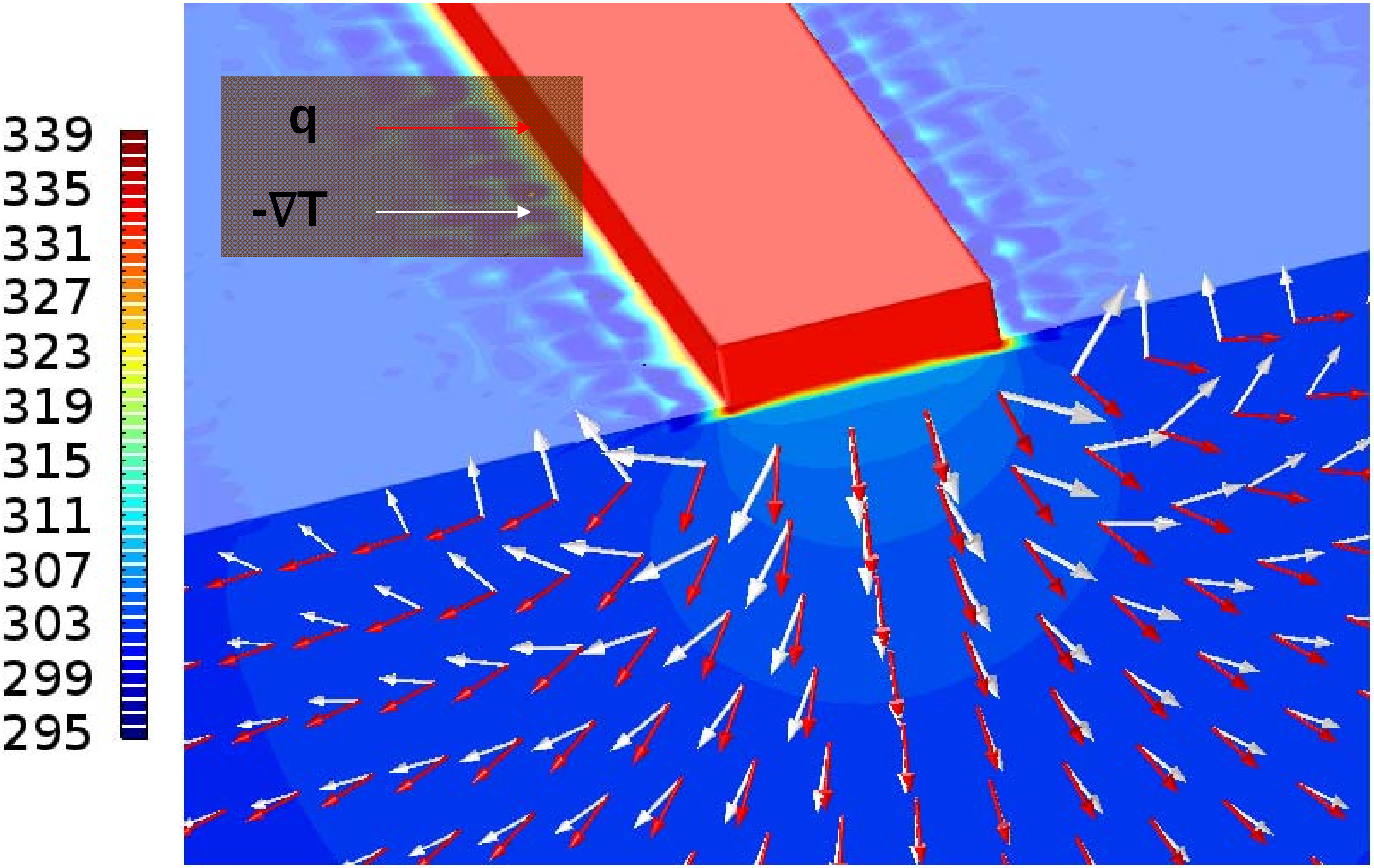
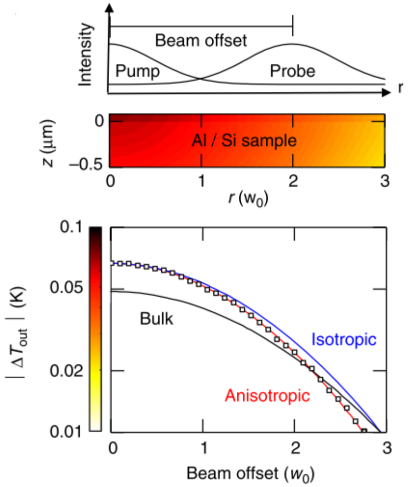


Torres et al. *Phys. Rev. Mat.*, **2**, 076001 (2018)

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.

