Hydrodynamic Behaviour in Thermal Transport

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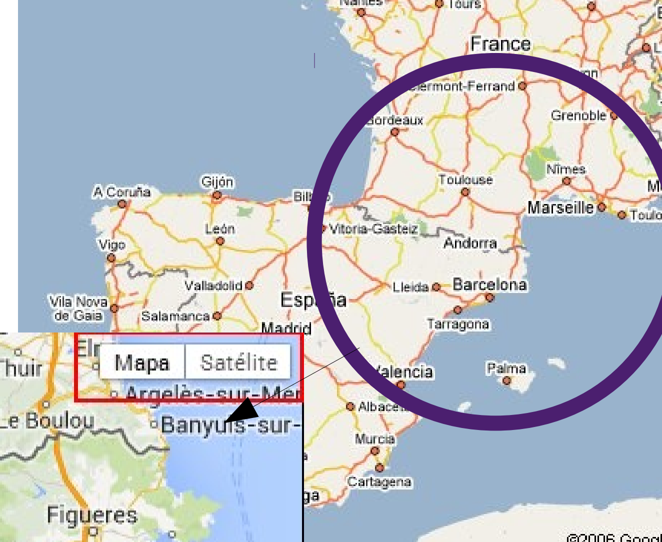
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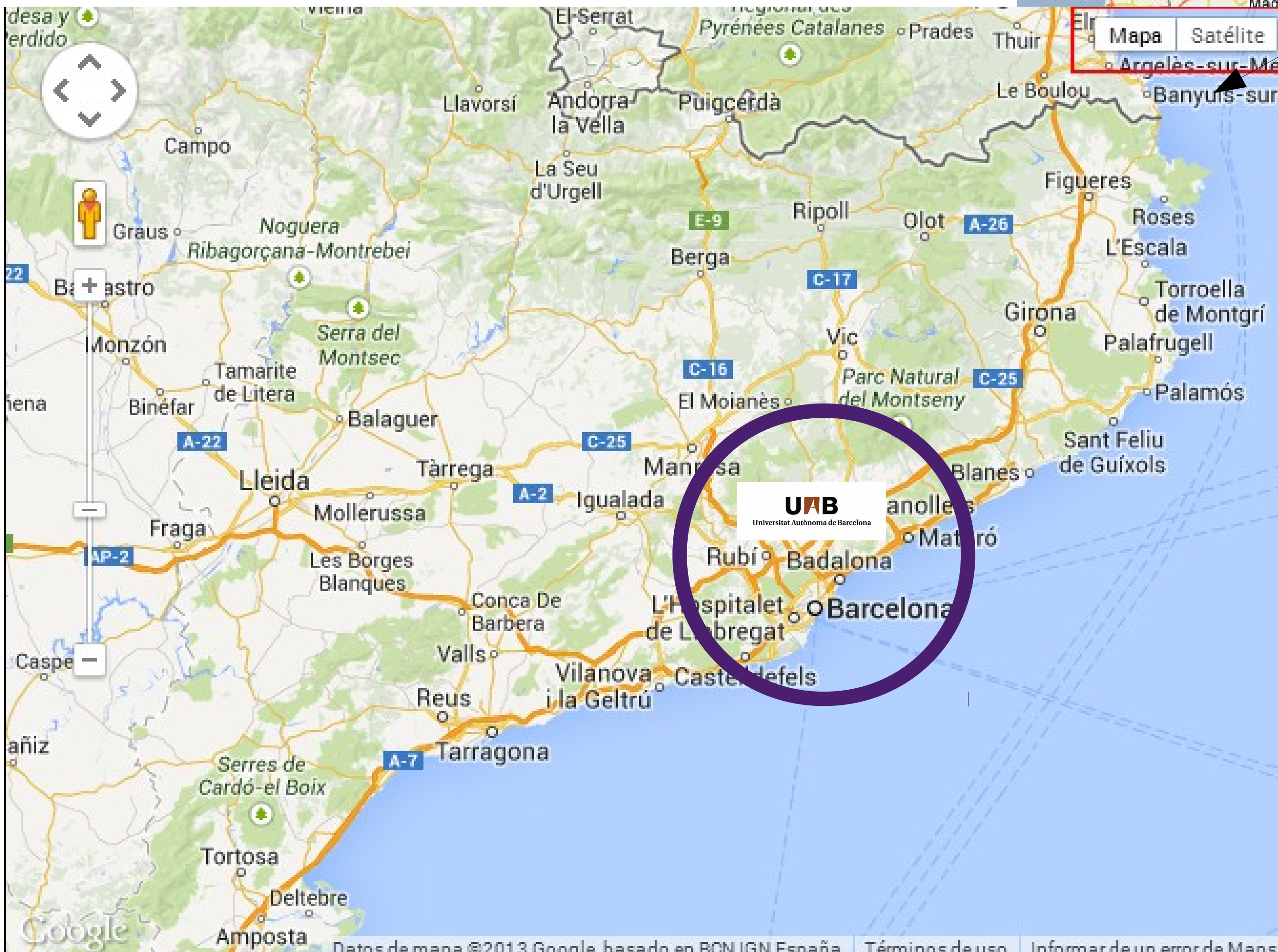
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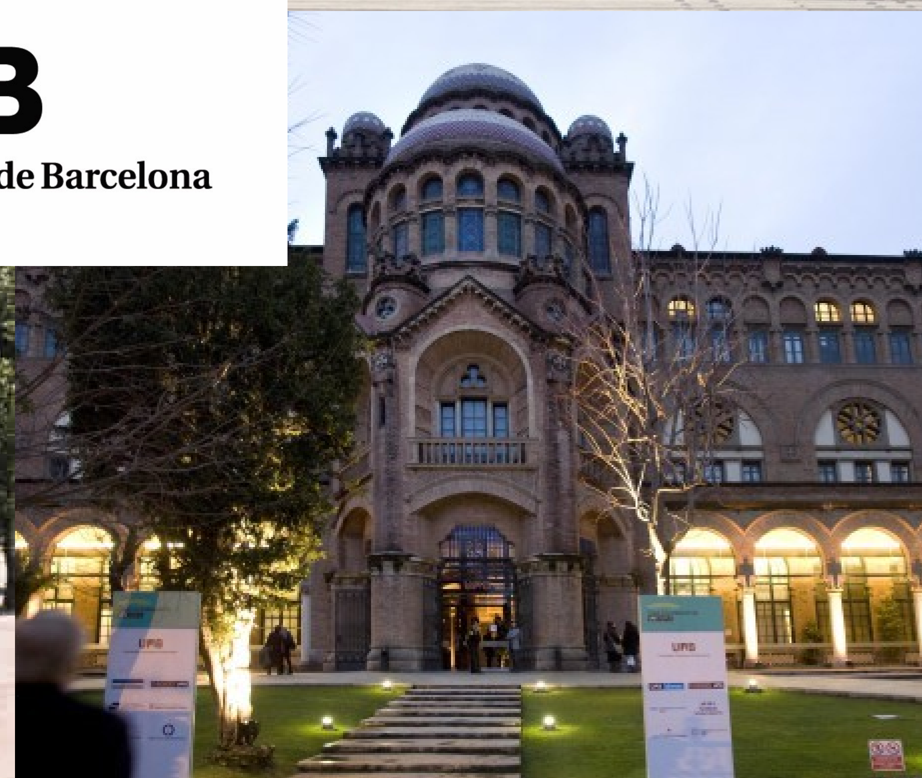
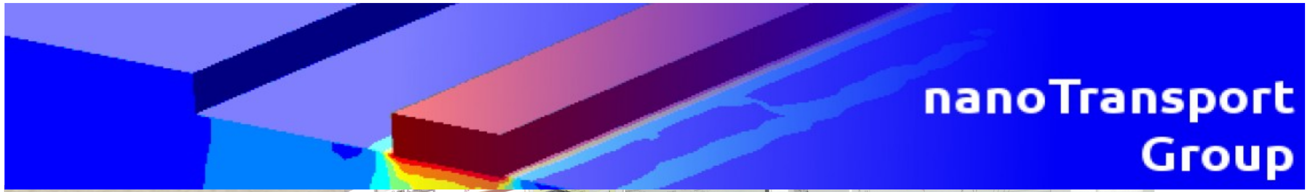
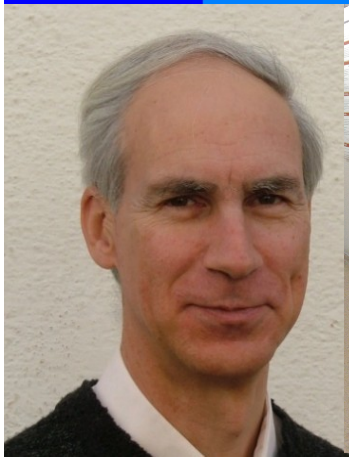
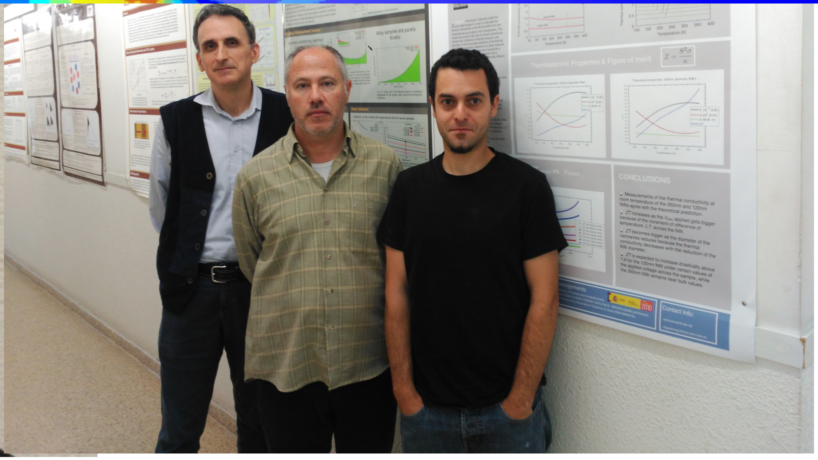


Collaborators







Theory Group: nanoTransport

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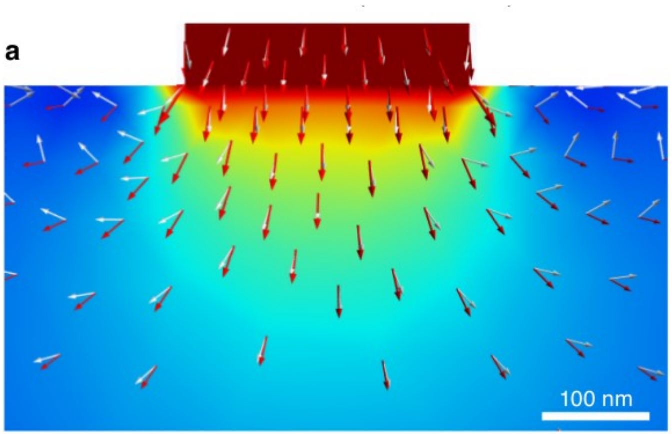
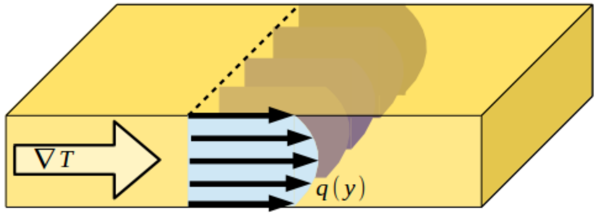
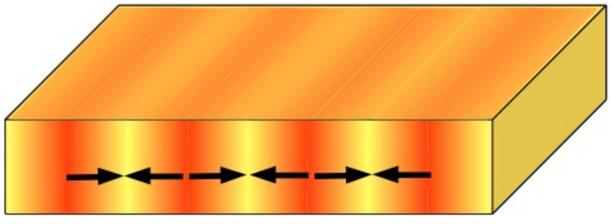
GNaM

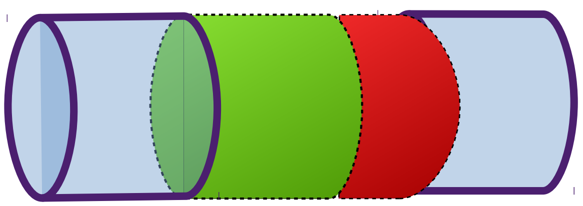
Summary

1. Thermal behaviour out of equilibrium
2. Extended Irreversible Thermodynamics (EIT)
3. Phonon Hydrodynamic Equations
4. Exact solutions of the BTE
5. Kinetic Collective Model (KCM)
6. Hydrodynamics + KCM - complex geometries







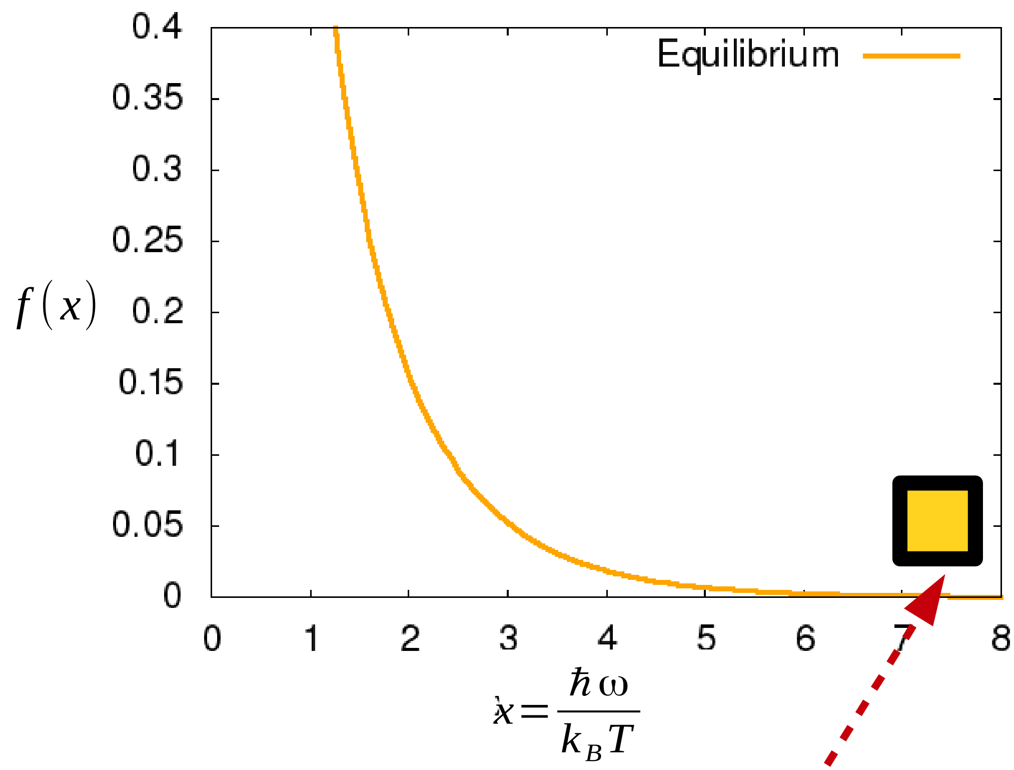


Thermal transport far from equilibrium

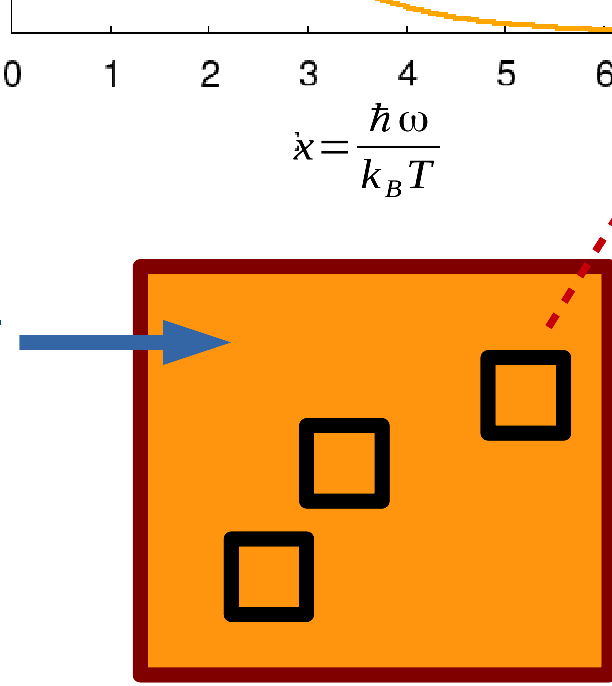
Equilibrium

In equilibrium, phonons follows the **Bose-Einsten** distribution function

$$f(\omega)=f_0(\omega)=\frac{1}{e^{\hbar\omega/k_B T}-1}$$



Homogeneous temperature T

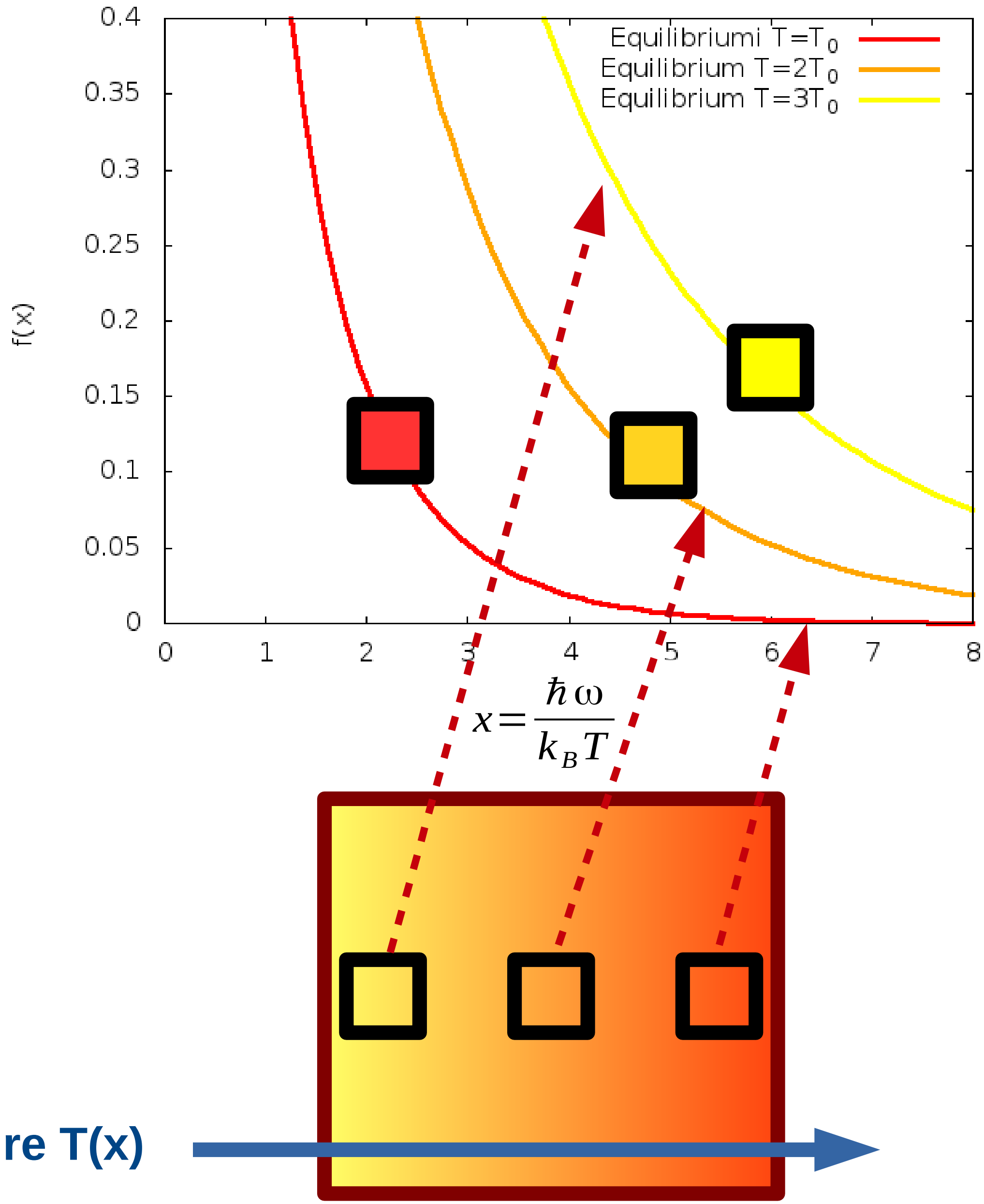


Local equilibrium

When inhomogeneties appear inside the system a global temperature **T** is no longer a good magnitude to describe the system

If these are not large a local equilibrium temperature **T(x)** can be defined

$$f_0(\omega, x) = \frac{1}{e^{\hbar\omega / k_B T(x)} - 1}$$

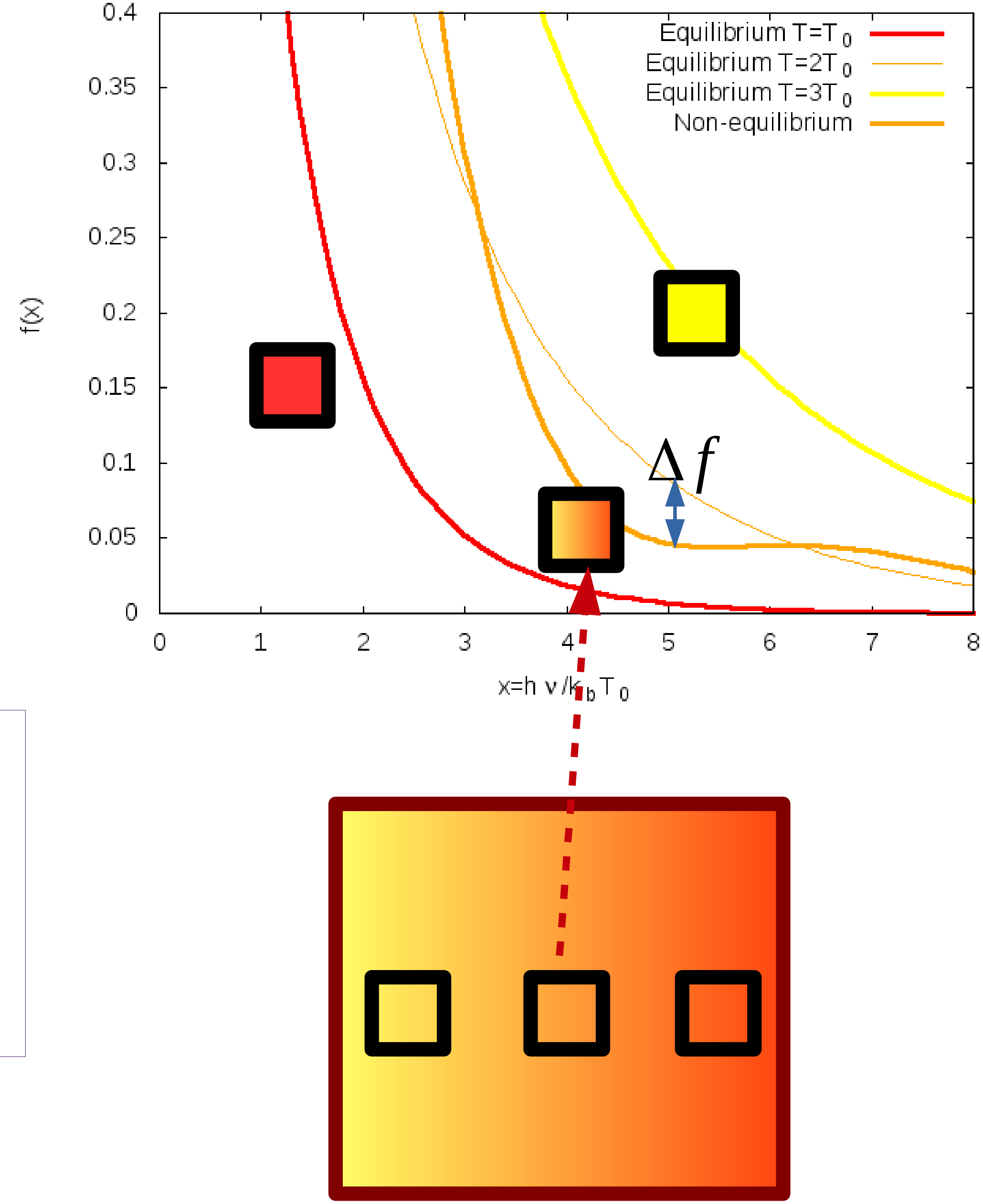


Inhomogeneous temperature T(x)

