Hydrodynamic heat transport model for semiconductors with complex geometries including interfaces

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Summary

- Motivation
- Kinetic Collective Model
- Hydrodynamic effects in heat transport
- Experimental Validation
- Conclusions

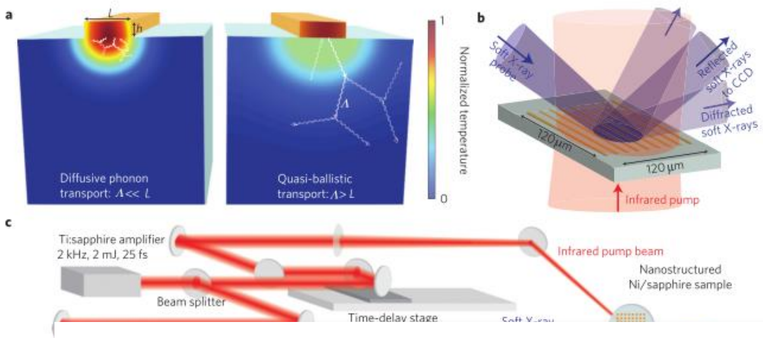
Motivation

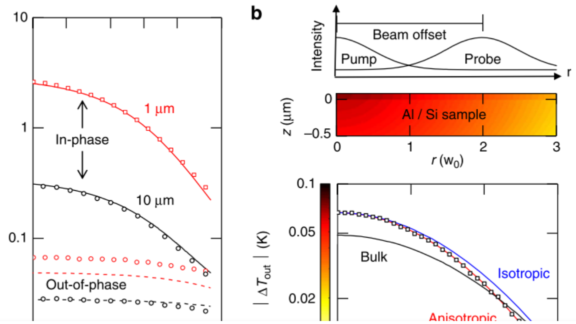
Siemens, M. E. *et al.*
Nat. Mater. **9,** 26–30 (2010)
Quasi-ballistic thermal transport from nanoscale interfaces observed using ultrafast coherent …

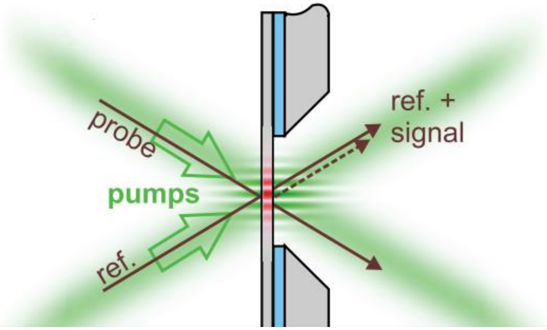
Wilson, R. B. and Cahill, D. G.
Nat. Commun. **5,** 5075 (2014)
Anisotropic failure of Fourier theory in time-domain thermoreflectance experiments

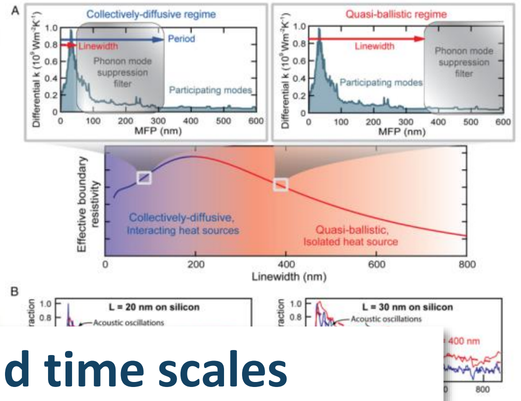
Hoogeboom-Pot, K. M. *et al.*
PNAS **112,** 201503449 (2015).
A new regime of nanoscale thermal transport: Collective diffusion increases dissipation efficiency

Johnson, J. A. *et al.*
Phys. Rev. Lett. **110,** 025901 (2013).
Direct Measurement of Room-Temperature Nondiffusive Thermal Transport Over Micron Distances in a Silicon Membrane.









Several recent experiments have shown the Fourier law is not valid at short length and time scales

Hydrodynamic heat transport equations

KINETIC COLLECTIVE MODEL

GUYER AND KRUMHANSL EQUATION

$$\boldsymbol{q} = -\lambda \nabla \mathrm{T} + \ell^2 (\nabla^2 \boldsymbol{q} + \mathbf{2} \boldsymbol{\nabla}\boldsymbol{\nabla} \cdot \mathbf{q})$$