Wilson and Cahill. Nat Comunic **5**, 5075 (2014)



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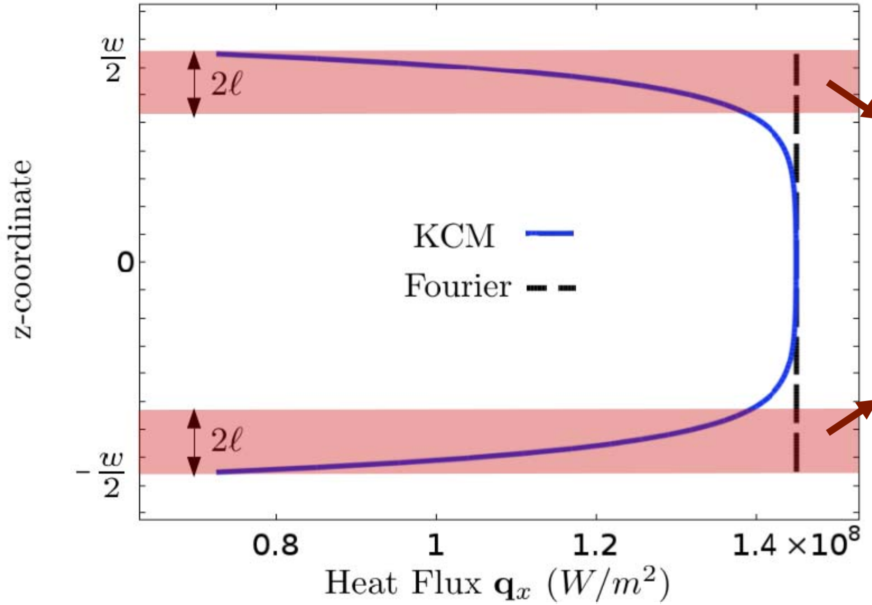
Silicon Thin Films

$$\kappa_{ef} = \frac{\int_\Gamma |\mathbf{q}| d\Gamma}{S \nabla T}$$

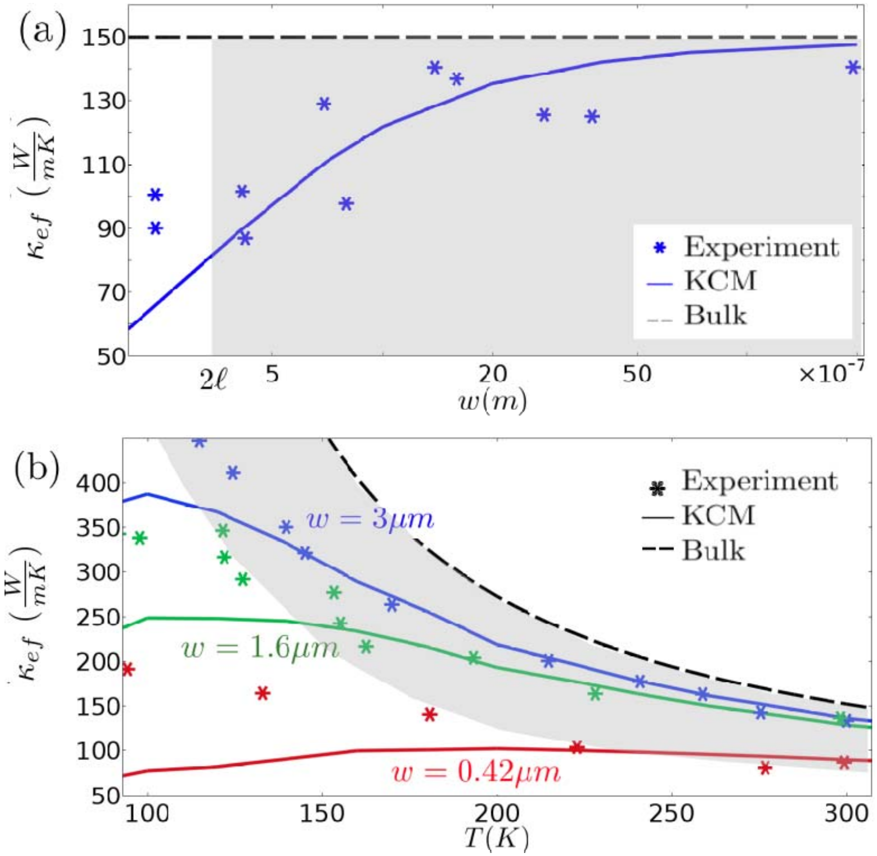
The effective thermal conductivity is lower than the Fourier prediction due to an effect analogous to **viscosity** in fluids.