Far from equilibrium

Sometimes the excitation of the distribution function cannot be expressed by a single parameter like a local temperature

$$f = f_0 + \Delta f$$



Which are the equations that determine the evolution of the excitation

$$\Delta f(k, x, t)?$$

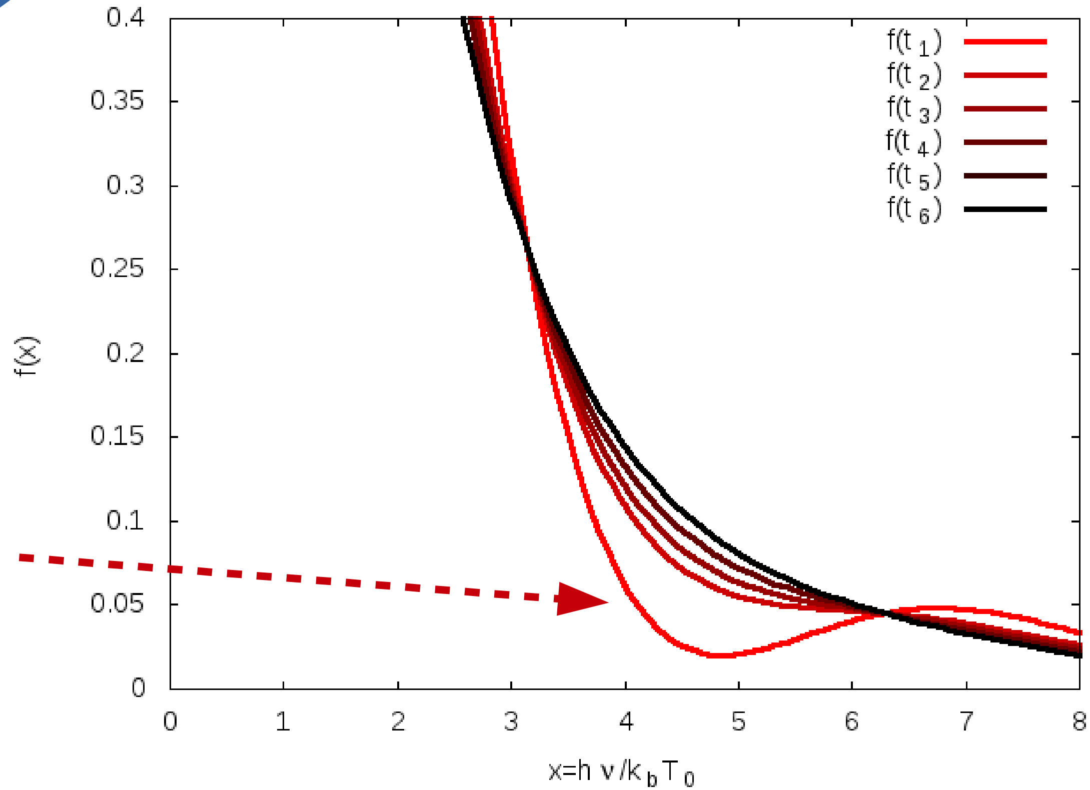
Boltzmann Tranport Equation (BTE)

The Boltzmann Transport Equation determines the spatial and temporal evolution of the distrubution fumction

$$\frac{\partial}{\partial t} + v \cdot \nabla f = \left(\frac{\partial f}{\partial t} \right)_{col}$$

Phonon group velocity

Starting from an initial condition, the distribution function changes in time



Extended Irreversible Thermodynamics

Moments of the distribution

From phonons $f(\kappa, x, t)$ **to moments** $M_i(x,t)$

$$\epsilon(x,t)=\int \hbar\omega_k f(\kappa,x,t)\frac{d^3k}{(2\pi)^3}$$

Zero order: **energy density**

$$q(x,t)=\int \hbar\omega_k \vec{v}_g f(\kappa,x,t)\frac{d^3k}{(2\pi)^3}$$

First order: **heat flux**

$$Q(x,t)=\int \hbar\omega_k (\vec{v}_{gx_1}\cdot\vec{v}_{gx_2}) f(\kappa,x,t)\frac{d^3k}{(2\pi)^3}$$

Second order: **flux of the flux**

...

$$Q^n(x,t)=\int \hbar\omega_k (\vec{v}_{gx_1}\cdots\vec{v}_{gx_n}) f(\kappa,x,t)\frac{d^3k}{(2\pi)^3}$$

n-order moment

Changing to moment equations

n equations for the n modes:
Boltzmann Transport Equation

BTE output

$$f(\kappa, x, t)$$

Change to moment description

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

n equations for the n moments
Grad/Chapman-Enskog equations

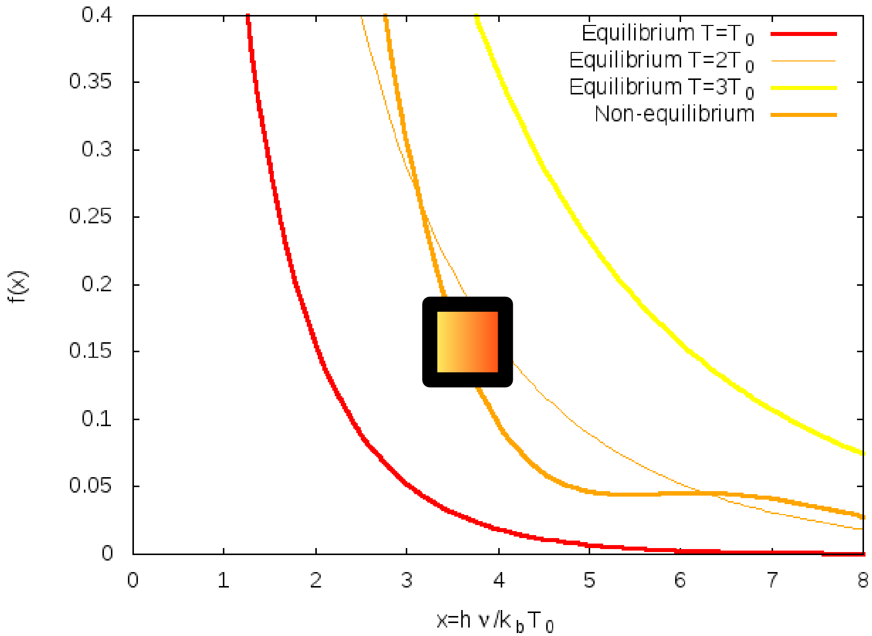
Thermodynamic output

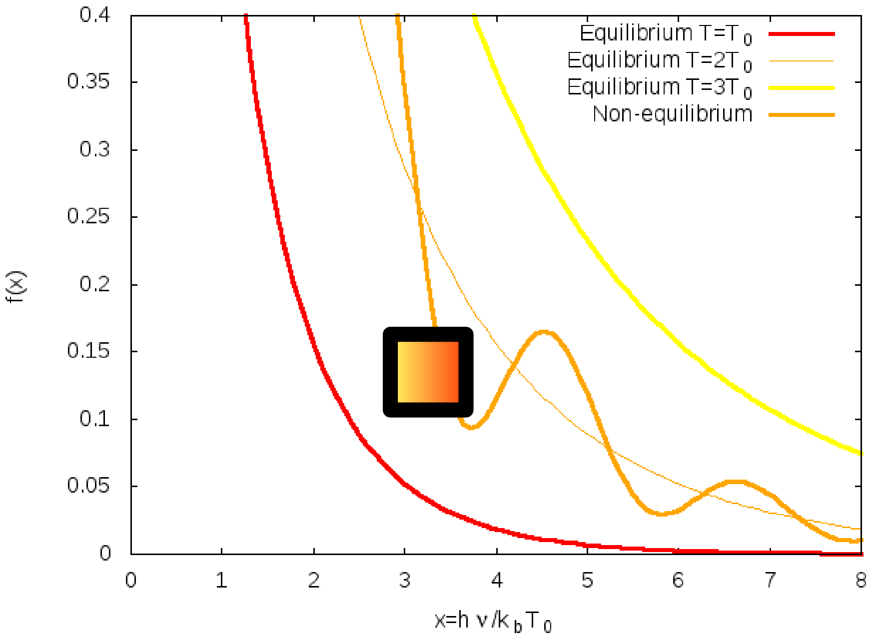
$$\Delta T(x,t), \vec{q}(x,t), Q(x,t)$$

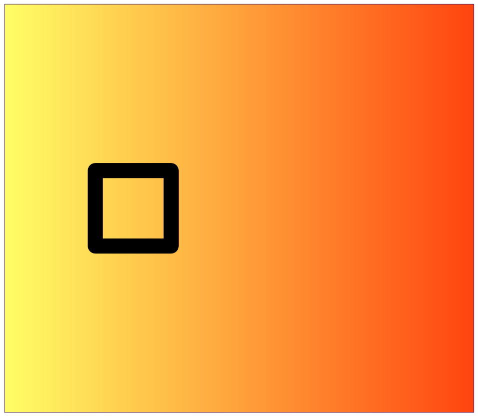
The experimental results are almost always the moments: Temperature, fluxes, etc...

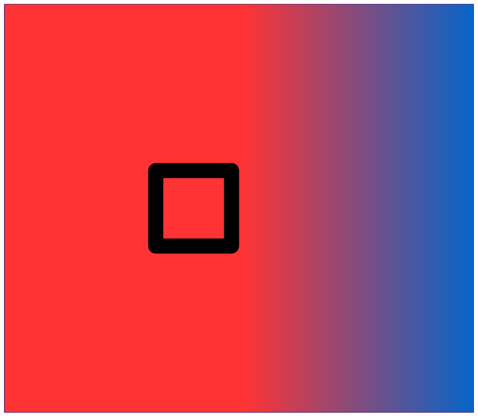
Moments needed for the description

Depending on the imposed conditions we may need higher number of orders to describe the system









Extended Irreversible Thermodynamics (EIT)

Temperature — **Heat Flux**

$$
\begin{aligned}
c_v \dot{T} & & &= -\frac{dq}{dx} & & \quad \text{Zero Order Eq.}\\
\alpha_1 \dot{q} & -\mu_1 q & &= -\beta_2 \frac{dQ^{(2)}}{dx} & -\lambda \frac{dT}{dx} & \quad \text{First Order Eq.}\\
\alpha_2 \dot{Q}^{(2)} & -\mu_2 Q^{(2)} & &= -\beta_3 \frac{dQ^{(3)}}{dx} & -\beta_1 \frac{dq}{dx} & \quad \text{Second Order Eq.}\\
\alpha_3 \dot{Q}^{(3)} & -\mu_3 Q^{(3)} & &= -\beta_4 \frac{dQ^{(4)}}{dx} & -\beta_2 \frac{dQ^{(2)}}{dx} & \\
& \dots & & & & \\
\alpha_n \dot{Q}^{(n)} & -\mu_n Q^{(n)} & &= -\beta_{n+1} \frac{dQ^{(n+1)}}{dx} & -\beta_n \frac{dQ^{(n-1)}}{dx} & \quad \text{n-Order Eq.}
\end{aligned}
$$

$$\alpha_n/\mu_n = \tau_n,\ \ell_n^2 = \beta_n^2/(\mu_n \mu_{n+1})$$

Extended Irreversible Thermodynamics (EIT) allows the description of any number of moments

First order: Fourier Law

Taking only the terms to first order we recover the Fourier Law

$$\begin{array}{lllll}
\boxed{c_v \dot{T}} & & = & \boxed{-\frac{dq}{dx}} & \\
\alpha_1 \dot{q} & \boxed{-\mu_1 q} & = & -\beta_2 \frac{dQ^{(2)}}{dx} & \boxed{-\lambda \frac{dT}{dx}} \\
\alpha_2 \dot{Q}^{(2)} & -\mu_2 Q^{(2)} & = & -\beta_3 \frac{dQ^{(3)}}{dx} & -\beta_1 \frac{dq}{dx} \\
\alpha_3 \dot{Q}^{(3)} & -\mu_3 Q^{(3)} & = & -\beta_4 \frac{dQ^{(4)}}{dx} & -\beta_2 \frac{dQ^{(2)}}{dx} \\
 & \ldots & & & \\
\alpha_n \dot{Q}^{(n)} & -\mu_n Q^{(n)} & = & -\beta_{n+1} \frac{dQ^{(n+1)}}{dx} & -\beta_n \frac{dQ^{(n-1)}}{dx}
\end{array}$$

Zero Order Eq.

First Order Eq.

Second Order Eq.

n-Order Eq.

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

Energy Conservation

$$\vec{q} = -\lambda \nabla T$$

Fourier Law

Second order: Guyer-Krumhansl equation

Taking only the terms to second order we recover the Guyer-Krumhansl equation

$$
\begin{aligned}
c_v \dot{T} & & &= -\frac{dq}{dx} & & \quad \leftarrow \text{Zero Order Eq.}\\
\alpha_1 \dot{q} & -\mu_1 q & &= -\beta_2 \frac{dQ^{(2)}}{dx} & -\lambda \frac{dT}{dx} & \quad \leftarrow \text{First Order Eq.}\\
\alpha_2 \dot{Q}^{(2)} & -\mu_2 Q^{(2)} & &= -\beta_3 \frac{dQ^{(3)}}{dx} & -\beta_1 \frac{dq}{dx} & \quad \leftarrow \text{Second Order Eq.}\\
\alpha_3 \dot{Q}^{(3)} & -\mu_3 Q^{(3)} & &= -\beta_4 \frac{dQ^{(4)}}{dx} & -\beta_2 \frac{dQ^{(2)}}{dx} & \\
& \cdots & & & & \\
\alpha_n \dot{Q}^{(n)} & -\mu_n Q^{(n)} & &= -\beta_{n+1} \frac{dQ^{(n+1)}}{dx} & -\beta_n \frac{dQ^{(n-1)}}{dx} & \quad \leftarrow \text{n-Order Eq.}
\end{aligned}
$$

$$C_v \frac{dT}{dt} = -\nabla \cdot q \quad \leftarrow \text{Energy Conservation}$$

$$\vec{q} = -\lambda \nabla T + l^2 \nabla^2 q \quad \leftarrow \text{Guyer-Krumhansl equation}$$

Continued fraction approach

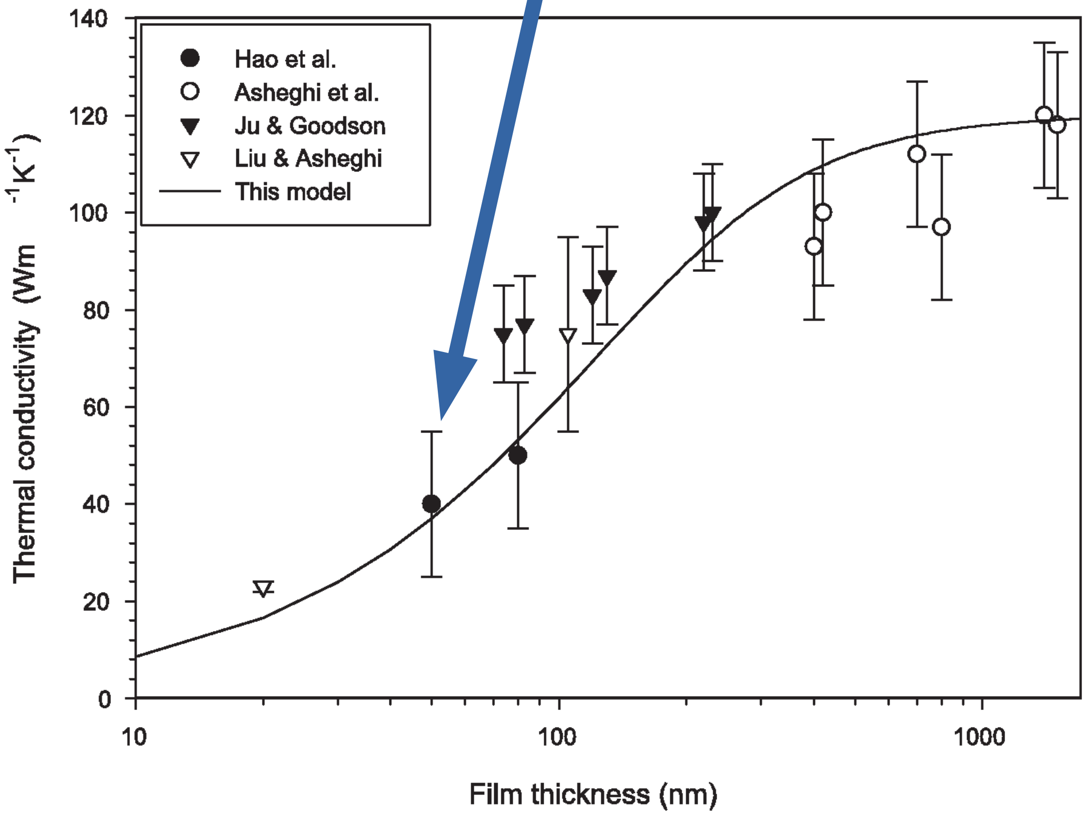
$$\hat{T} = \left(s + \frac{D\xi^2}{1 + \frac{\ell^2\xi^2}{1 + \frac{\ell^2\xi^2}{1 + \frac{\ell^2\xi^2}{1+\dots}}}} \right)^{-1}$$

$$\lambda = \lambda_0 \frac{-1 + \sqrt{1 + (\xi l)^2}}{1/2(\xi l)^2}$$

Alvarez and Jou, APL 90, 83109 (2007)

Application to nanowires

Nonlocalities give an interpretation for the reduction of effective thermal conductivity at the nanoscale



Alvarez and Jou, APL 90, 83109 (2007)

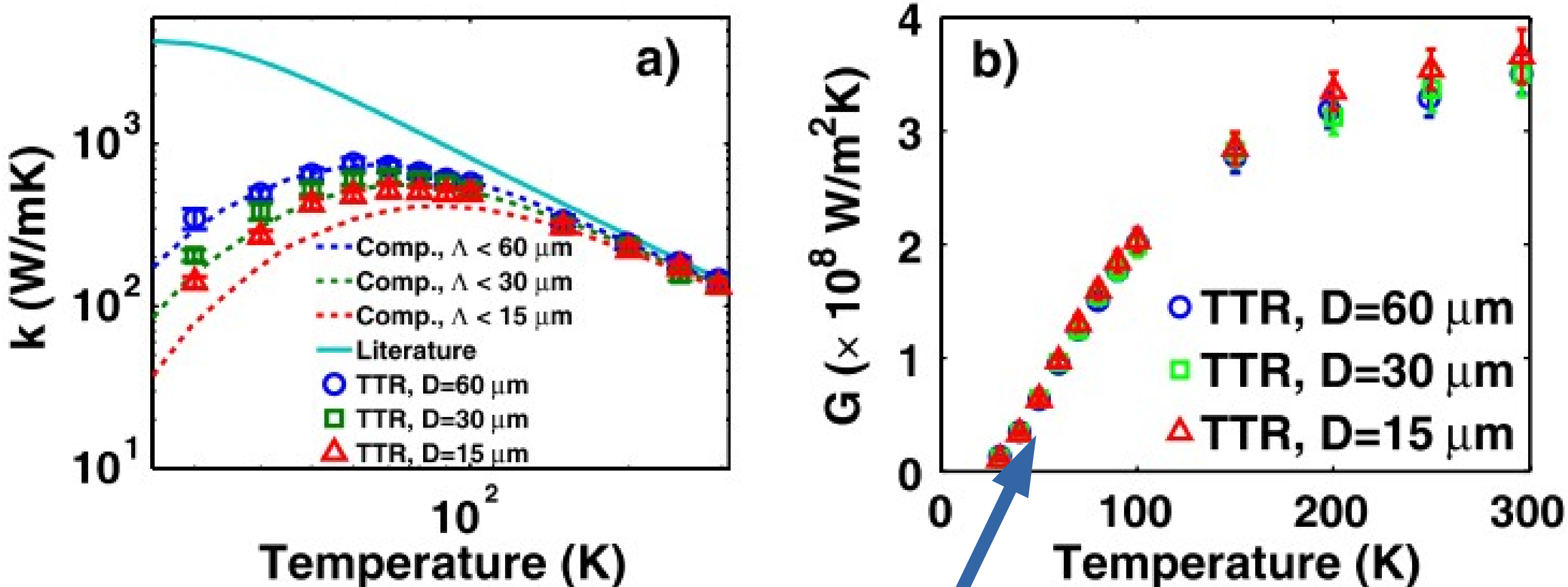
$$\lambda = \lambda_0 \frac{-1+\sqrt{1+(\xi l)^2}}{1/2(\xi l)^2}$$

$$\xi = \frac{2\pi}{L}$$

$$\lambda = \frac{\lambda_0 L^2}{2\pi^2 l^2}\left[\sqrt{1+4\left(\frac{\pi l}{L}\right)^2}-1\right]$$

Application TDTR experiments

Reduction of the effective thermal conductivity with the laser spot radius.