BOUNDARY CONDITIONS

TANGENTIAL SLIP FLOW

$$\boldsymbol{q_t} = -C\ell \frac{\partial \boldsymbol{q_t}}{\partial n}$$

INTERFACE NORMAL FLUX

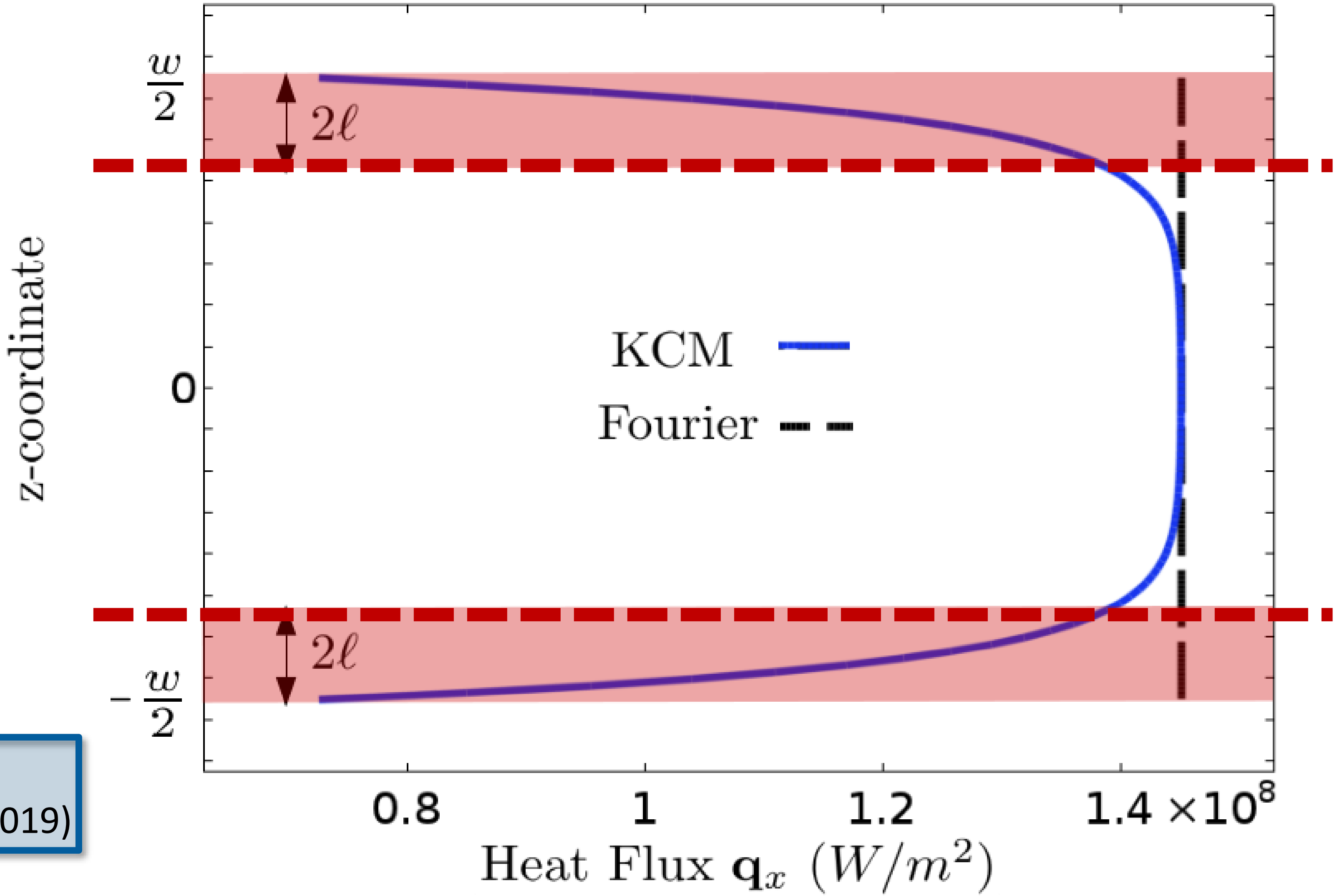
$$\boldsymbol{q_n} = -\frac{\Delta T}{R} + \beta \nabla \cdot \boldsymbol{q} - \chi : \nabla \boldsymbol{q}$$

MATERIAL PROPERTIES

Ab initio calculated parameters

$\lambda, \ell, \beta, \chi, C, R$

Hydrodynamic effects I: Viscosity



HEAT FLUX REDUCTION

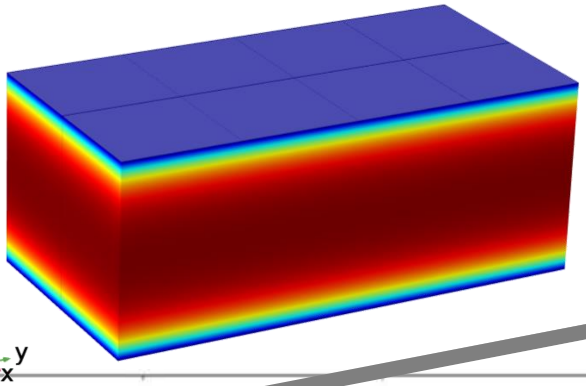
Heat flux needs a distance l to change from the value at the boundary to that on the inner parts of the sample

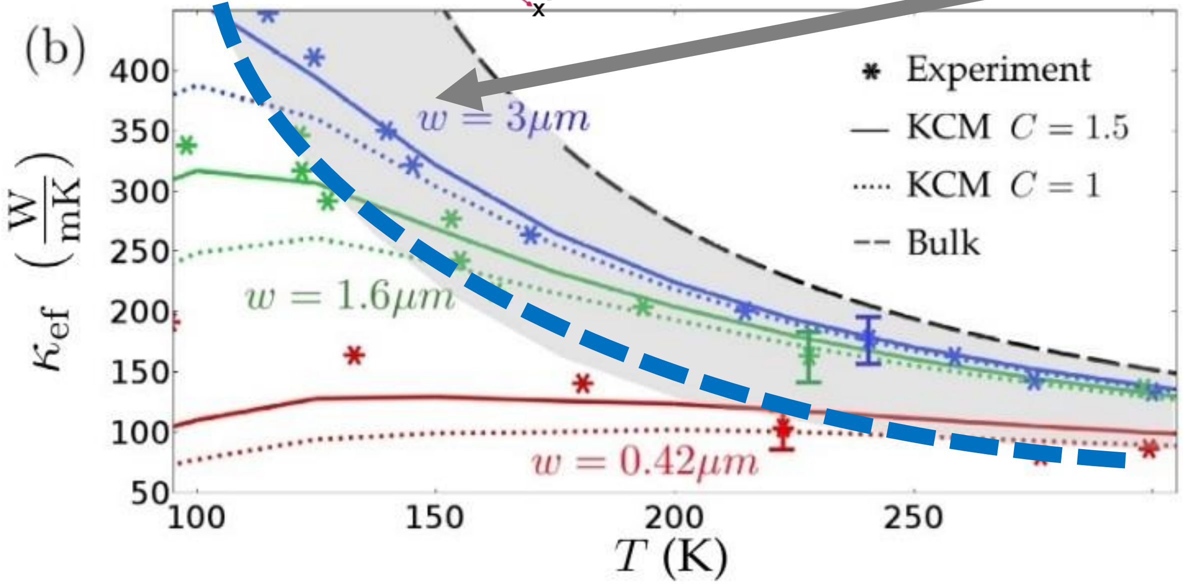
Beardo et al.
Phys. Rev. Appl. **11**, 034003 (2019)