Boundary conditions produce a non local reduction of the heat flux

Region of applicability is indicated in gray.

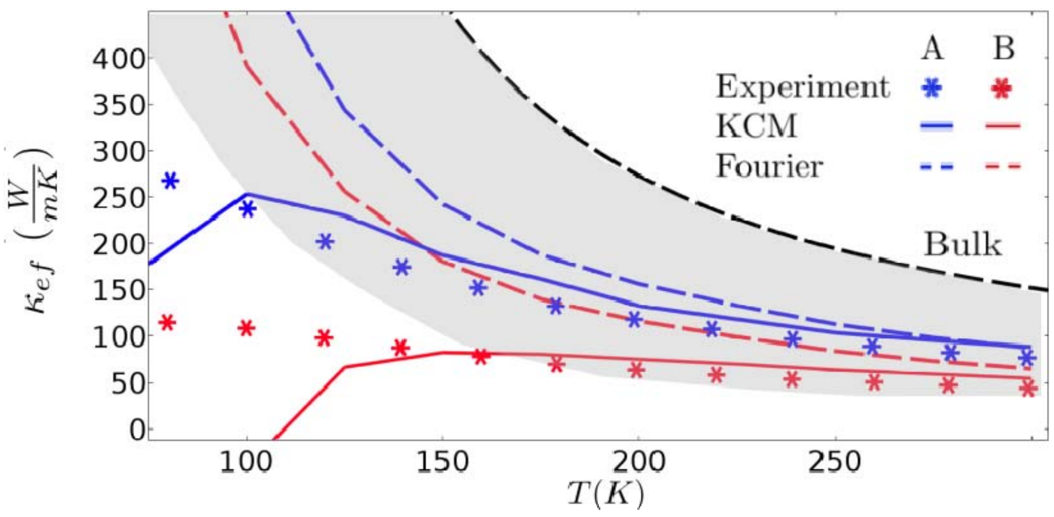
$$2\ell < w$$

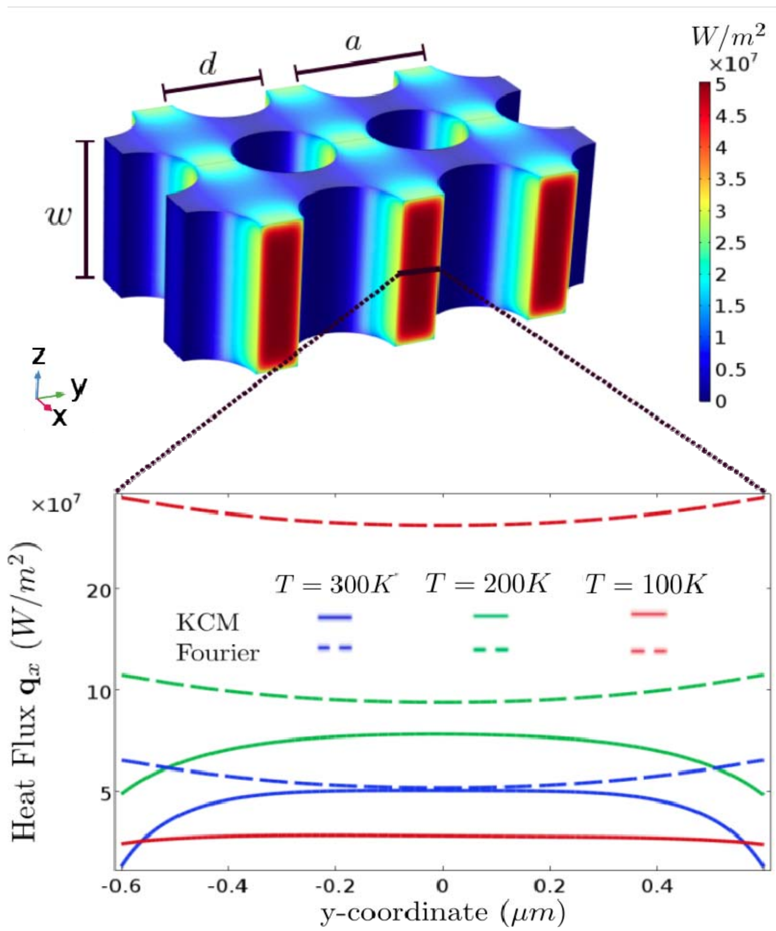


Beardo et al. submitted

 Experimental validation.

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