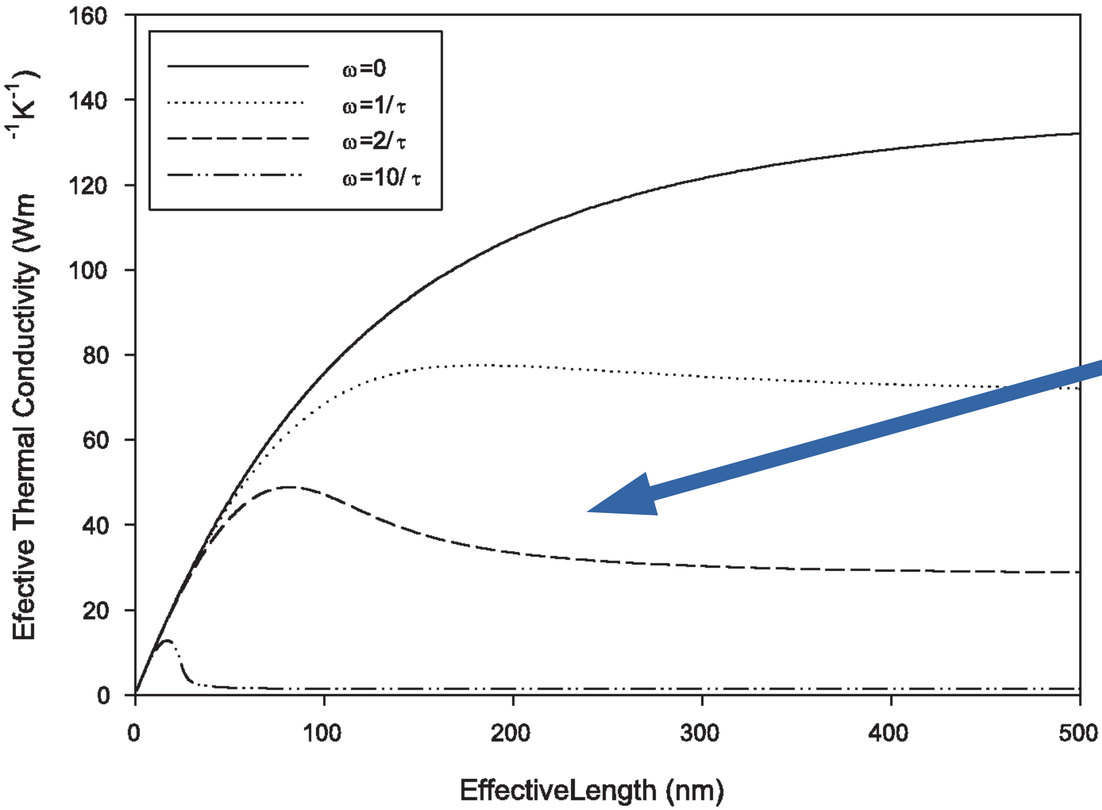
Minnich et al, PRL 107, 095901 (2011)

The reduction is due to the inhomogeneous heating in combination with the laplacian term. No boundaries

$$l^2 \nabla^2 q$$

Memory effects

$$\lambda = \lambda_0 \frac{-(1+i\omega\tau)+\sqrt{(1+i\omega\tau)^2+(kl)^2}}{1/2(kl)^2}$$



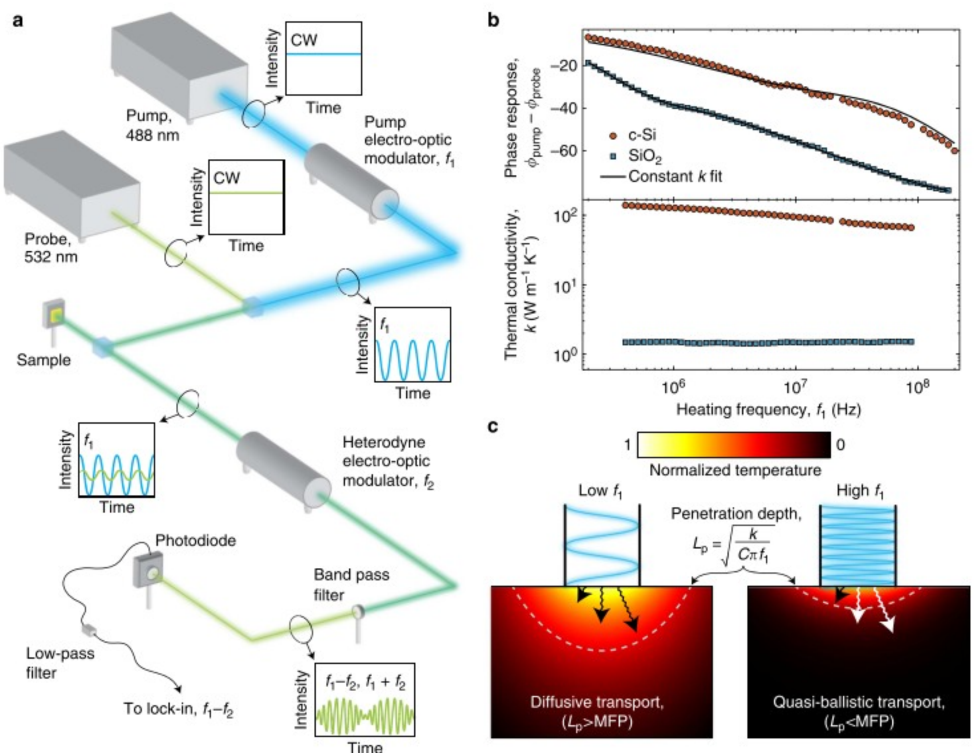
Memory also changes the effective thermal conductivity.

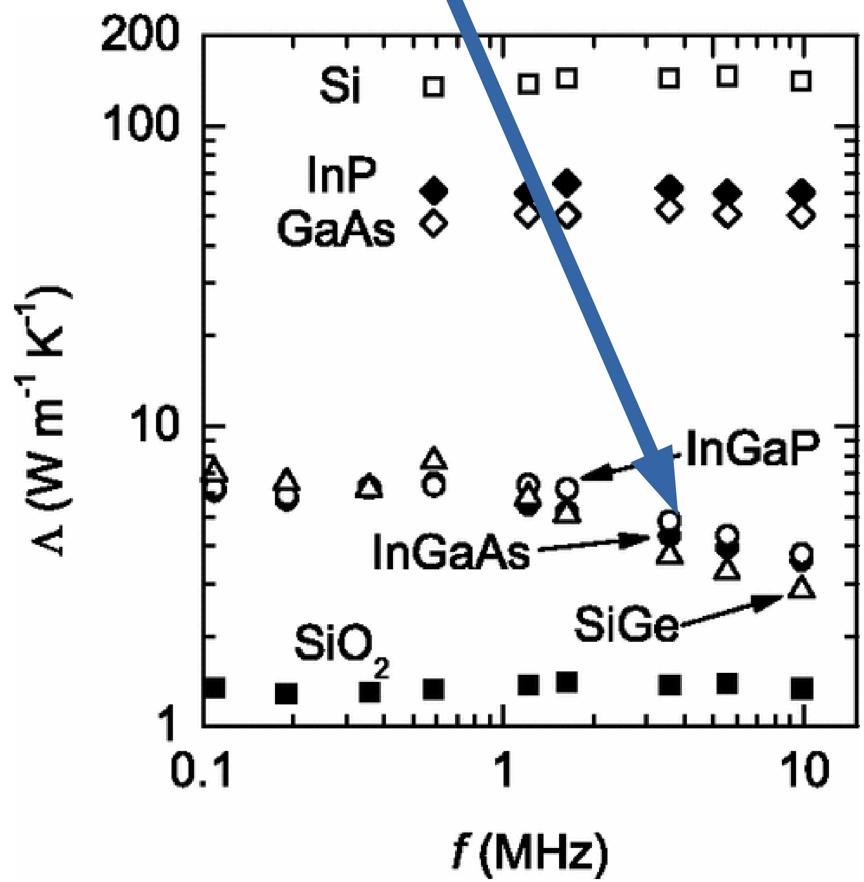
Higher excitation frequencies give smaller thermal conductivities

Alvarez and Jou, JAP 103, 94321 (2008).

Application to TDTR experiments

Experimental evidence of the reduction of the effective thermal conductivity with excitation frequency





Regner et al, Nat. Comm. 4, 1640 (2013)
Koh and Cahill, PRB, 76, 075207 (2007)

Take Home Idea

Fourier law can be extended by including memory and nonlocal effects

The number of terms needed depend on how far we are from local equilibrium

Phonon Hydrodynamic Equations

Phonon hydrodynamic equation

Guyer-Krumhansl equation

$$\tau \dot{q} + q = -\lambda \nabla T + l^2 \left(\nabla^2 q + 2 \nabla \nabla \cdot q \right)$$

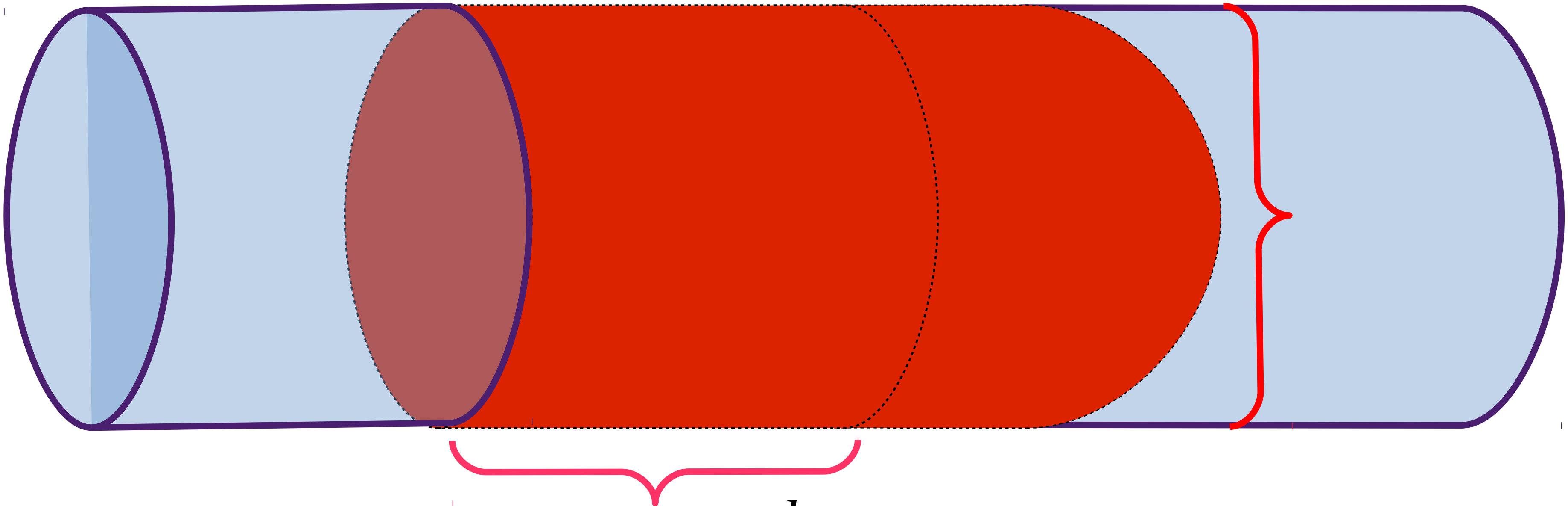
Similarities between GK and NS equations

$l^2 \left(\nabla^2 q + 2 \nabla \nabla \cdot q \right)$ **Acts as a friction term**

Navier-Stokes equation

$$\dot{v} = -\frac{1}{\rho} \nabla p + \left(\nu \nabla^2 v + \frac{\nu}{3} \nabla \left(\nabla \cdot v \right) \right)$$

Boundaries



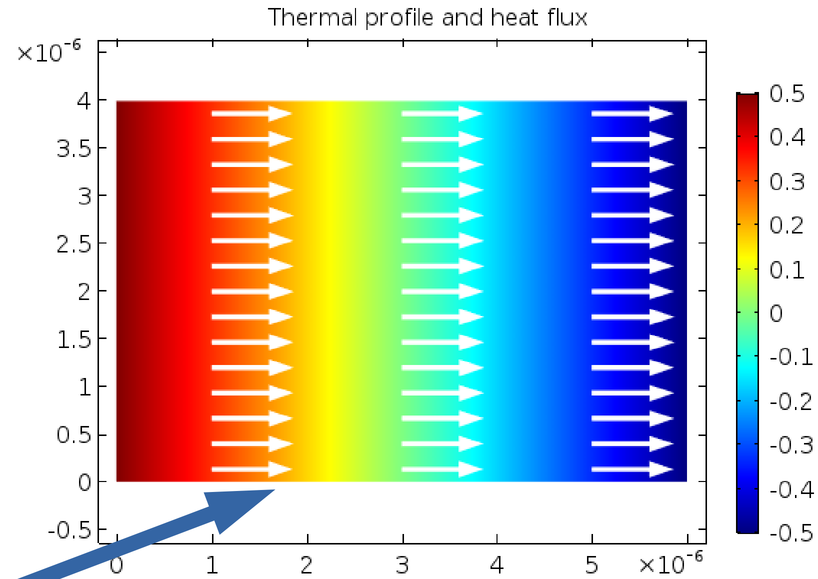
$$q_b = -C\, l \frac{dq}{dr}$$

GK equation should be combined with the proper boundary conditions to obtain a solution

Alvarez, Jou and Sellitto, JAP 105, 14317 (2009).
Sellitto, Alvarez and Jou, JAP 107, 114312 (2010).
Alvarez, Jou and Sellitto, J. Heat Transfer 133, 22402 (2011).

Specularity

$$q_b = -C\, l \frac{dq}{dr} \qquad C = \frac{2-\sigma}{\sigma}$$

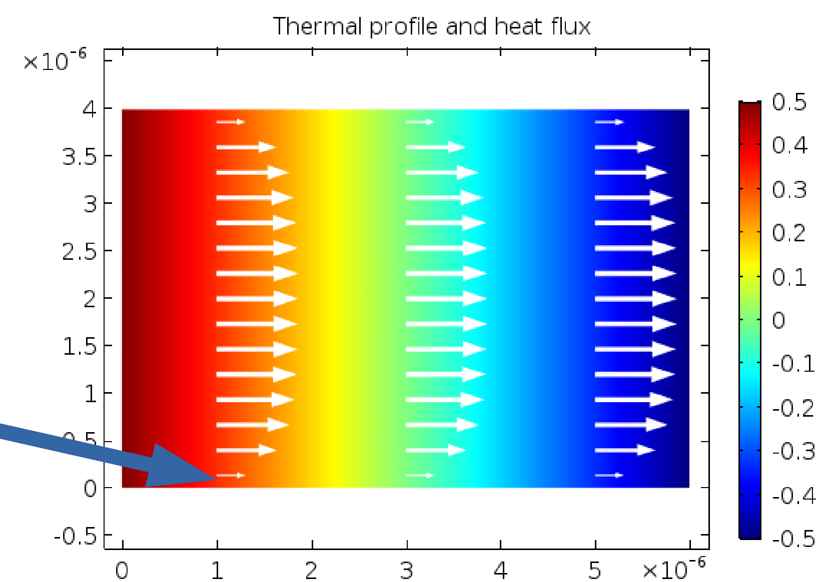


For specular boundary:

$$\sigma \rightarrow 0 ; C \rightarrow \infty$$

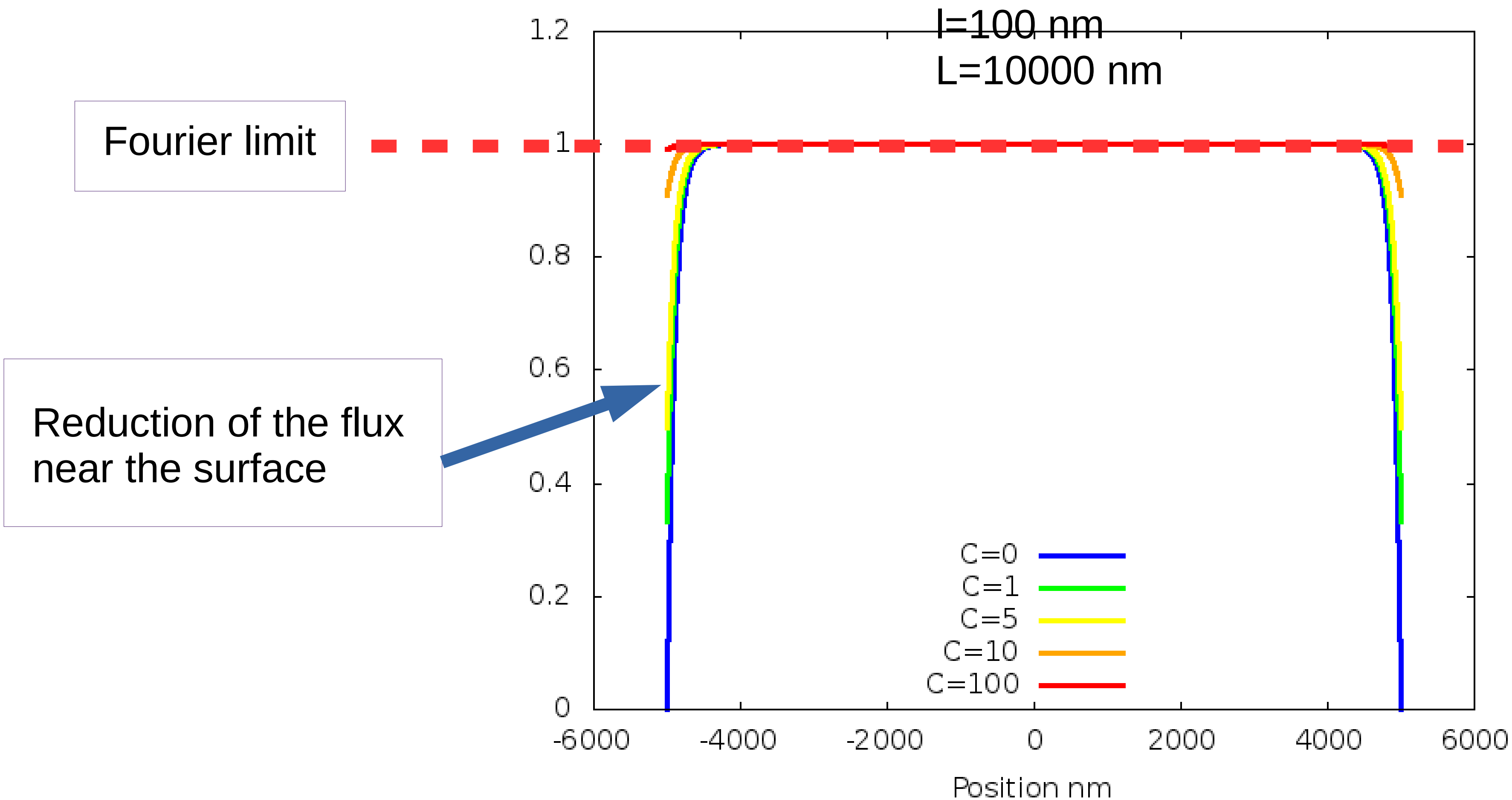
For diffuse boundary:

$$\sigma \rightarrow 1 ; C \rightarrow 1$$



Boundary effect L>>l

$$\lambda_{eff} = \frac{\int q(r)\, dA}{A \nabla T}$$



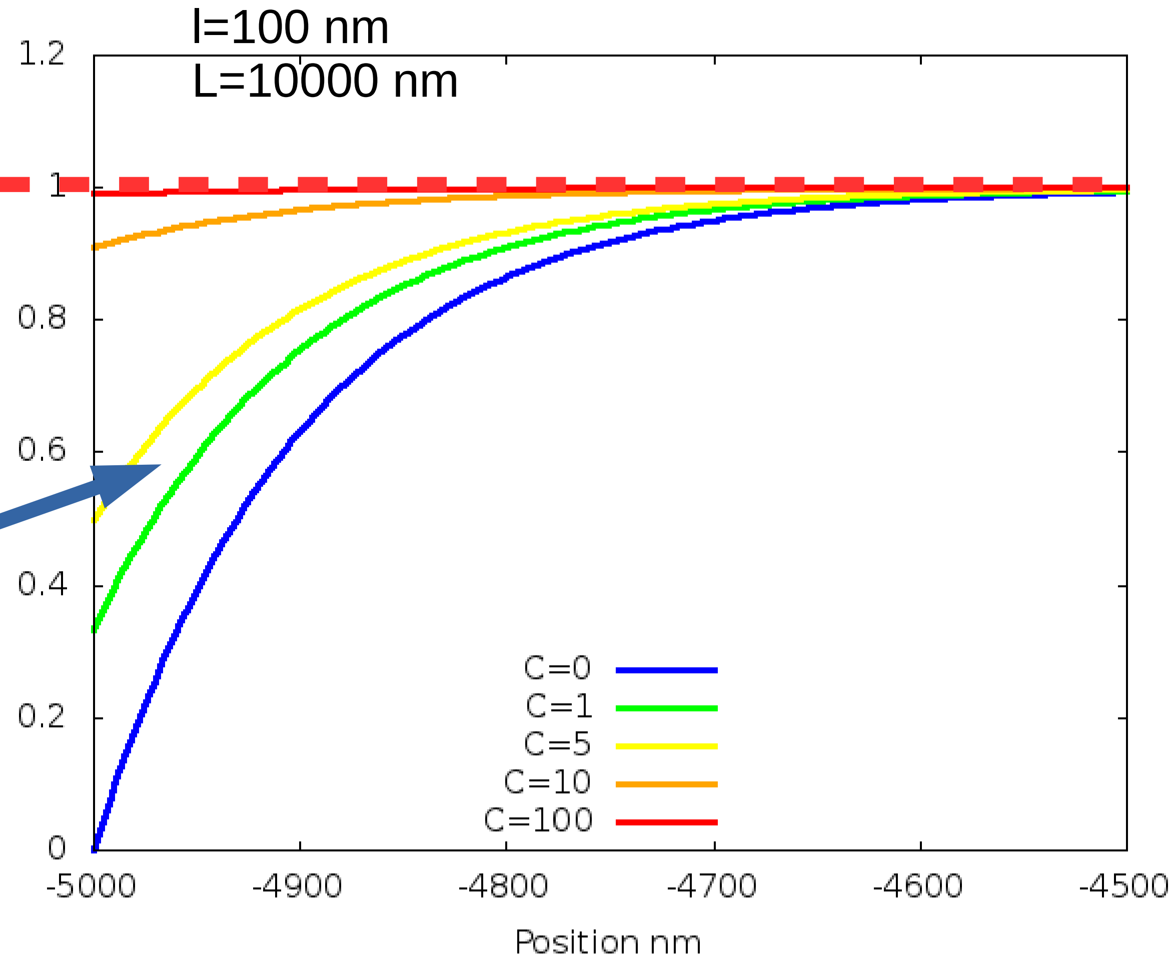
In the limit of small Knudsen number the obtained profile is very similar to a Fourier profile with a reduction near the surface