Applicability of hydrodynamic ab initio model

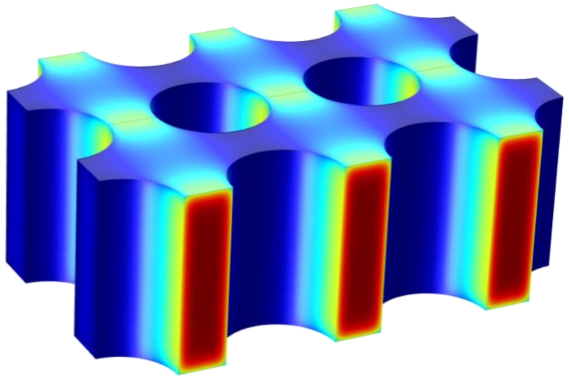
Thin films

$$k_{\text{eff}} = \frac{|\boldsymbol{q}|}{|\nabla T|}$$

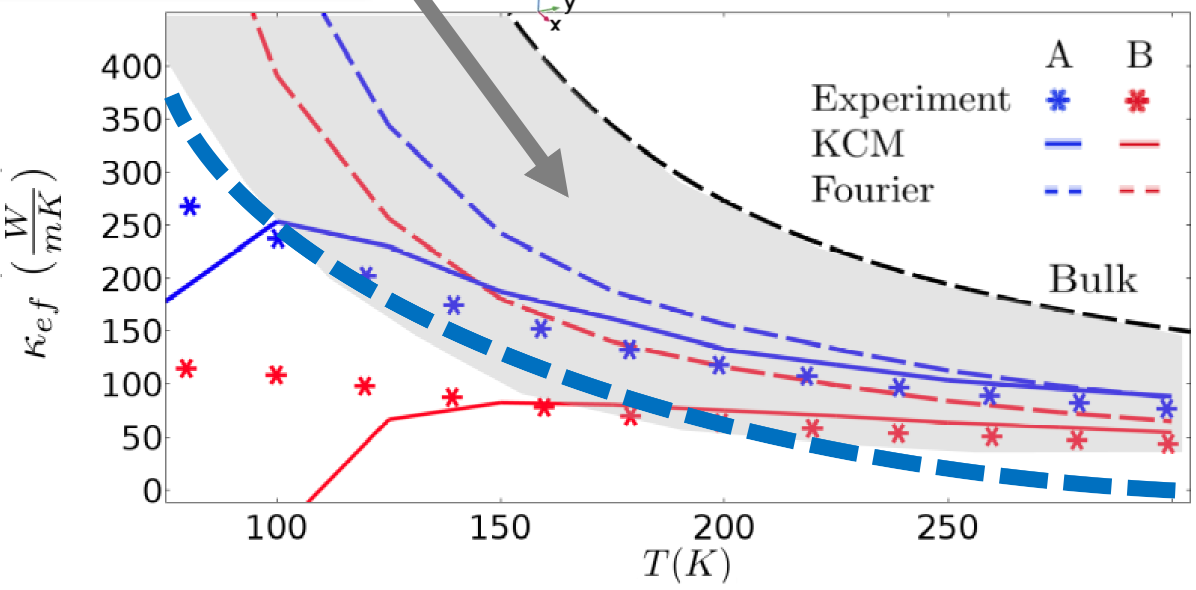




Holey films



Region of predictability
$L > 2\ell$



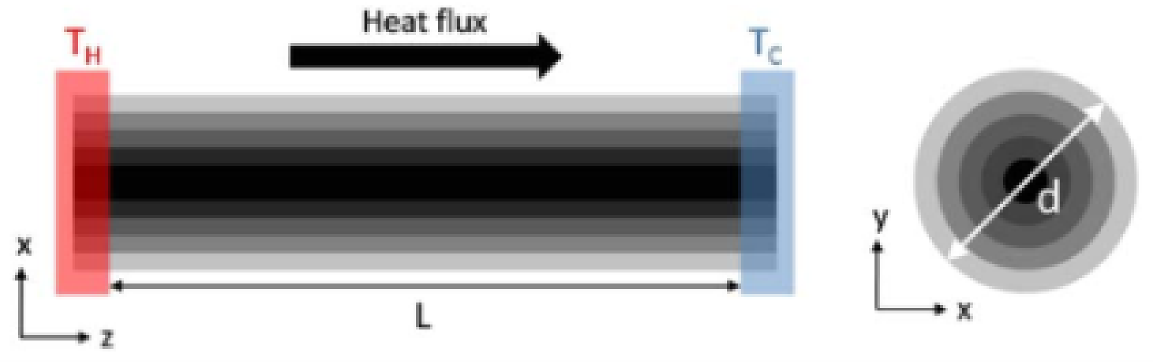
Silicon ℓ =180 nm at 300K