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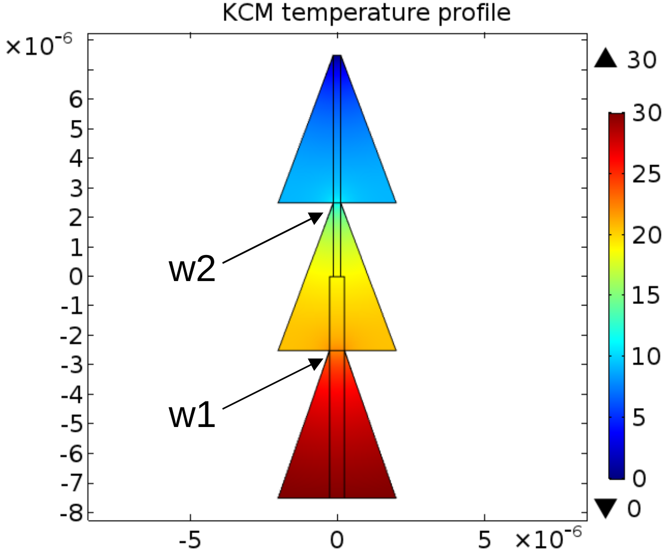
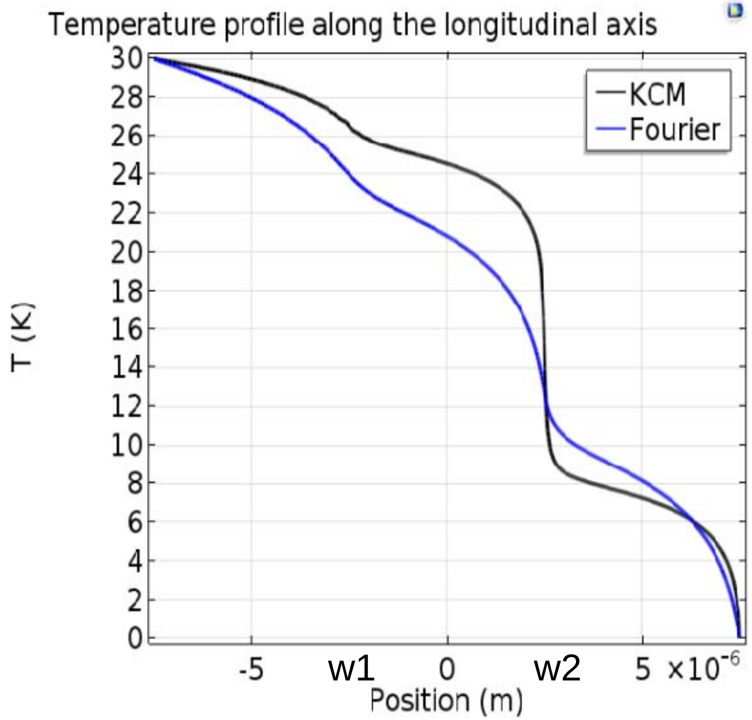
Suspended Silicon Structures





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.

Acknowledgements

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Thanks for your attention.