Boundary effect L>>l

$$\lambda_{eff} = \frac{\int q(r)\, dA}{A \nabla T}$$

Fourier limit

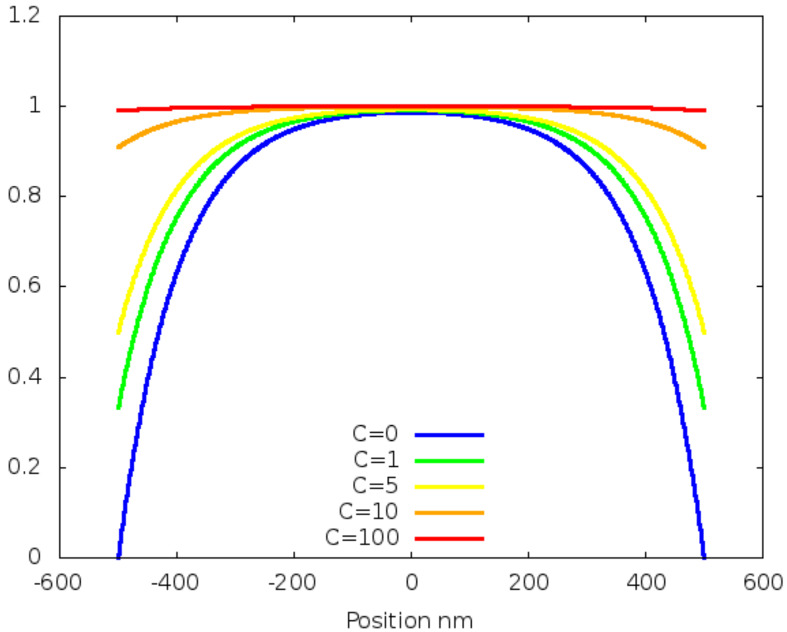
Reduction of the flux near the surface



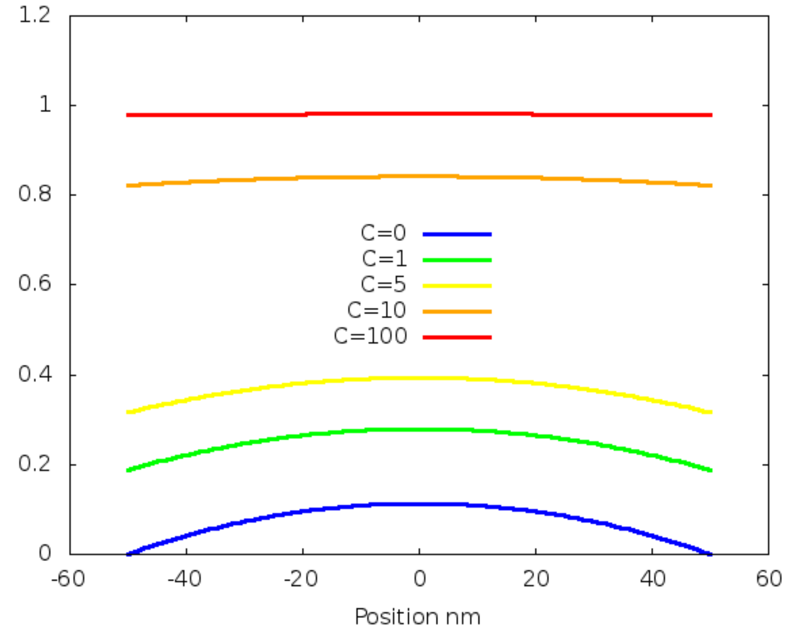
Boundary effect L~l

$$\lambda_{eff} = \frac{\int q(r)\, dA}{A \nabla T}$$

l=100 nm
L=1000 nm



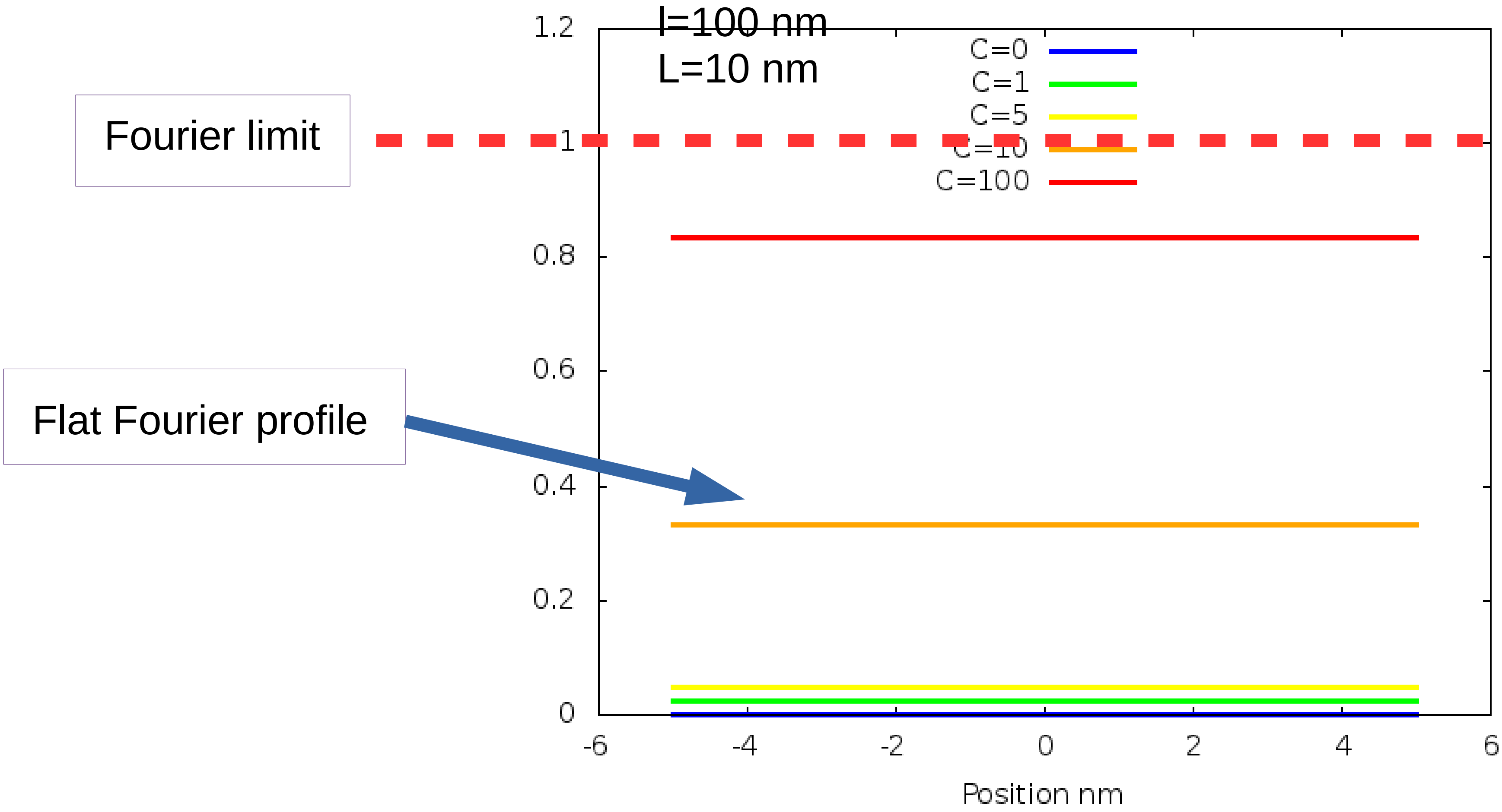
l=100 nm
L=100 nm



If the Knudsen number increases, the reduction is noticed in a larger region of the wire

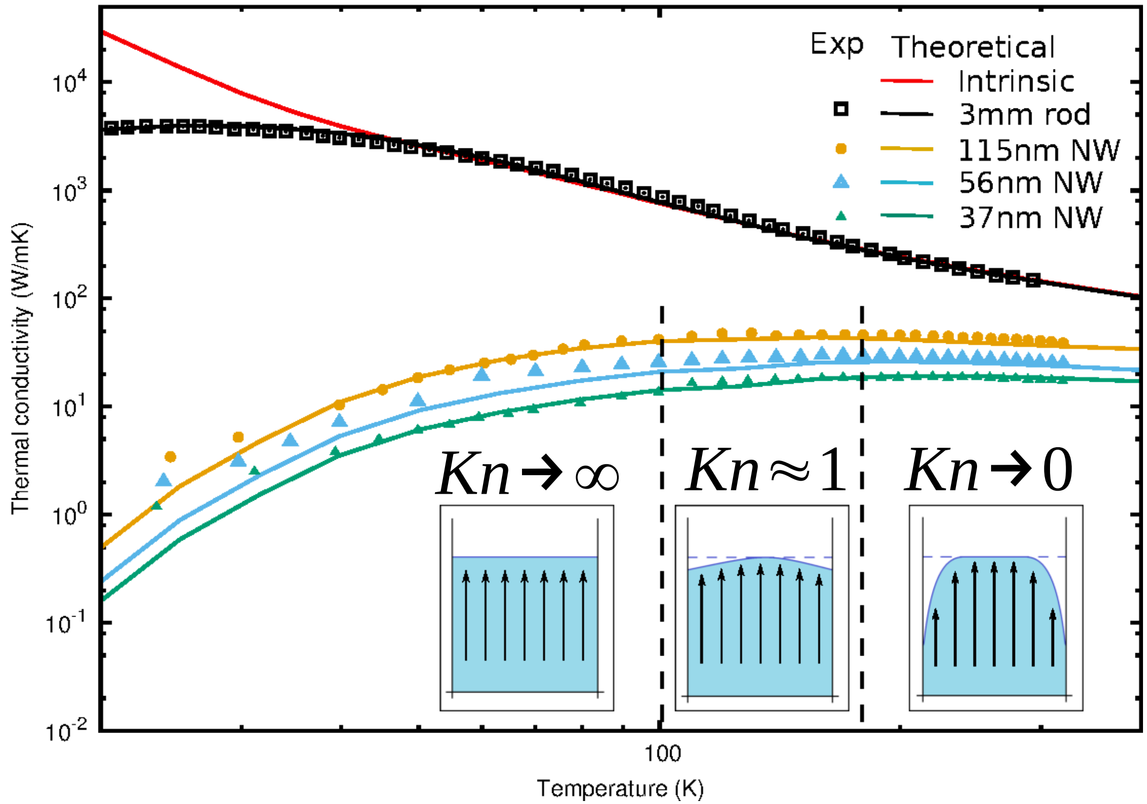
Boundary effect L<<l

$$\lambda_{eff} = \frac{\int q(r)\, dA}{A \nabla T}$$



In the limit of high Knudsen number the obtained profile is very similar to an effective Fourier profile

Predictions for nanowires



$$Kn = \frac{l}{L}$$

Hydrodynamic model allows a description of nanoscale simple geometries

Take Home Idea

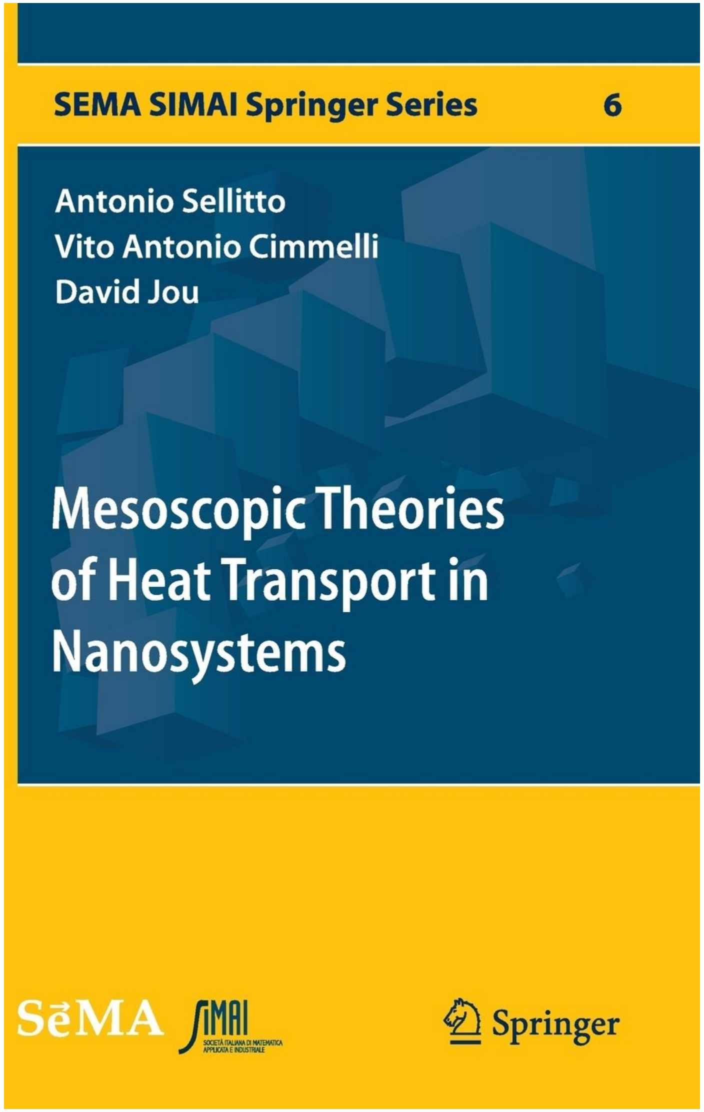
The hydrodynamic equation gives a simple picture of the reduction of heat transport

Boundary conditions are key to understand reduced size samples

In hydrodynamic models the way to incorporate this is through the slip flow condition

Hydrodynamic model

Alvarez, Jou and Sellitto, JAP 105, 14317 (2009).
Sellitto, Alvarez and Jou, JAP 107, 114312 (2010).
Alvarez, Jou and Sellitto, J. Heat Transfer 133, 22402 (2011).

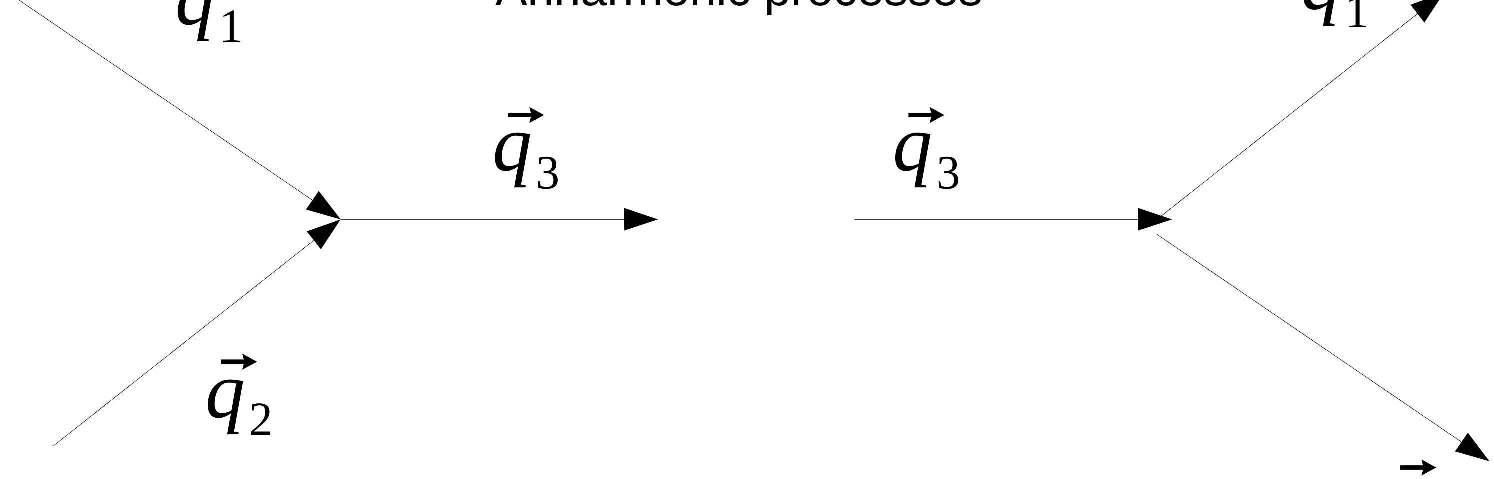


Exact Solutions of the BTE

Anharmonic effects in collision term

$$\left(\frac{\partial}{\partial t} + v\cdot\nabla\right) f = \left(\frac{\partial f}{\partial t}\right)_{col}$$

Anharmonic processes



$$\left(\frac{\partial f}{\partial t}\right)_{col} = \iint f_{\vec{q}_1} f_{\vec{q}_2}\left(f_{\vec{q}_3}+1\right)\Gamma^{\vec{q}_3}_{\vec{q}_1\vec{q}_2} - \left(f_{\vec{q}_1}+1\right)\left(f_{\vec{q}_2}+1\right) f_{\vec{q}_3}\Gamma^{\vec{q}_1\vec{q}_2}_{\vec{q}_3}\, d\vec{q}_2\, d\vec{q}_3$$

f is a nonequilibrium function depending on q

Boltzmann equation is generally nonlinea

Relaxation time approximation (RTA)

$$\left(\frac{\partial f}{\partial t}\right)_{col} = \iint \left(\Phi_{\vec{q}_1} + \Phi_{\vec{q}_2} - \Phi_{\vec{q}_3}\right) P_{\vec{q}_1 \vec{q}_2}^{\vec{q}_3} \, d\vec{q}_2 \, d\vec{q}_3$$

$$D_{\vec{q}} f_{\vec{q}} = \sum_{\vec{q}\,'} C_{\vec{q},\vec{q}\,'} f_{\vec{q}\,'}$$

Linearized collision term

Diagonal in q

Nondiagonal in q

$$\left(\frac{\partial f}{\partial t}\right)_{col} = \iint \Phi_{\vec{q}_1} P_{\vec{q}_1 \vec{q}_2}^{\vec{q}_3} \, d\vec{q}_2 \, d\vec{q}_3 \qquad \Phi_{\vec{q}_1} \neq 0 \qquad \Phi_{\vec{q}_2} = 0 \qquad \Phi_{\vec{q}_3} = 0$$

$$D_{\vec{q}} f_{\vec{q}} = C_{\vec{q}} f_{\vec{q}\,'}$$

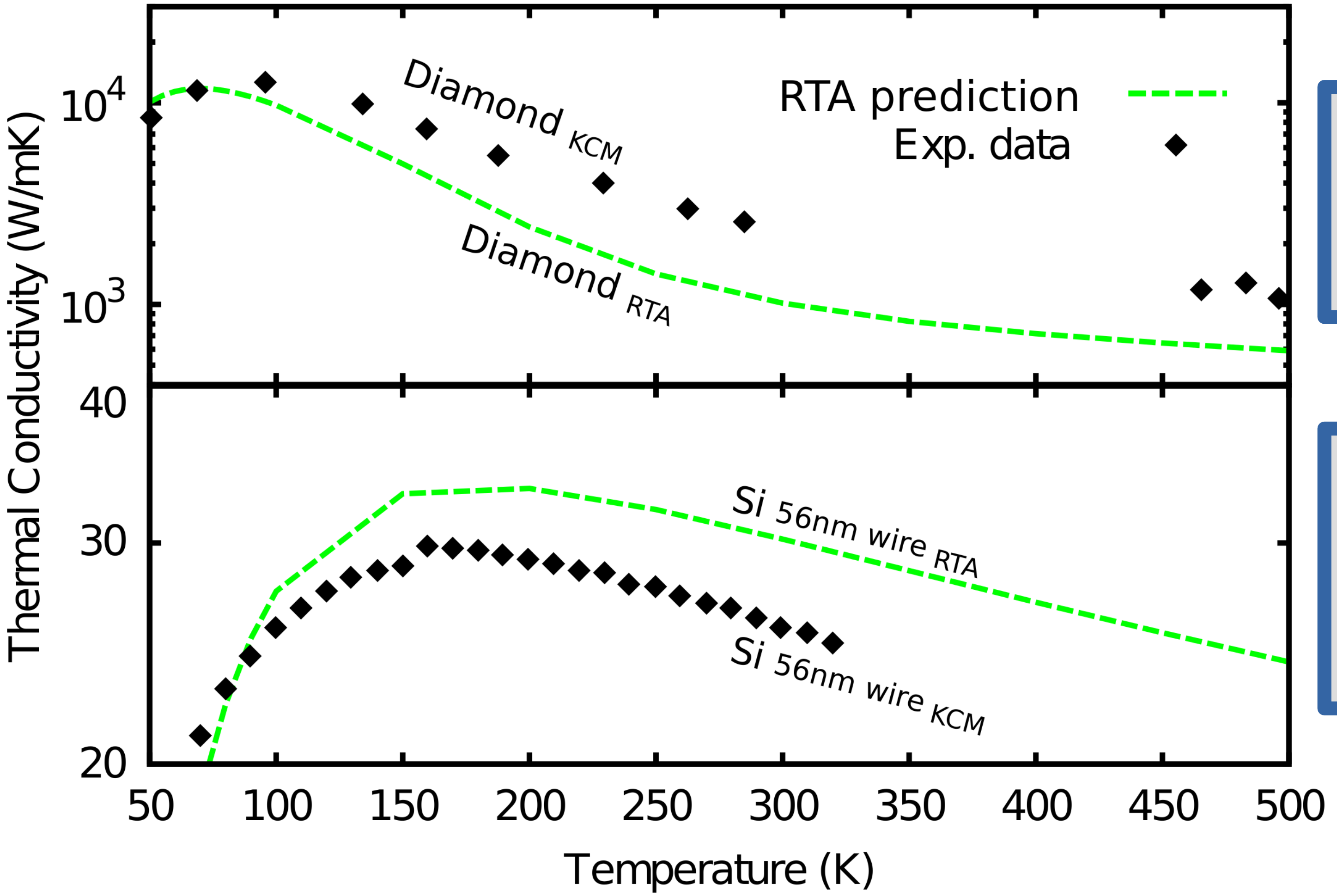
RTA collision term

Diagonal in q

Diagonal in q

$$\frac{\partial f}{\partial t} + v \cdot \nabla f_{\vec{q}} = \frac{f_{\vec{q}} - f_{\vec{q}0}}{\tau_{\vec{q}}}$$