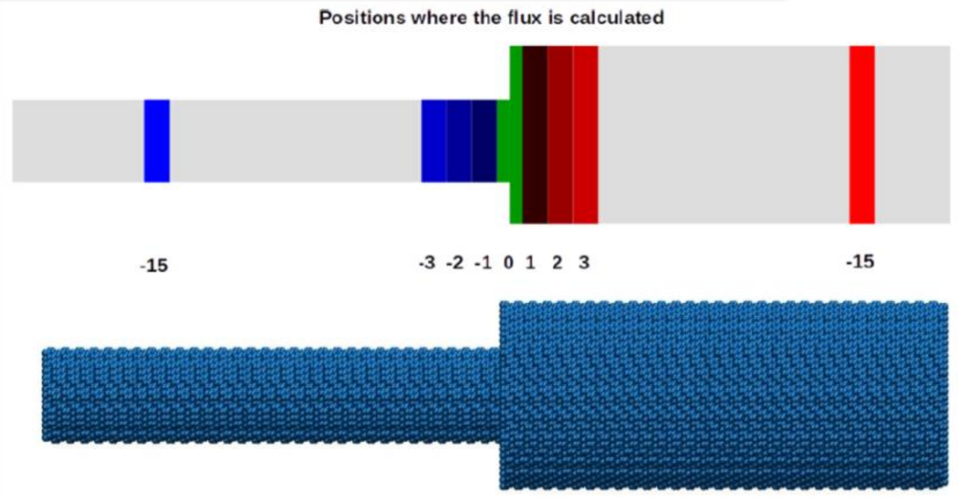
Beardo et al.
Phys. Rev. Appl. **11**, 034003 (2019)

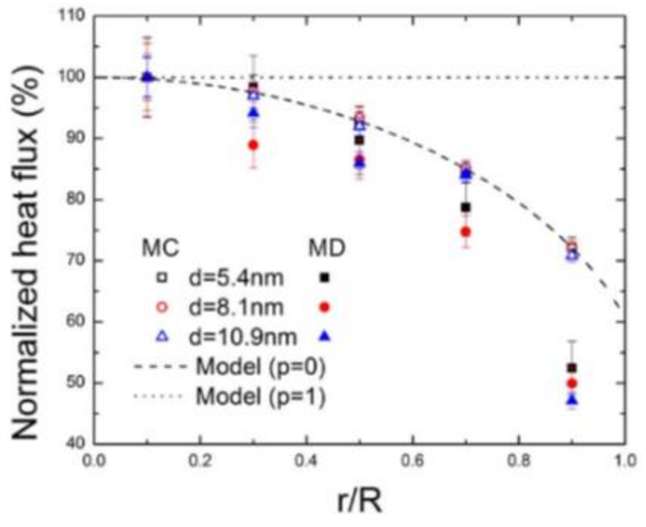
Curved heat flow in MC, MD and FE

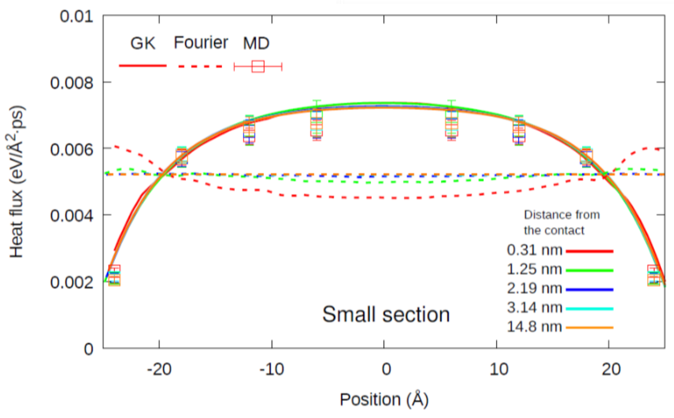
Verdier et al.
J. Phys. Mat., **2** 015002 (2019)

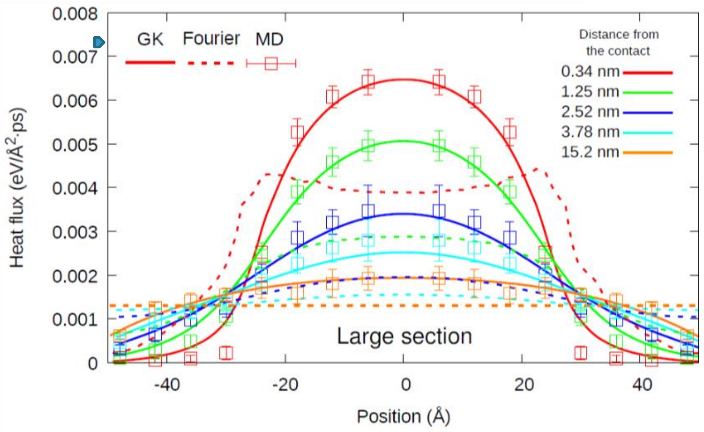
Melis et al.
Phys. Rev. Appl, ***11*** *054059 (2019)*