Failures of RTA

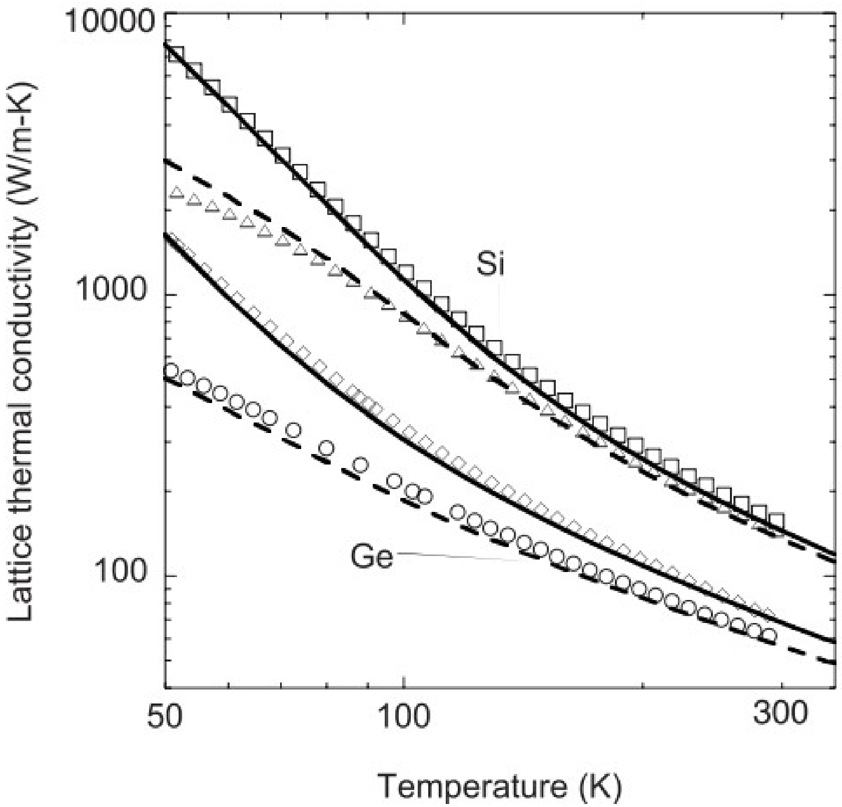


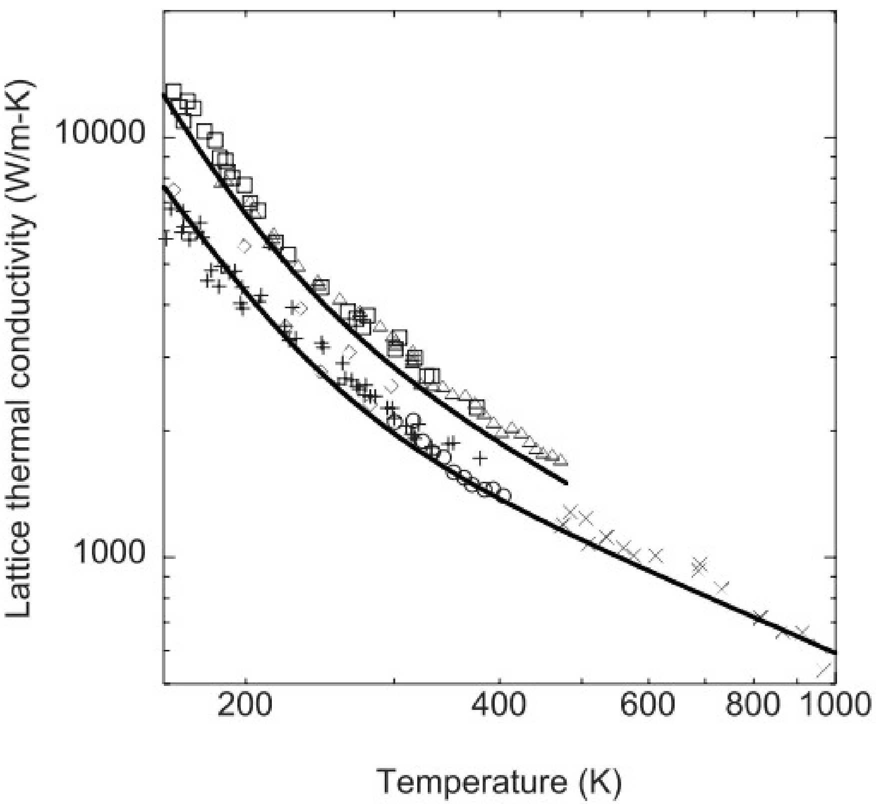
Materials where normal scattering is important

Samples where boundary scattering is important

Iterative BTE (IBTE)

$$f_{q(\vec{i}+1)} = f_{\vec{q}i} + \tau_{\vec{q}i}\left(\frac{\partial}{\partial t} + v\nabla\right) f_{\vec{q}i}$$

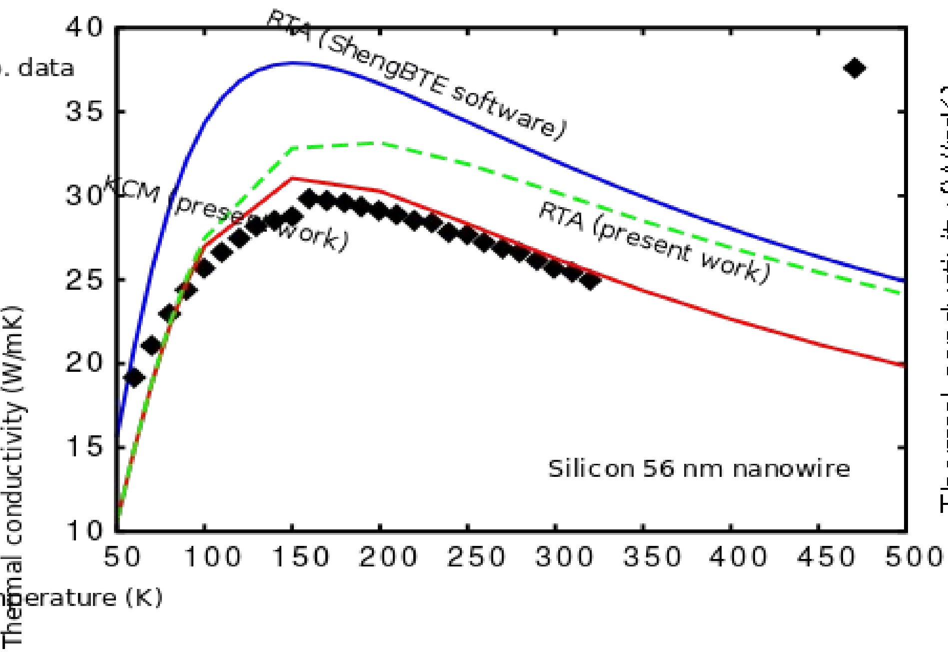


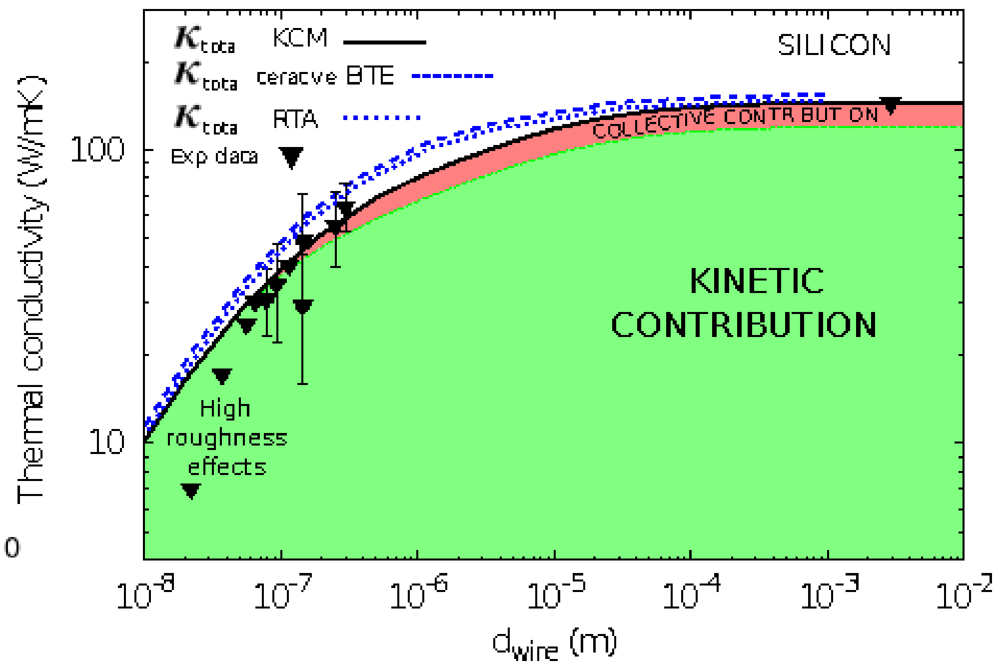


Significant improvement for bulk materials

Ward et al. PRB **80**, 125203 (2009)

Iterative BTE (IBTE)





Li et al. PRB **85**, 195436 (2012)

Linearized BTE – Relaxons. R-LBTE

$$D_{\vec q} f_{\vec q} = \sum_{\vec q'} C_{\vec q, \vec q'} f_{\vec q'}$$

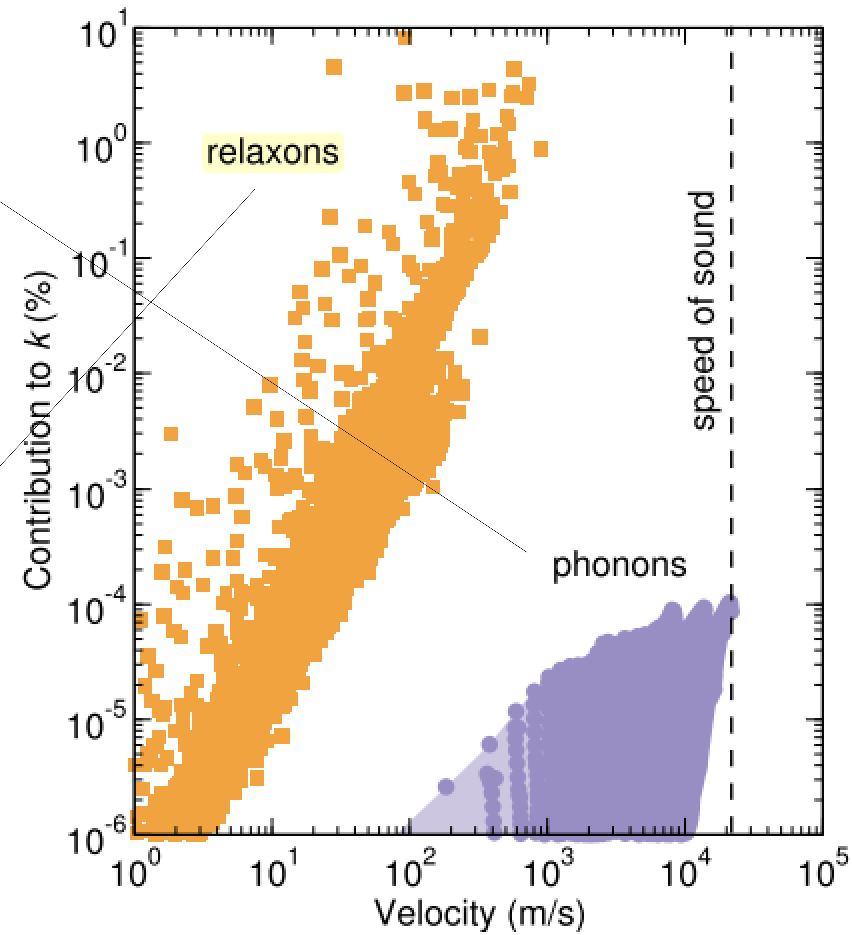
$$\vec k = \sum_{\vec q'} A_{\vec q \vec q'} \vec q'$$

$$\sum_{\vec k'} D_{\vec k \vec k'} f_{\vec k} = C_{\vec k} f_{\vec k'}$$

Non-diagonal in k

Diagonal in k

Cepellotti and Marzari , PRX, 6(4), 41013 (2016)



In steady state it can be solved because D simplifies

Objective

Can we find a solution of the BTE that simplifies the collision term without complicate in excess the drift term?

Kinetic Collective Model

Guyer-Krumhansl

$$\frac{\partial f}{\partial t} + v \cdot \nabla f = \left(\frac{\partial f}{\partial t} \right)_{col}$$

Split the collision term in two: R/N

Momentum basis

Diagonalizes Normal scattering

$$D f = \left(R + N \right) f$$

$$\begin{pmatrix} D_{00} & D_{01} & 0 \\ D_{10} & D_{11} & D_{12} \\ 0 & D_{21} & D_{22} \end{pmatrix} \begin{pmatrix} a_0 \\ a_1 \\ a_2 \end{pmatrix} = \left(\begin{pmatrix} 0 & 0 & 0 \\ 0 & R_{11} & R_{12} \\ 0 & R_{21} & R_{22} \end{pmatrix} + \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & N_{22} \end{pmatrix} \right) \begin{pmatrix} a_0 \\ a_1 \\ a_2 \end{pmatrix}$$

Guyer-Krumhansl

For a bulk homogeneous system in steady state

$$a_1 = \left(R_{11} + R_{12}\left(R_{22} + N_{22}\right)^{-1} R_{21}\right)^{-1} D_{10}\, a_0$$

$$\vec{q} = -\kappa \nabla T$$

Kinetic Regime $N_{22} = 0$

$$a_1 = \left(R_{11} + R_{12} R_{22}^{-1} R_{21}\right)^{-1} D_{10}\, a_0$$

$$\left(R^{-1}\right)_{11} D_{10}\, a_0 = a_1$$

$$\vec{q} = -\kappa_{kin} \nabla T$$

Collective Regme $N_{22} = \infty$

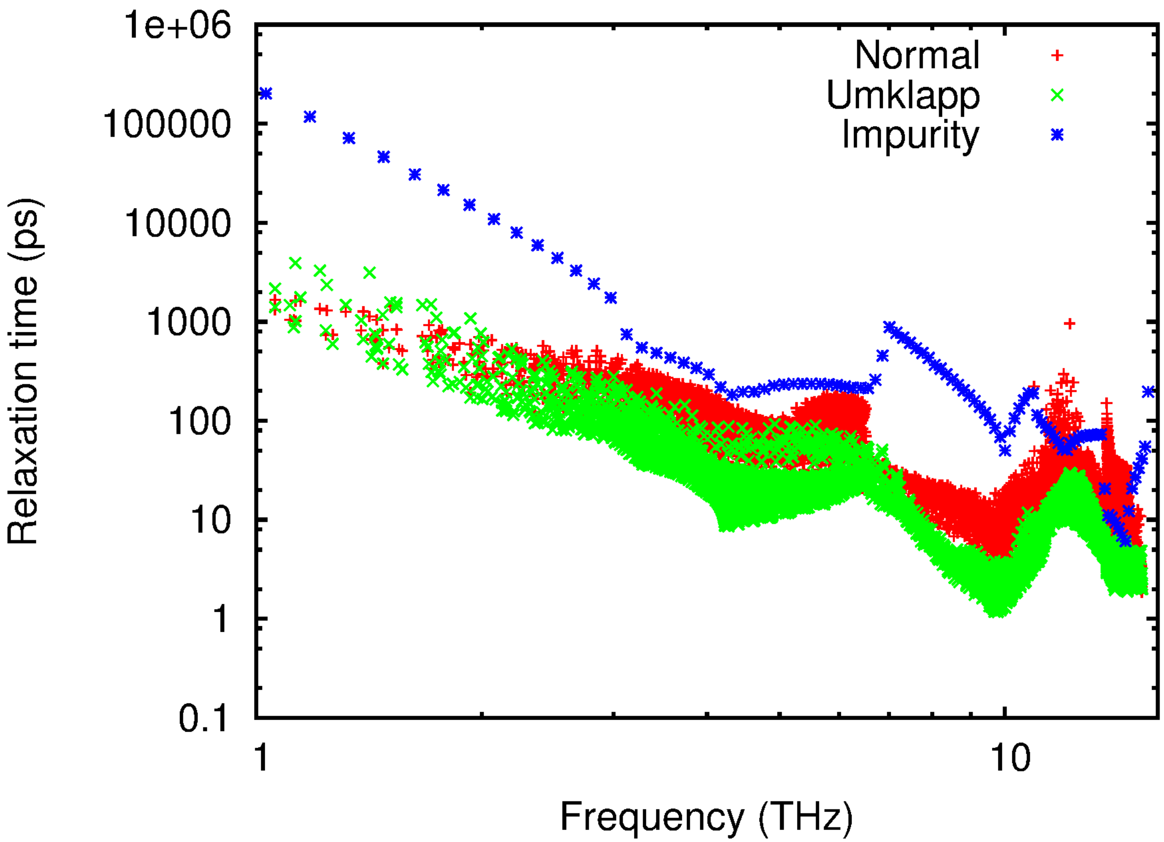
$$a_1 = R_{11}^{-1} D_{10}\, a_0$$

$$D_{10}\, a_0 = R_{11}\, a_1$$

$$\vec{q} = -\kappa_{col} \nabla T$$

Relaxation times

Relaxation times from ab-initio calculations



Scattering Rates

Non-Resistive Normal
Resistive Umklapp Impurity Boundary

Predictions for nanowires

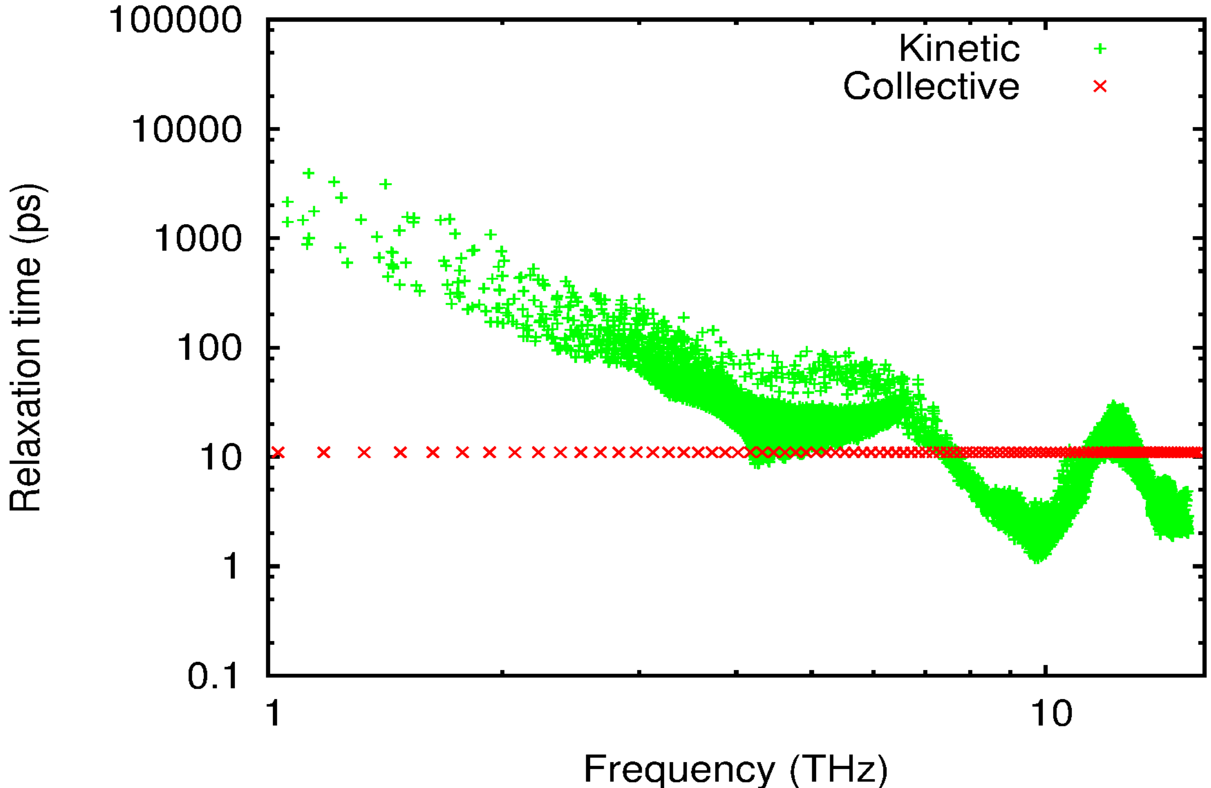
$$\vec{q}_{kin/col} = -\kappa_{kin/col} \nabla T \qquad \kappa_{kin/col} = \int \frac{1}{3} C_v v^2 \tau_{kin/col}$$

Kinetic

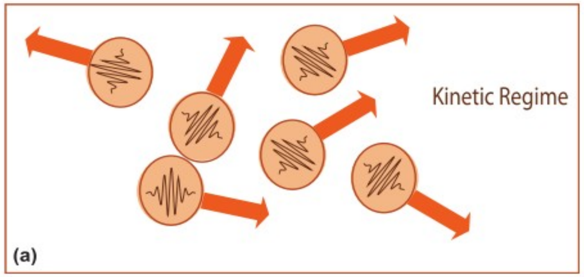
$$\tau_{kin} = \tau_R$$

Collective

$$\tau_{col} = \left\langle \tau_R^{-1} \right\rangle^{-1} = \left(\frac{\int C_v \tau_R^{-1}}{\int C_v} \right)^{-1}$$



Entropic justification. Kinetic Term



$$\dot{s}_{\mathbf{q}}\big|_{\rm scat} = \frac{\Phi_{\mathbf{q}}}{T}\left.\frac{\partial f_{\mathbf{q}}}{\partial t}\right|_{\rm scat}$$

$$\dot{s}_{\mathbf{q}}\big|_{\rm drift} = \frac{\mathbf{j}_{\mathbf{q}}^2}{\kappa_{\mathbf{q}} T^2}$$

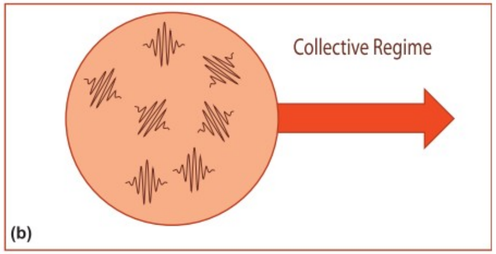
$$\kappa_{\mathbf{q}} = \frac{\mathbf{j}_{\mathbf{q}}^2}{T\Phi_{\mathbf{q}} \left.\frac{\partial f_{\mathbf{q}}}{\partial t}\right|_{\rm scat}}$$

Kinetic thermal conductivity

$$\kappa_{\rm kin} = \frac{1}{3}\int \hbar\omega\tau_\omega v_g^2 \frac{\partial f_\omega^0}{\partial T} D_\omega d\omega$$

De Tomas et al. JAP **115**, 164314 (2014)

Entropic justification. Collective Term



$$\dot{s}_{\text{tot}}\big|_{\text{scat}} = \int \frac{\Phi_{\mathbf{q}}}{T} \frac{\partial f_{\mathbf{q}}}{\partial t}\bigg|_{\text{scat}} d\mathbf{q}$$

$$\dot{s}_{\text{tot}}\big|_{\text{drift}} = \frac{\left[\int \hbar\omega_{\mathbf{q}} \mathbf{v}_g f_{\mathbf{q}}^0 (f_{\mathbf{q}}^0 + 1) \frac{\Phi_{\mathbf{q}}}{k_B T} d\mathbf{q}\right]^2}{\kappa T^2}$$

$$\kappa_{\text{coll}} = \frac{\left[\int \hbar\omega_{\mathbf{q}} \mathbf{v}_g f_{\mathbf{q}}^0 (f_{\mathbf{q}}^0 + 1) \frac{\Phi_{\mathbf{q}}}{k_B T} d\mathbf{q}\right]^2}{T^2 \int \frac{\Phi_{\mathbf{q}}}{T} \frac{\partial f_{\mathbf{q}}}{\partial t}\Big|_{\text{scat}} d\mathbf{q}}$$

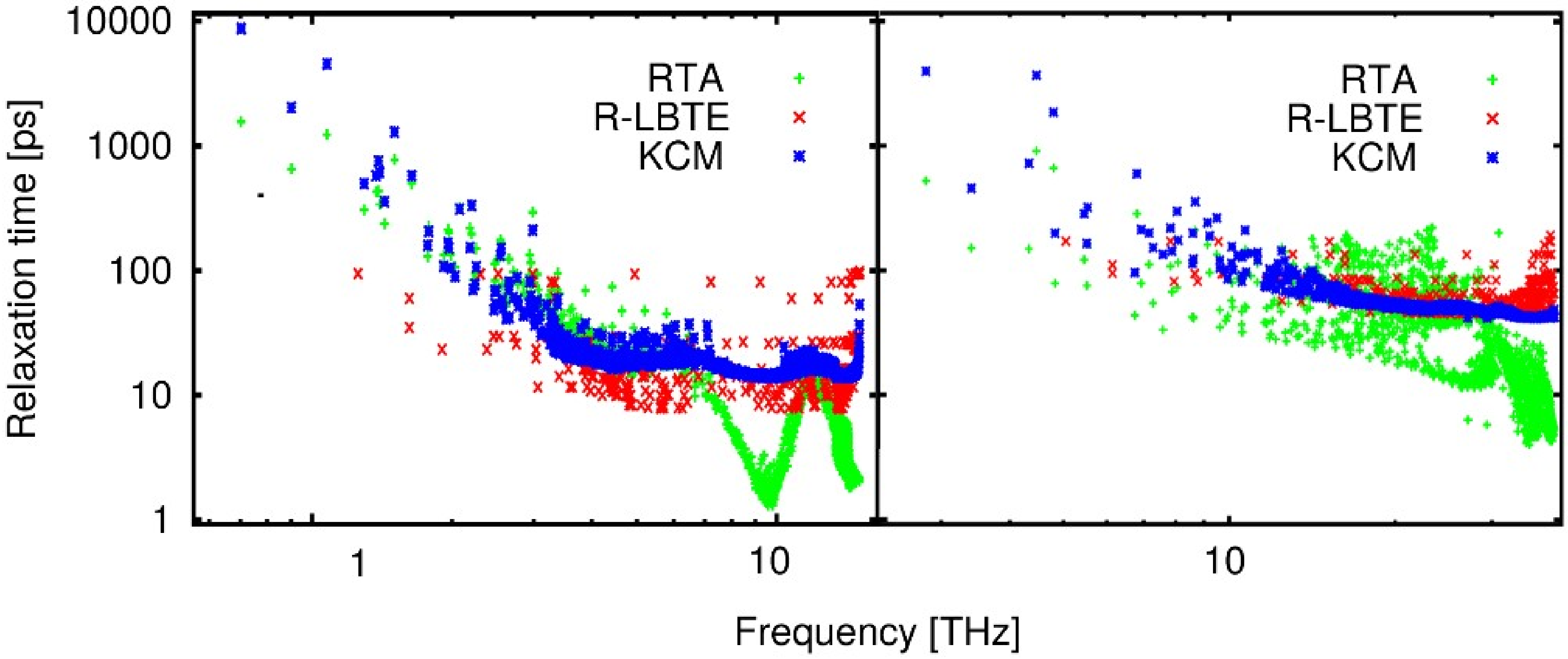
Collective thermal conductivity

$$\kappa_{\text{coll}} = \frac{1}{3} \frac{\left(\int v_g q_\omega \frac{\partial f_\omega^0}{\partial T} D_\omega d\omega\right)^2}{\int \frac{q_\omega^2}{\hbar\omega} \frac{1}{\tau_\omega} \frac{\partial f_\omega^0}{\partial T} D_\omega d\omega}$$

De Tomas et al. JAP **115**, 164314 (2014)

Predictions for nanowires

KCM captures most o the anharmonic effects through the proper treatment of Normal Scattering



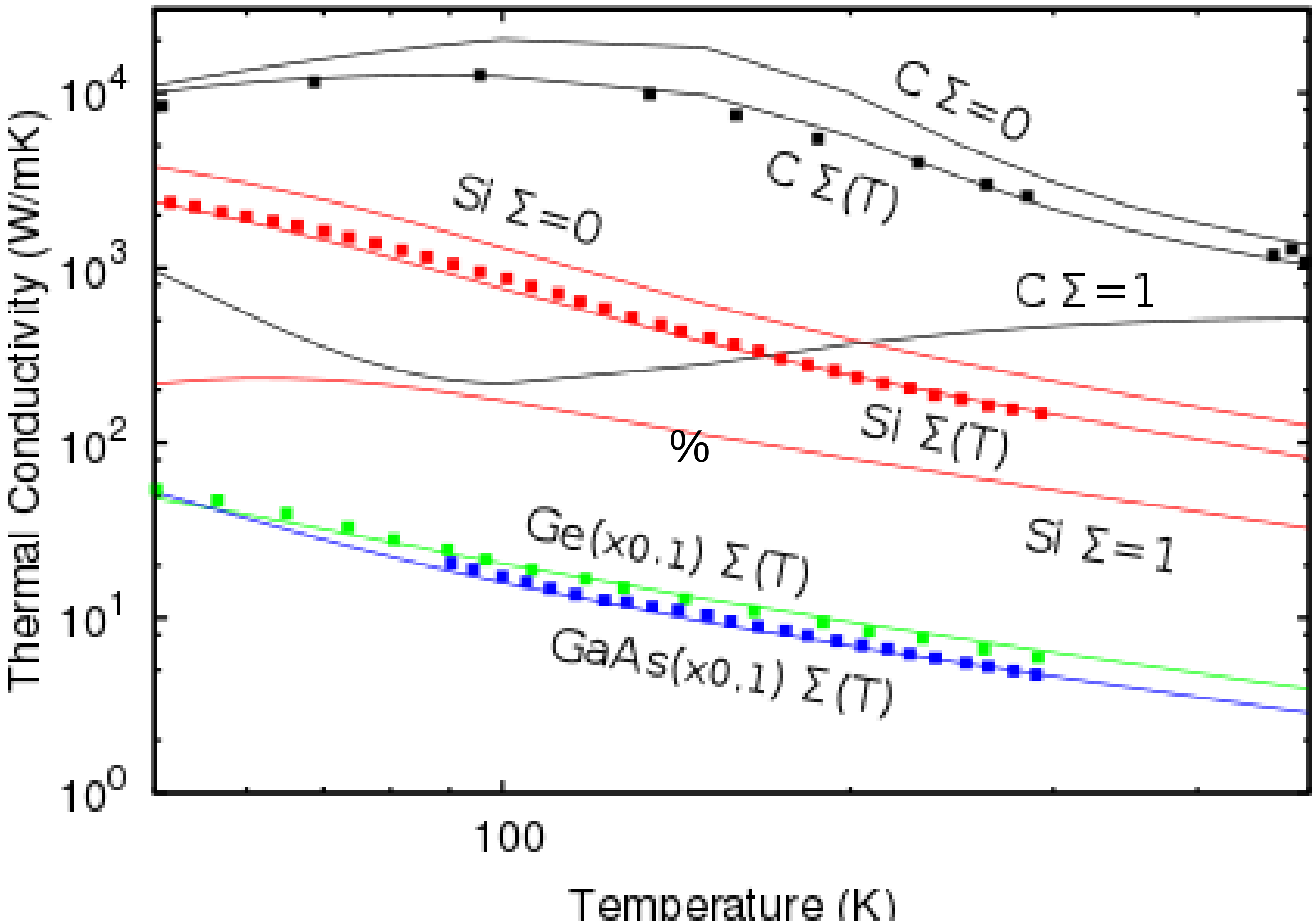
Predictions for bulk

In a general case

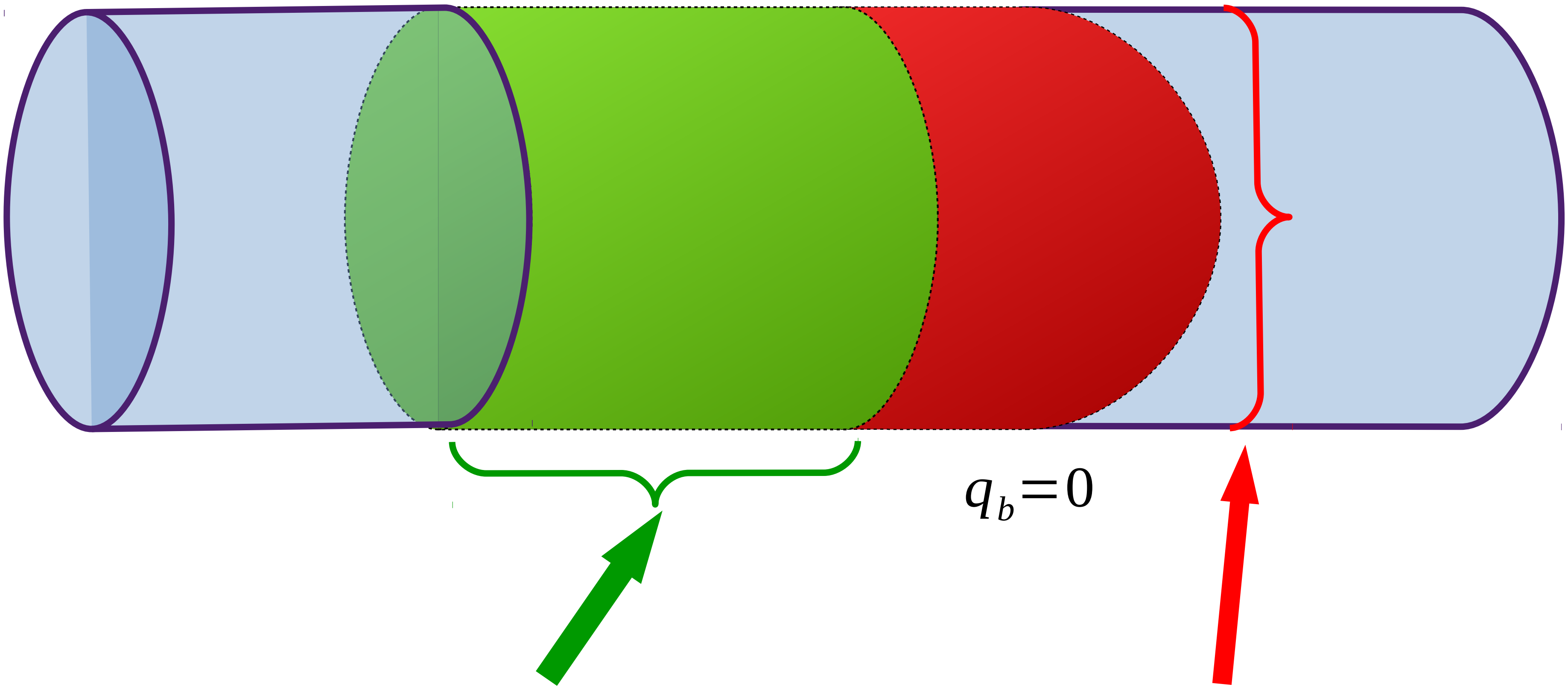
$$\vec{q} = -\left(\left(1-\Sigma\right)\kappa_{kin} + \Sigma\kappa_{col}\right)\nabla T$$

$$\Sigma = \frac{1}{1+\frac{\tau_N}{\tau_{kin}}}$$

Remarkable agreement with bulk data



Predictions for nanowires



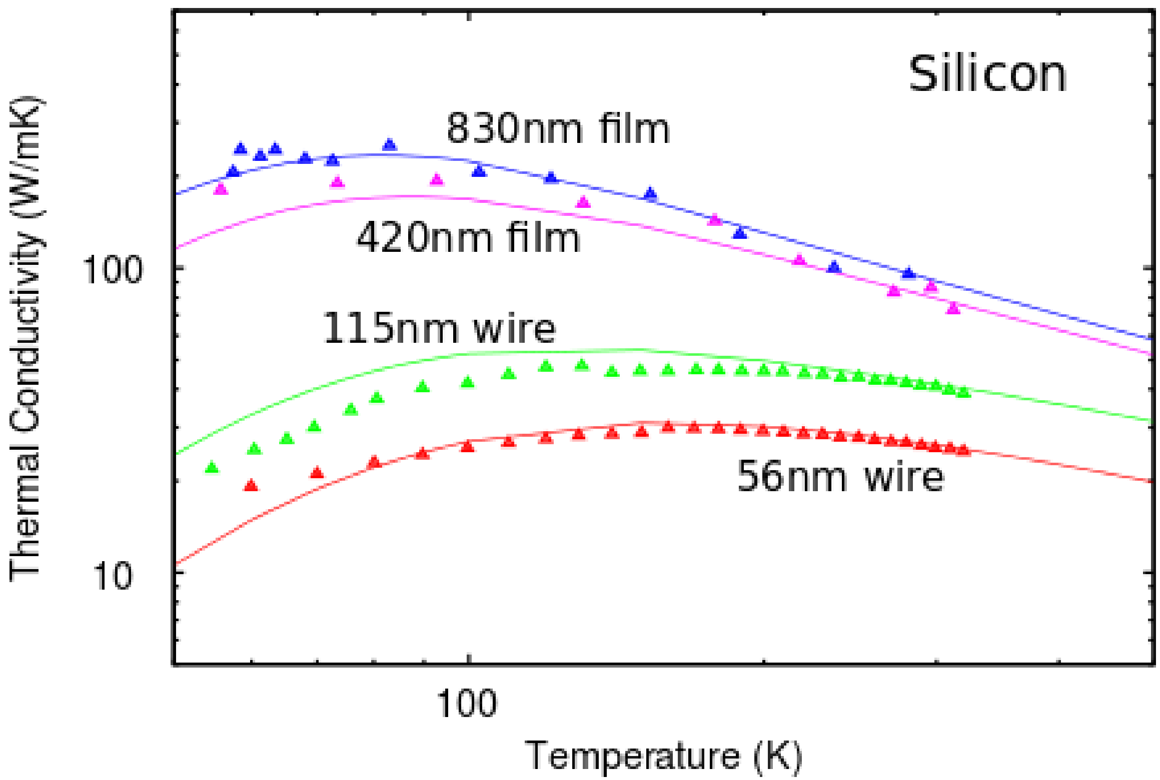
The kinetic contribution is reduced by the combination of the boundary term with the rest of the collisions

$$\frac{1}{\tau}=\frac{1}{\tau_I}+\frac{c}{L}$$

Form factor modulates the profile of the collective contribution

$$\tau\dot{q}+q=-\lambda\nabla T+l^2\left(\nabla^2 q+2\nabla\nabla\cdot q\right)$$

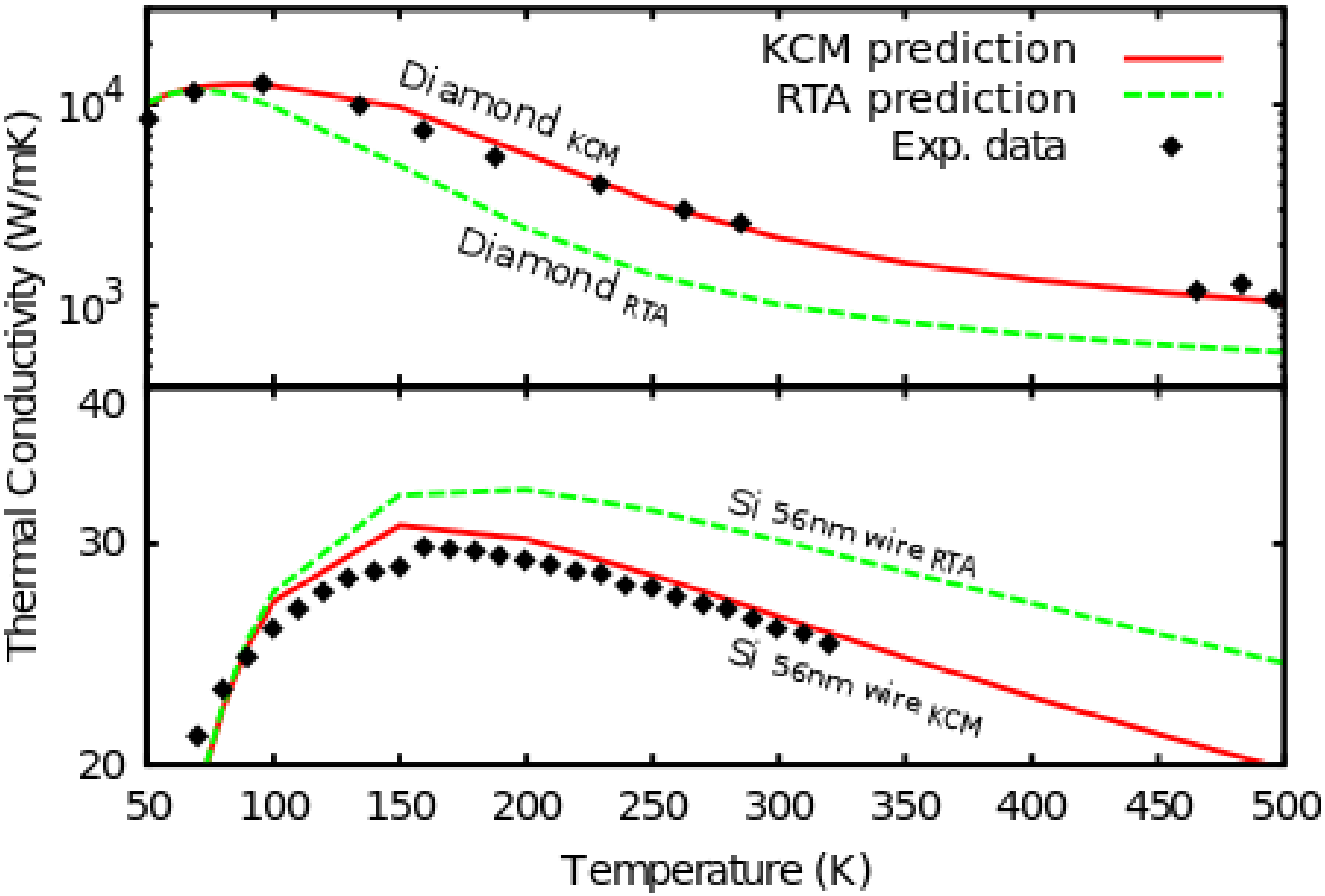
Predictions for nanowires



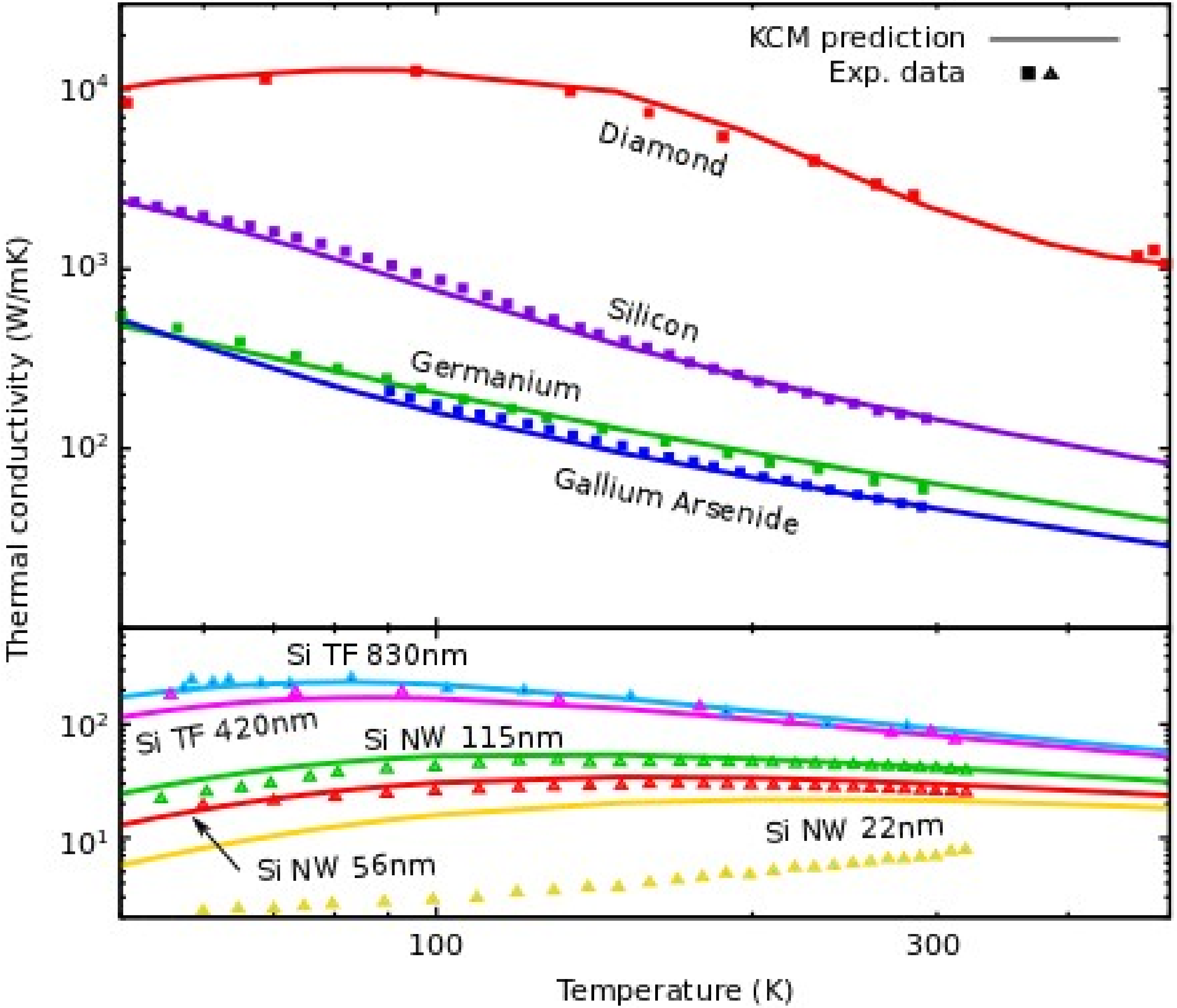
In combination with hydrodynamic model
Good prediction for nanoscale experimental data

Improvements of KCM

The same simplicity as RTA with improved performance



Overview of KCM results



KCM package for phonopy

KINETIC COLLECTIVE MODEL   KCM ▼ USER GUIDE ▼ RESOURCES ▼ NANOTRANSPORT GROUP

Kinetic Collective Model

BTE-based hydrodynamic model for thermal transport

The Kinetic Collective Model (KCM), developed by the nanoTransport group of the Universitat Autònoma de Barcelona, is a generalization of the Guyer and Krumhansl solution of the phonon Boltzmann Transport Equation. KCM allows to compute t conductivity of semiconductors in a fast and low memory way from *first principl* calculations.