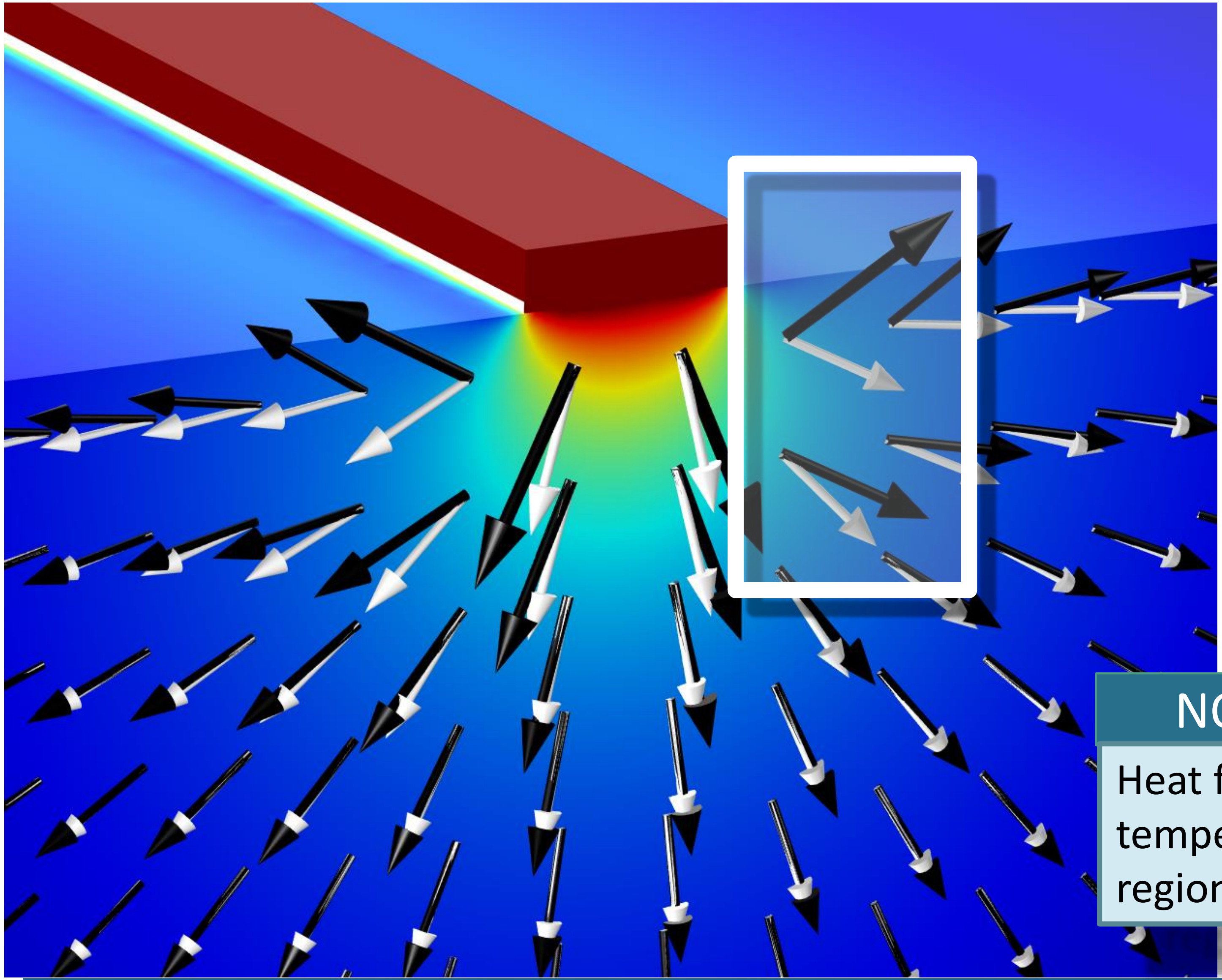




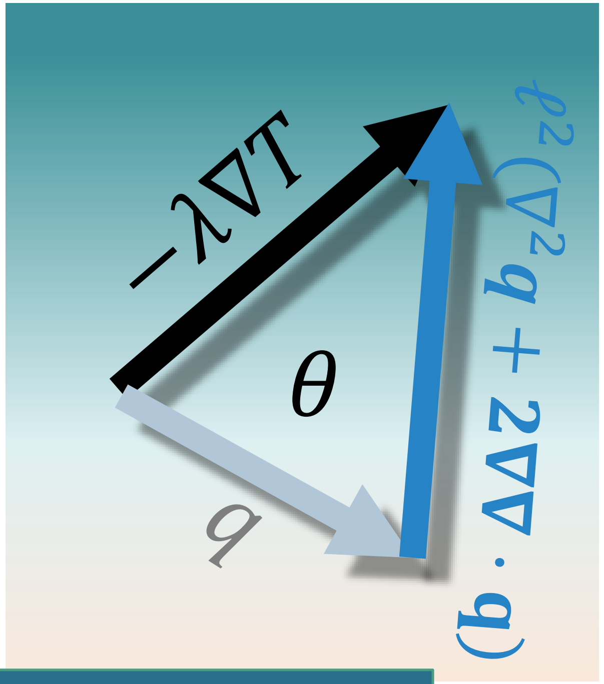




Hydrodynamic effects II. Vorticity



$$q = -\lambda\nabla T + \ell^2(\nabla^2 q + 2\nabla\nabla\cdot \mathbf{q})$$

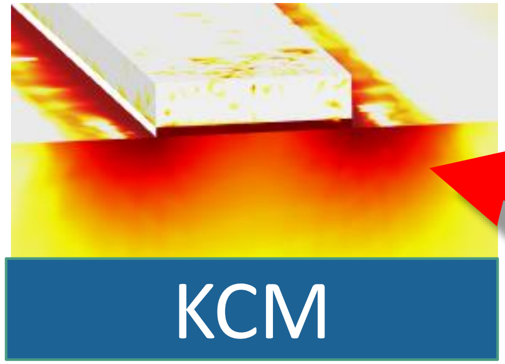


NON-PARAL·LEL VECTORS

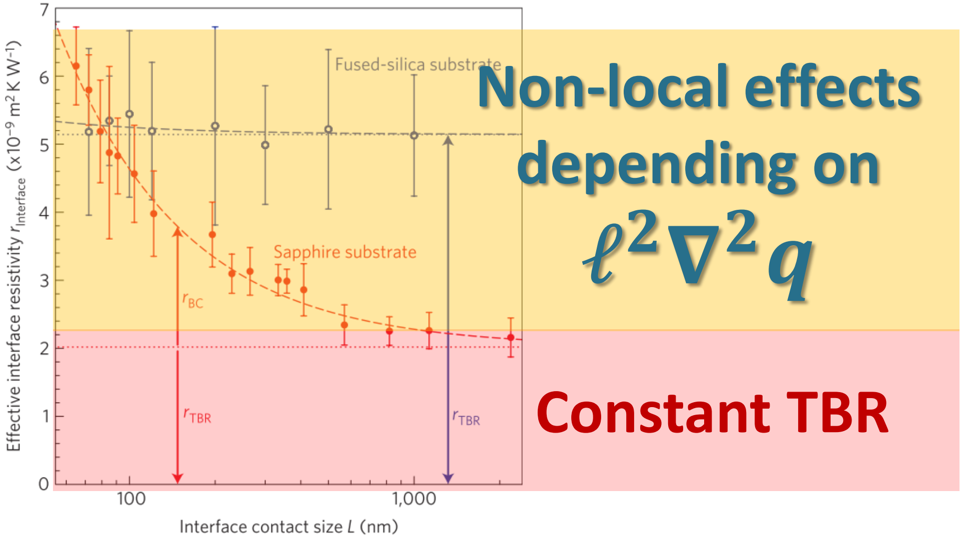
Heat flux is not parallel to temperature gradient near the regions with large curvature

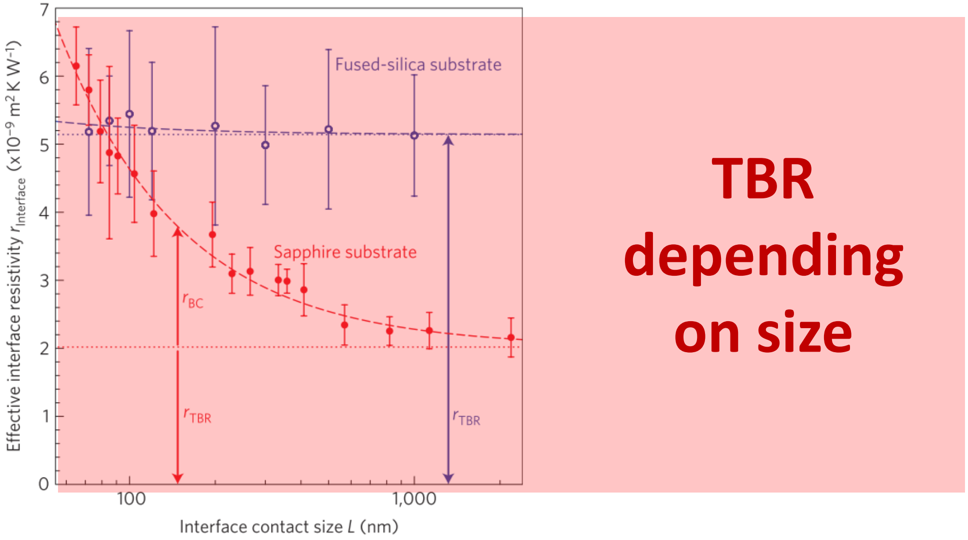
Thermal Boundary Resistance

Torres et al.,
Phys. Rev. Mat. **3,** 076001 (2018)