The KCM:

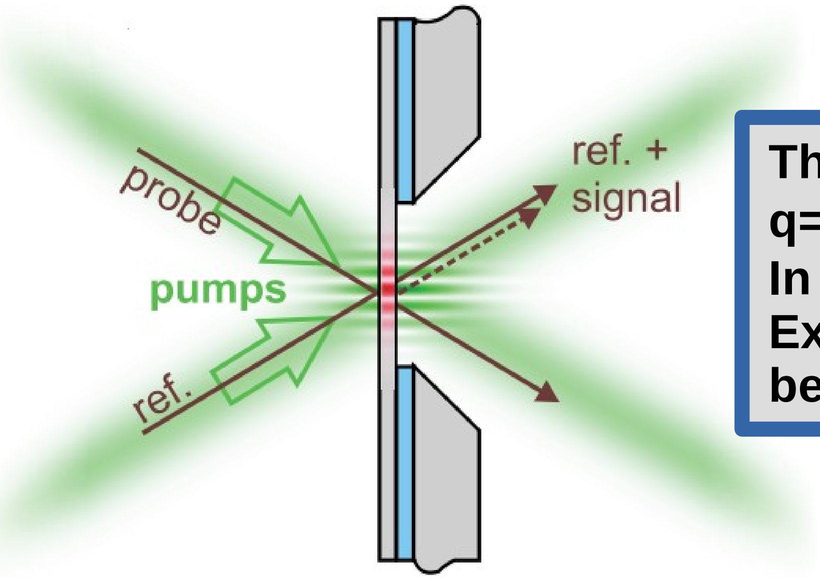
- Properly accounts for the effect of normal scattering processes.
- Uses *first principles* calculations.
- Allows fast calculations of thermal conductivity with low memory and time u
- Defines an hydrodynamic heat flux equation able to be used in finite elemen simulations for thermal calculations in complex geometries (See the hydrod equation in THEORY).

http://physta.github.io

```
KINETIC  COLLECTIVE    MODEL    Version 1.0

-------------------------------

Running calculation of thermal conductivity on a  20x20

Temp[k]  Kappa[W/mK]  Sigma  NL-lenght[nm]

10.0     1971.069     0.011    1012395.247
15.0     3670.769     0.049    512610.045
20.0     4707.944     0.106    278024.104
25.0     5151.292     0.179    159608.791
30.0     5168.565     0.260    97801.267
40.0     4566.568     0.412    44399.319
50.0     3719.696     0.531    24254.132
60.0     2902.404     0.620    14696.933
70.0     2214.747     0.682    9424.408
```

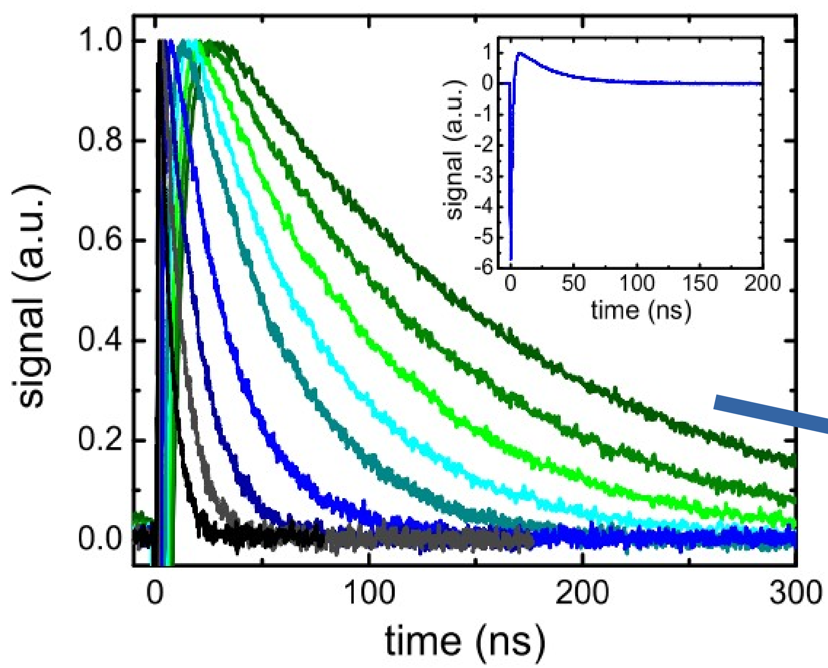
Complex Geometries

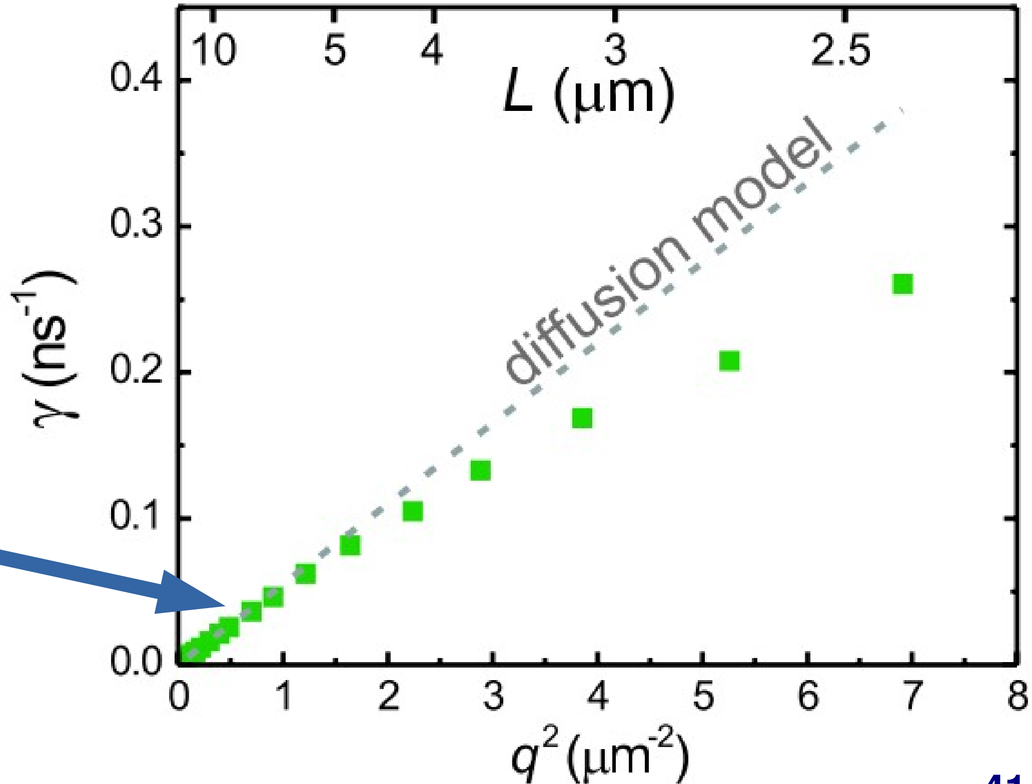
Thermal Grating Experiment



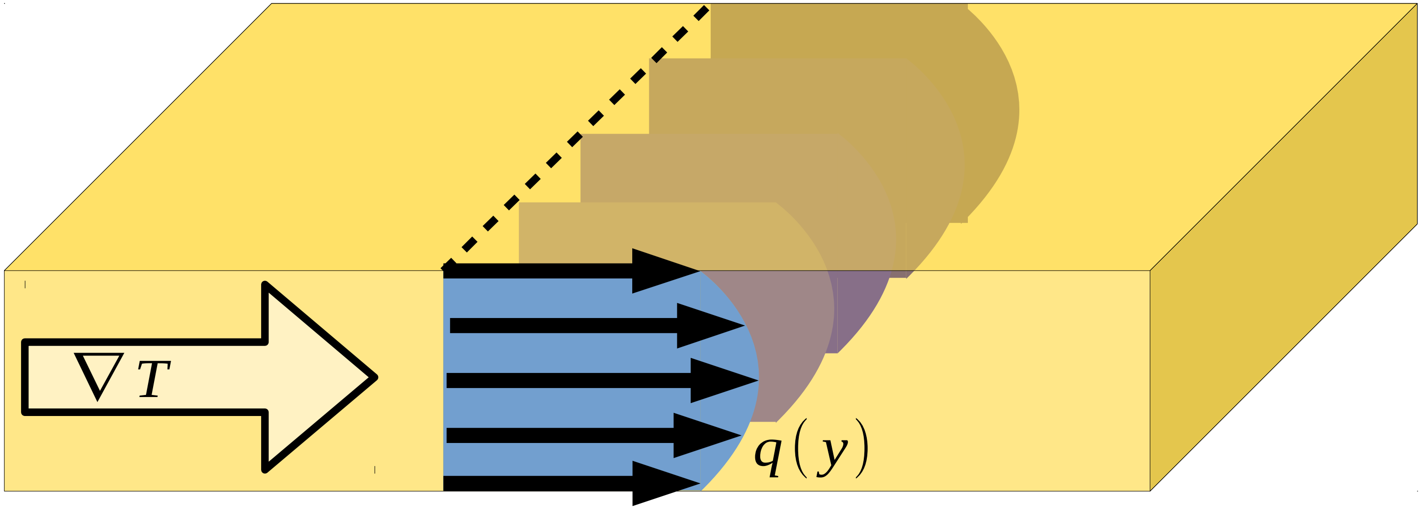
Johnson *et al.* PRL 110, 025901 (2013)

The decay rate depend on the heating wavector $q=2\pi/L$
In Fourier model the dependance is quadratic
Experimental results show nonquadratic behaviour



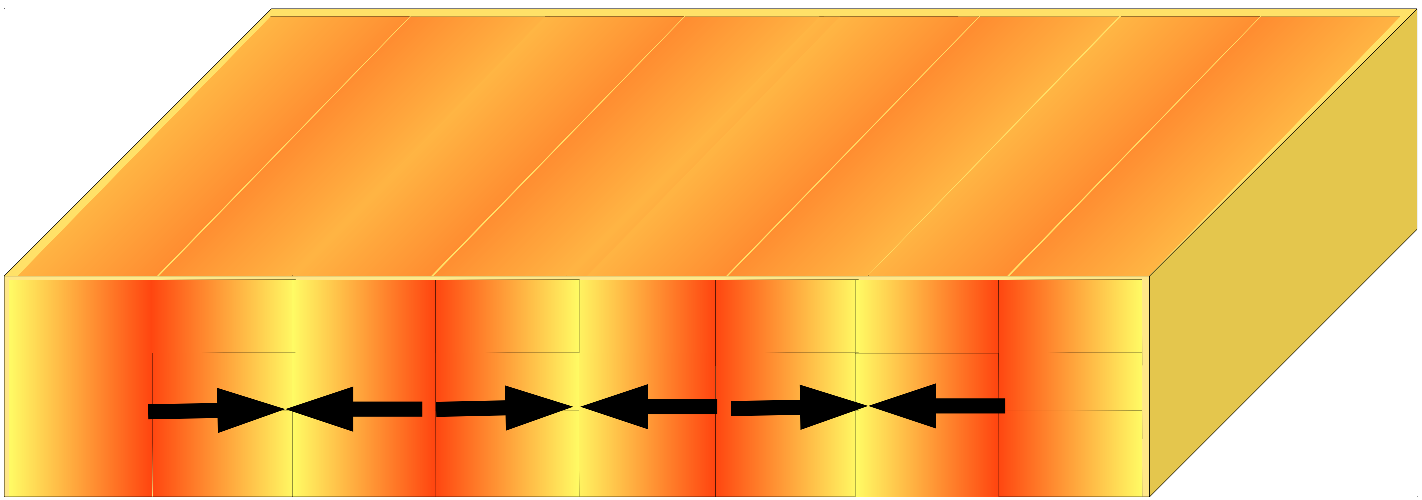


Thermal Grating in the KCM



Nonlocal correction due to boundary effect

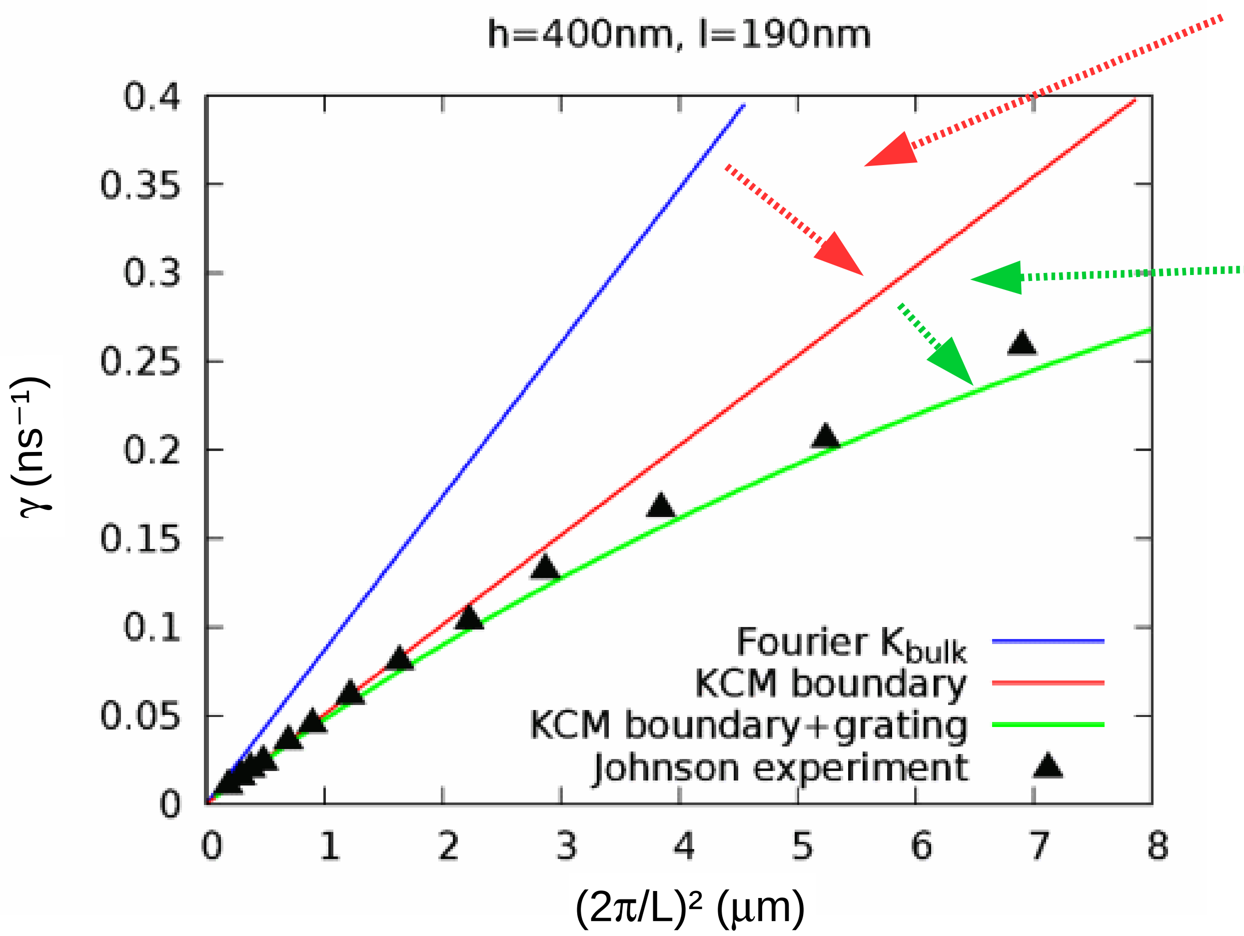
$$q_b = -C\,l\,\frac{dq}{dy}$$

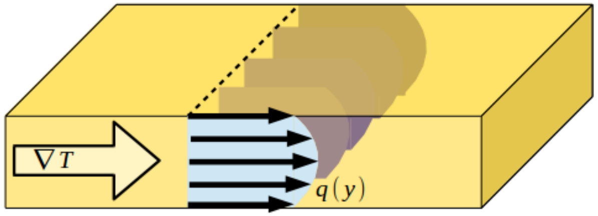


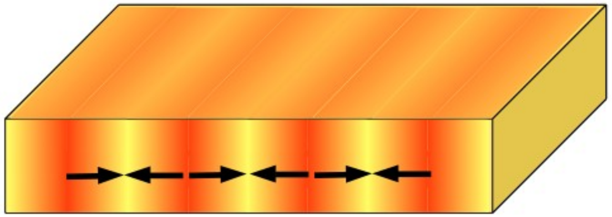
Nonlocal correction due to periodic heating

$$\nabla^2 q(x)$$

Thermal Grating in the KCM



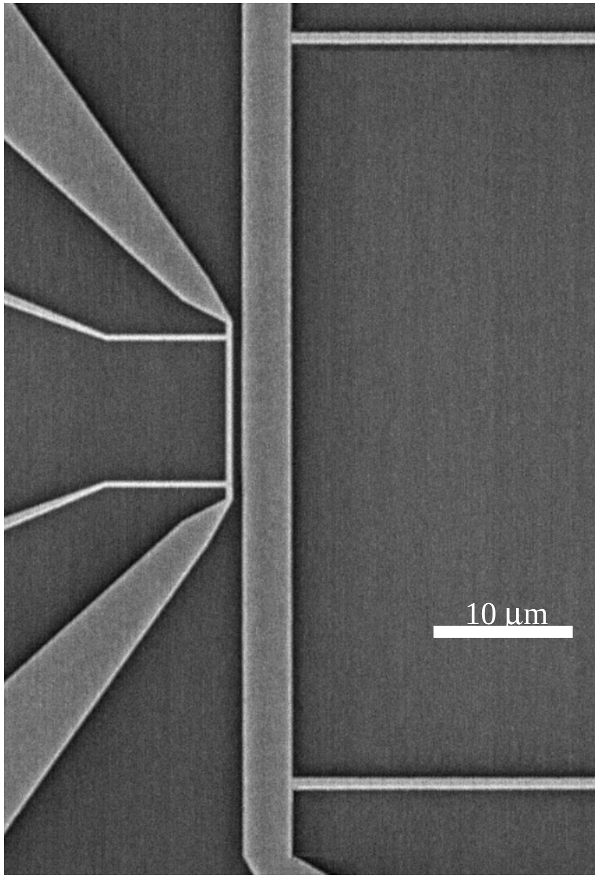


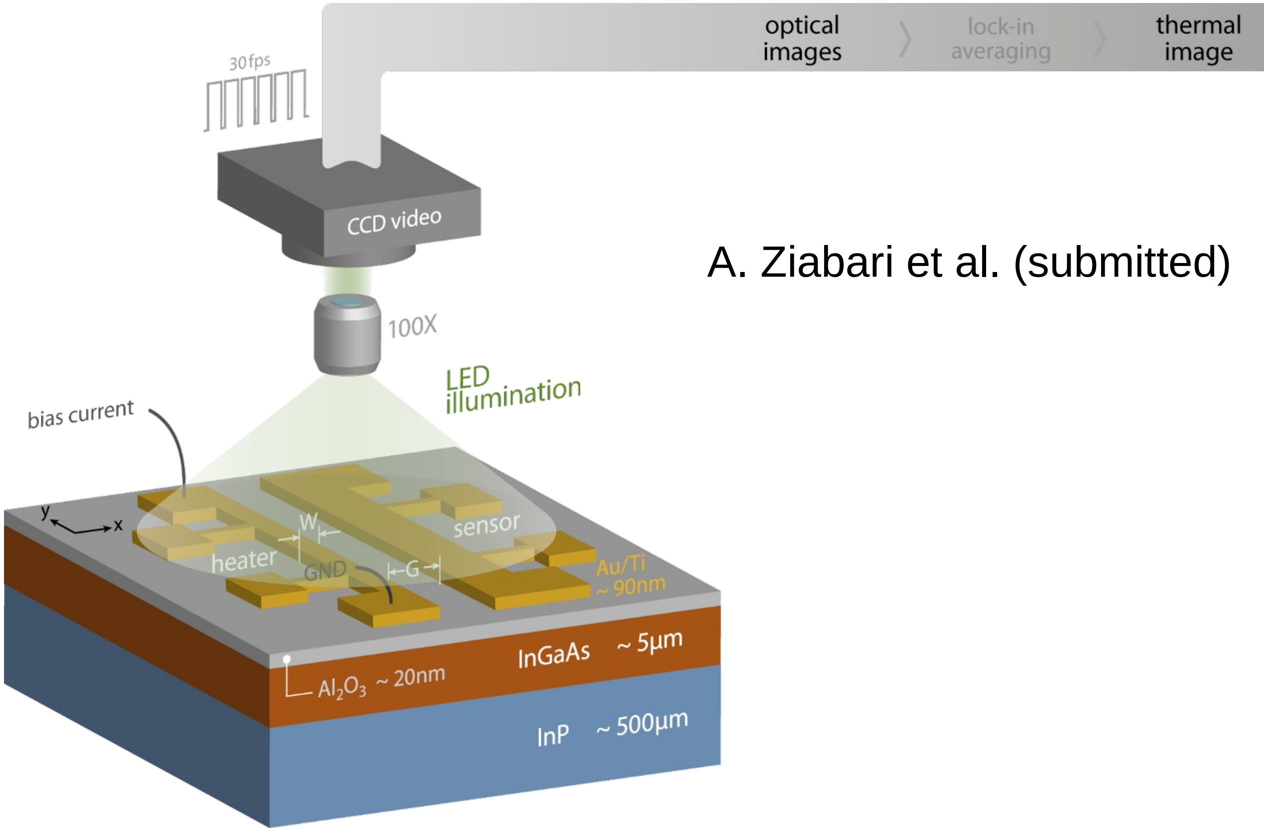


The combination of effects allows to explain the experimental results

Thermo Reflectance Imaging (TRI)