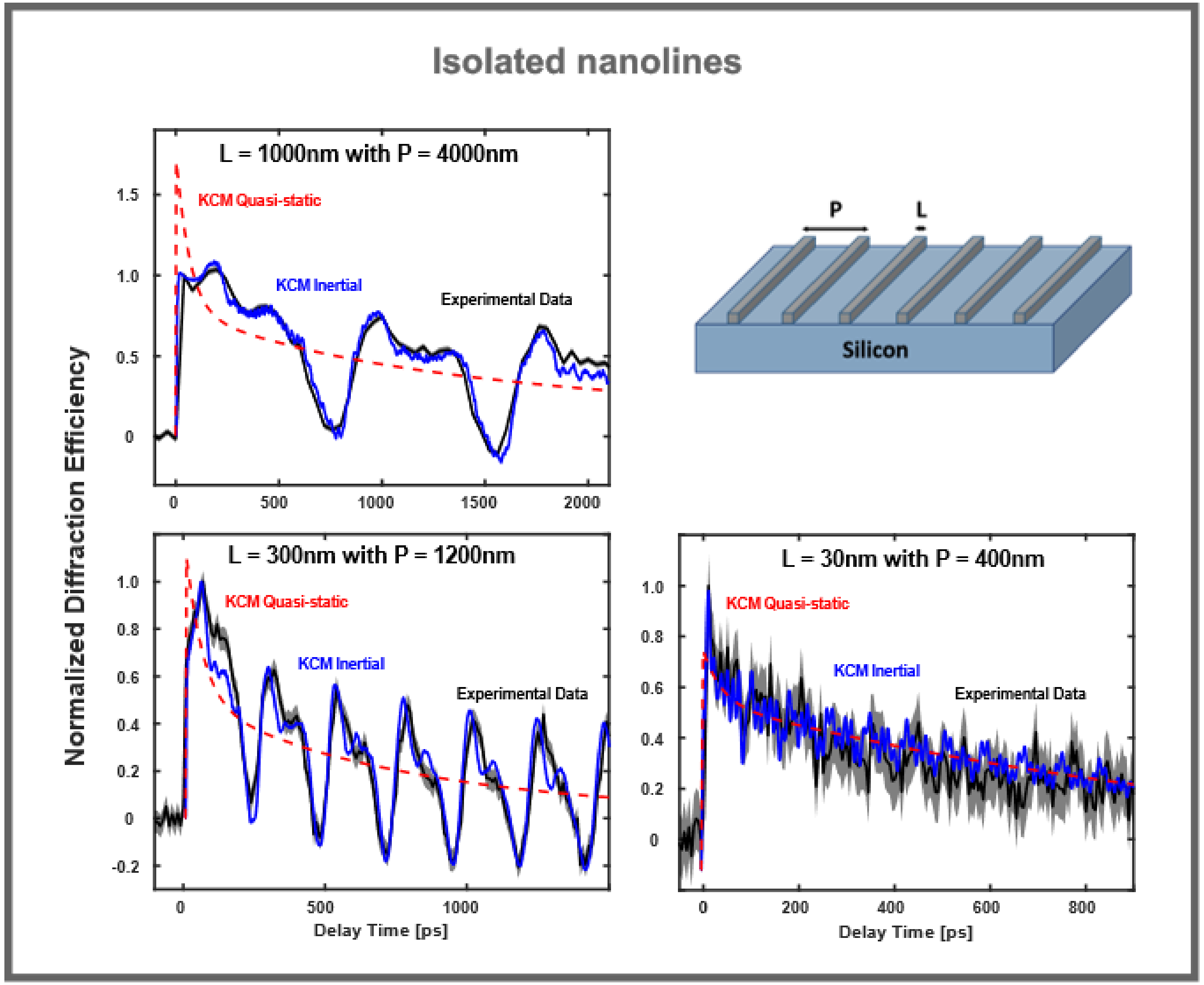


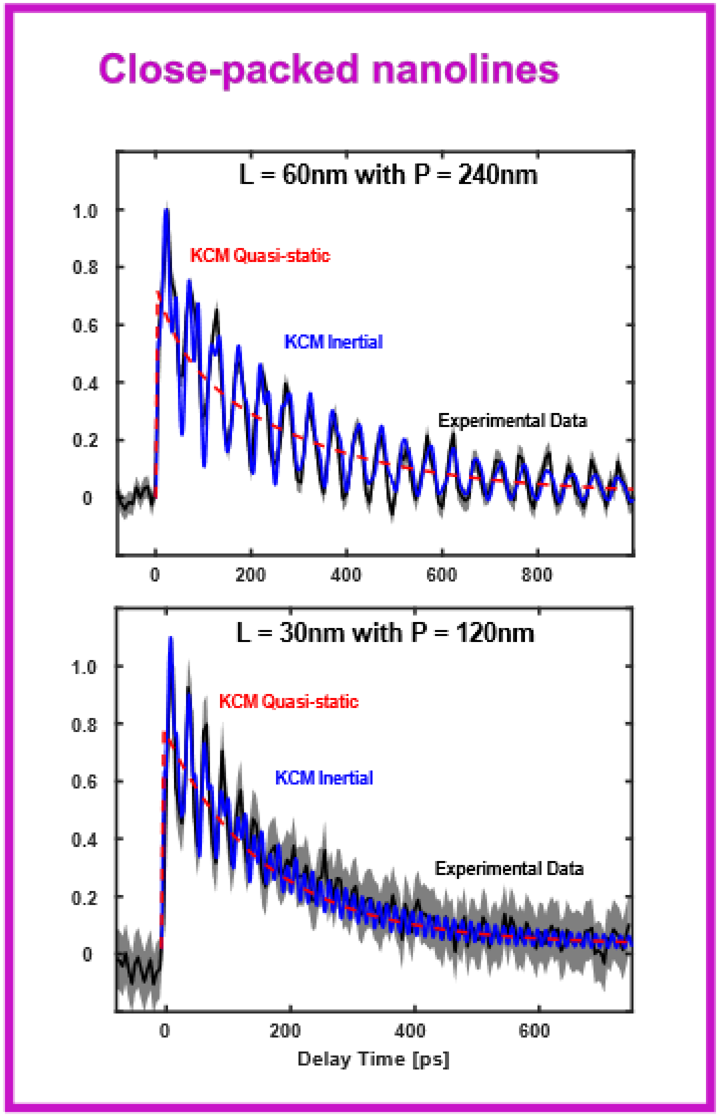
$$k_{\text{eff}} = \frac{|\boldsymbol{q}|}{|\nabla T|}$$



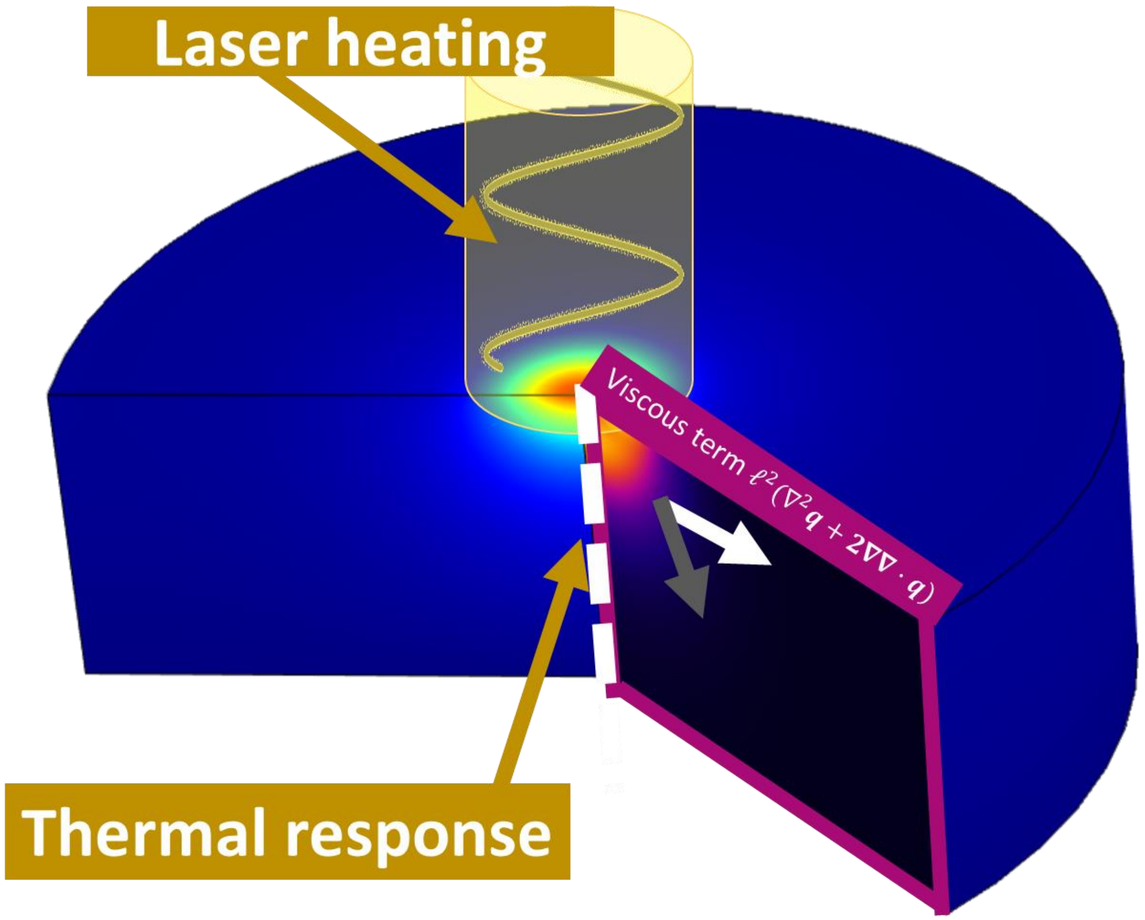


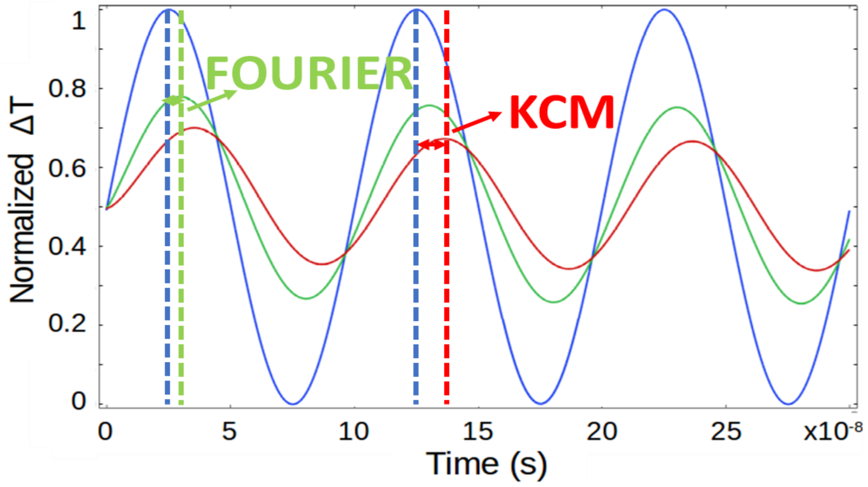
EUV metrology

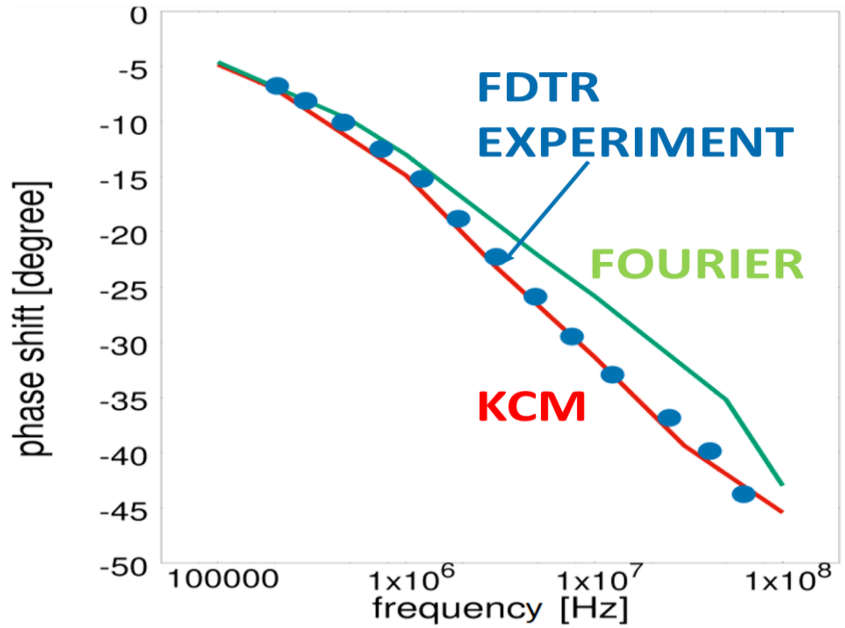




Frequency Domain Thermoreflectance (FDTR)







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Conclusions

- Phonon hydrodynamics is a generalization of Fourier with improved predictability at the nanoscale
- Phonon vorticity and viscosity appear as a phenomenological explanations for the thermal behavior of nanoscale samples allowing to explain the new experiments
- In some experiments hydrodynamics can be observed as an increase of a the Thermal boundary resistance when analyzed with a Fourier model
- The simplicity of the equations allows an easy implementation in COMSOL

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Thanks
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