Nano-Heater Lines



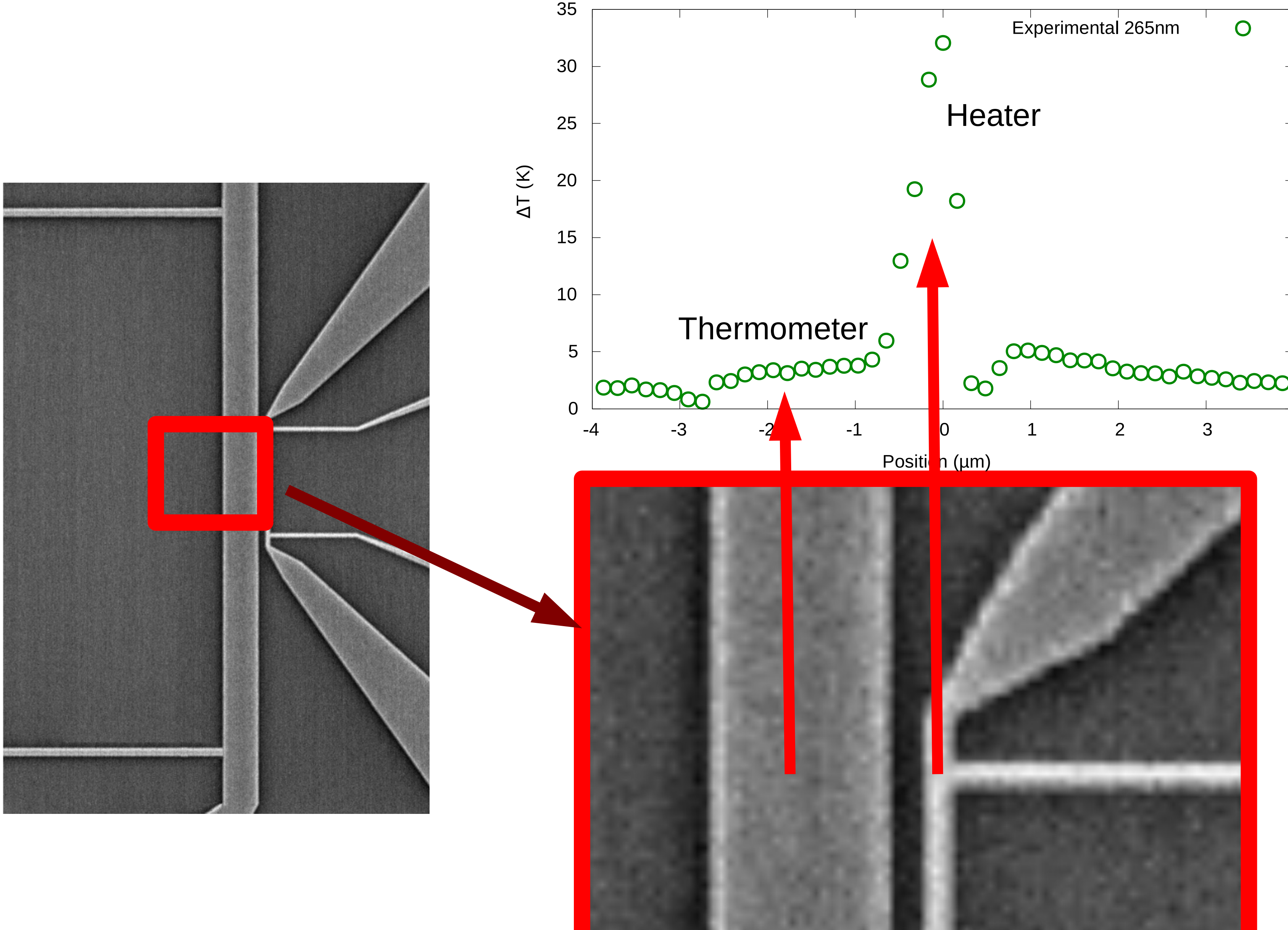


A. Ziabari et al. (submitted)

- ❑ Width: 100nm - 10µm
- ❑ Length/Width ratio = 40
- ❑ Spacing: 0.3, 0.5, and 20µm
- ❑ Both InGaAs and Si were studied
- ❑ Static and Transient TR imaging

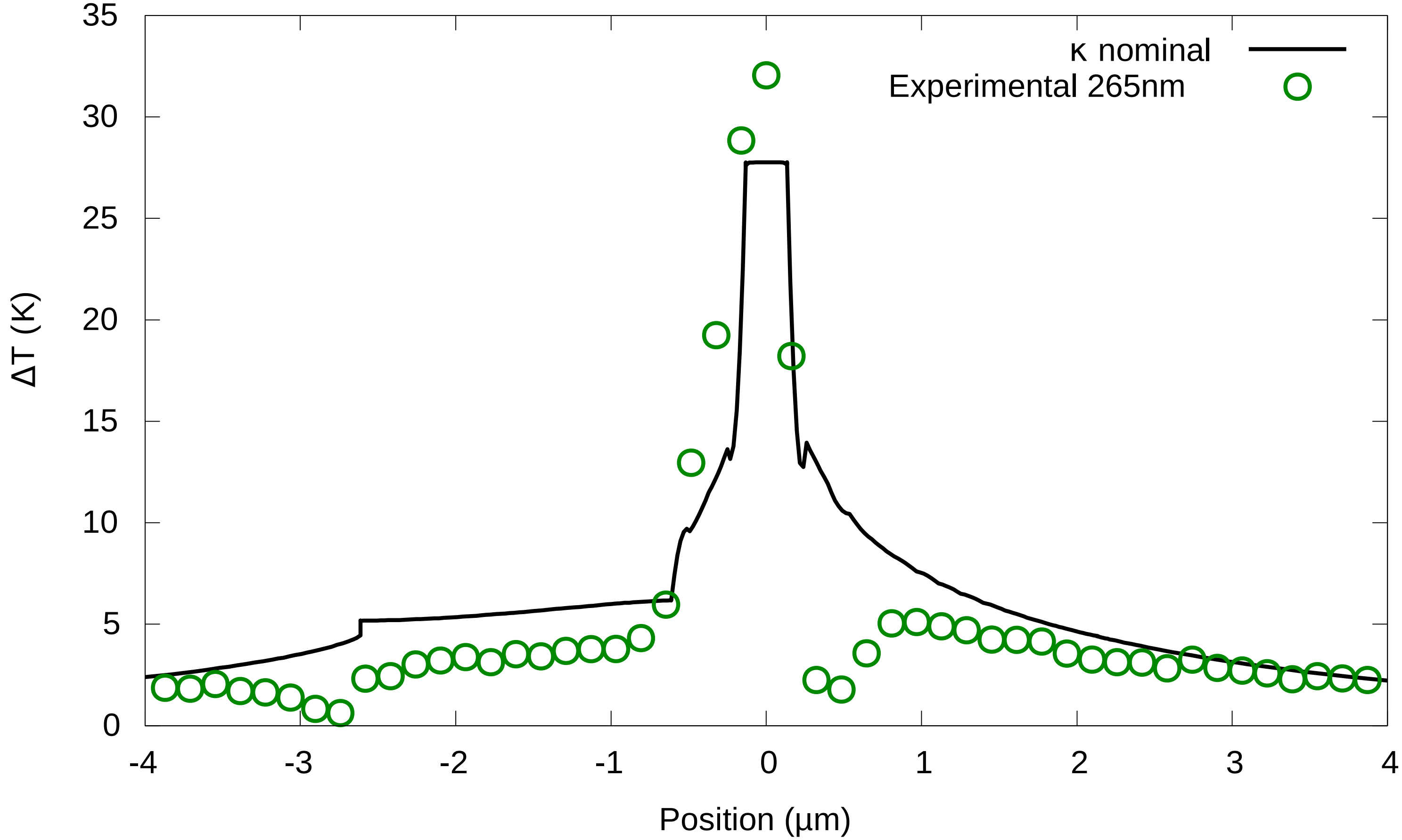
Objective:
Obtain the thermal profile

Thermo Reflectance Imaging (TRI)



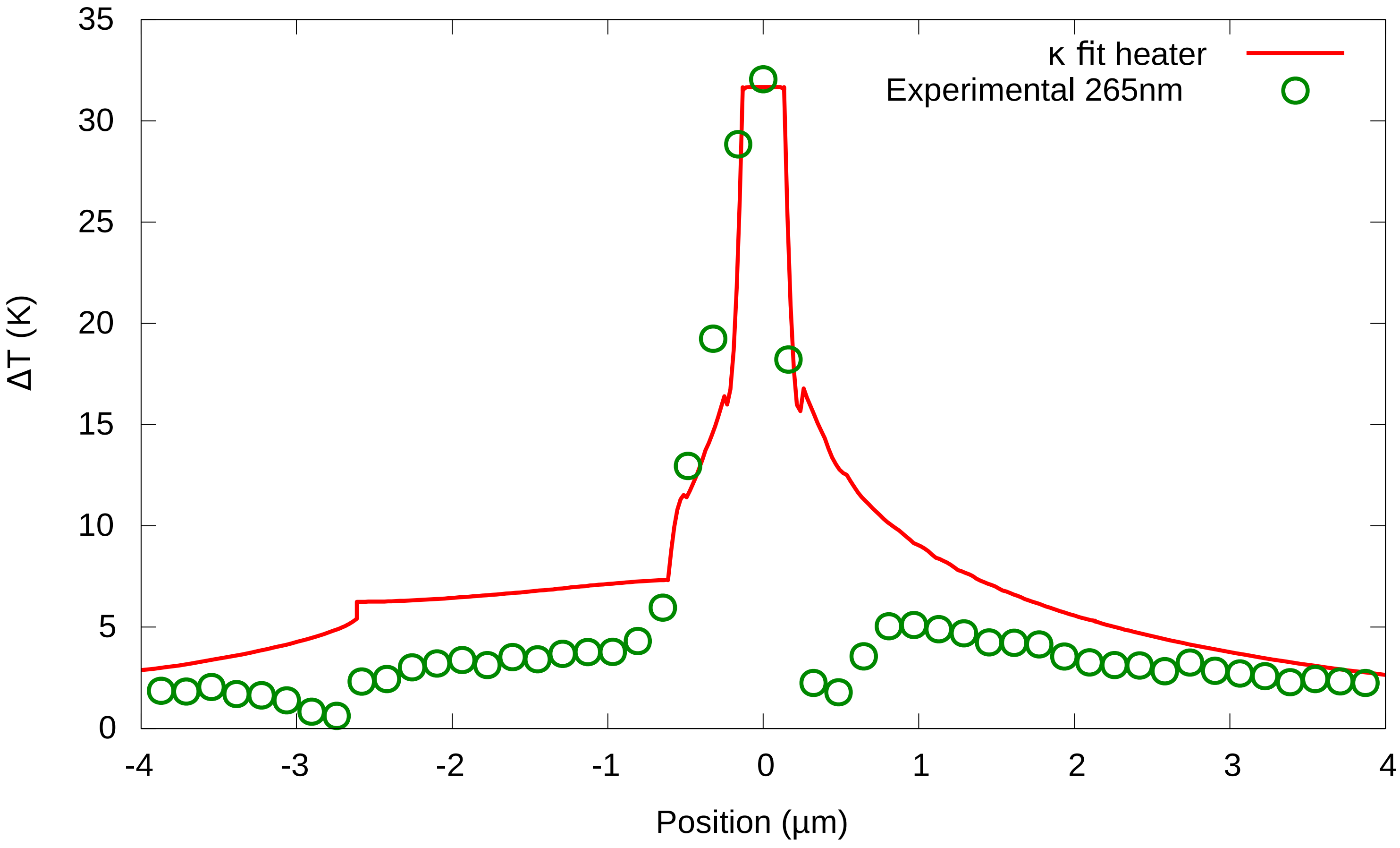
Fourier modelization of TRI experiment

Nominal value of the thermal conductivity (κ=5.5 W/mK)
Underpredict the heater and overpredict the thermometer



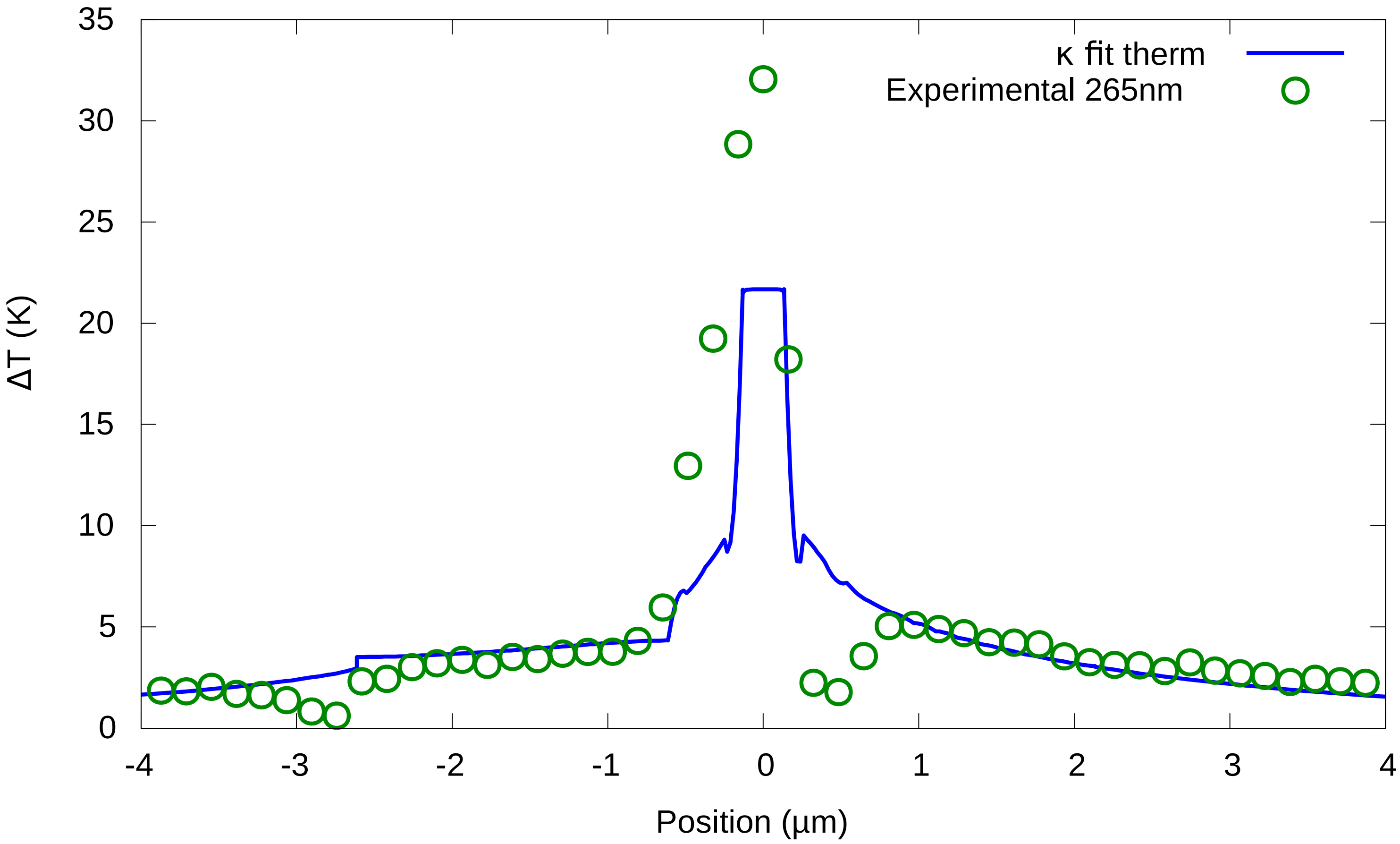
Fourier modelization of TRI experiment

Reducing the conductivity to fit the heater te (κ=4.5 W/mK)
We obtain a larger overprediction in the thermometer



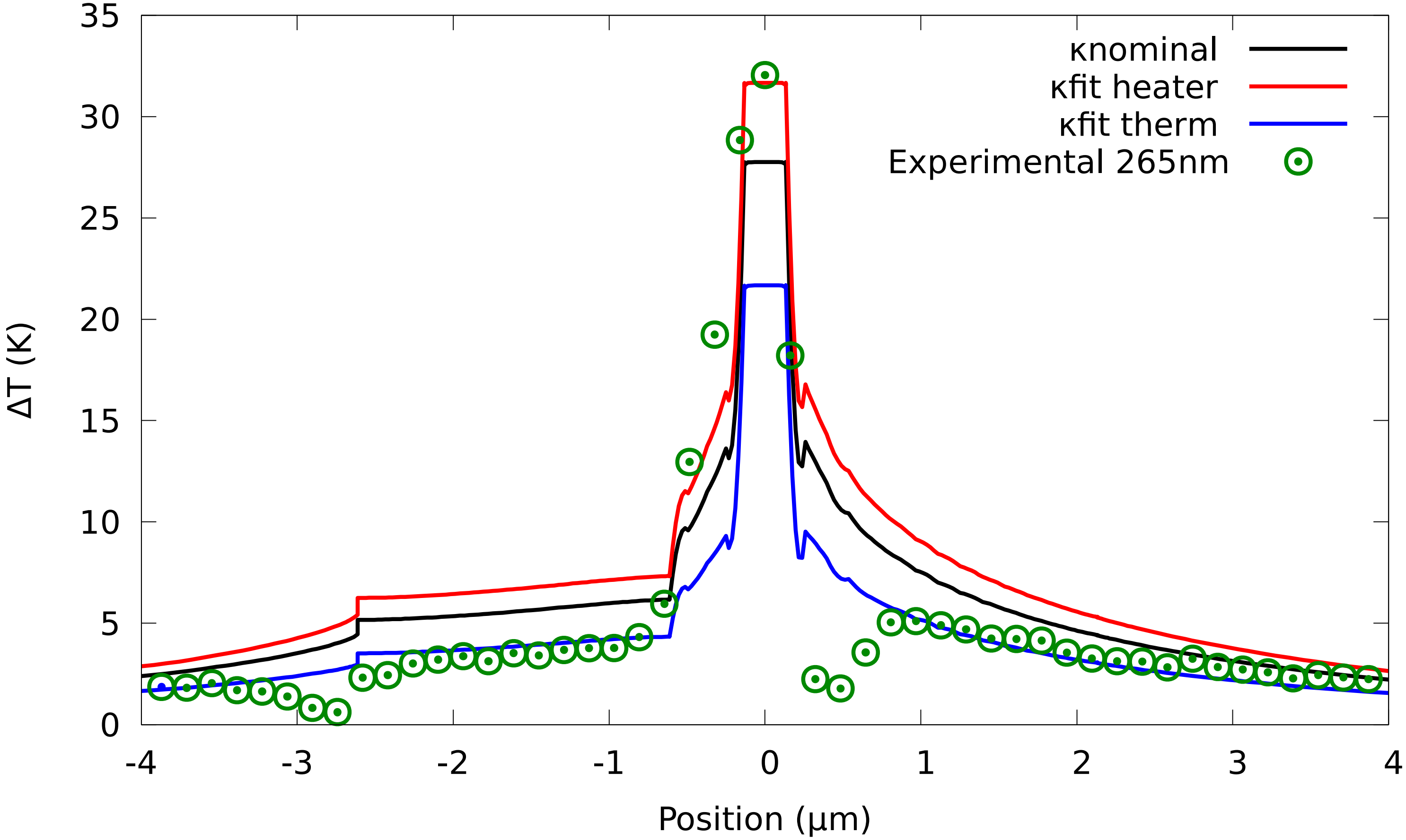
Fourier modelization of TRI experiment

Increasing the conductivity to fit the thermometer (κ=6.7 W/mK)
We obtain a larger underprediction in the heater



Fourier modelization of TRI experiment

There is not a single value for the thermal conductivity
That works in the entire domain for Fourier



TDTR experiments

nature
COMMUNICATIONS

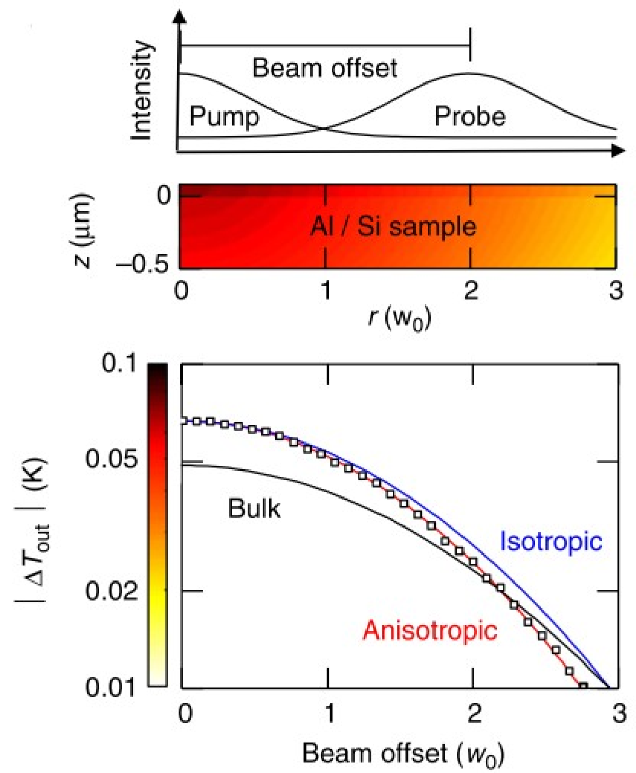
ARTICLE

Received 3 Dec 2013 | Accepted 26 Aug 2014 | Published 1 Oct 2014

DOI: 10.1038/ncomms6075

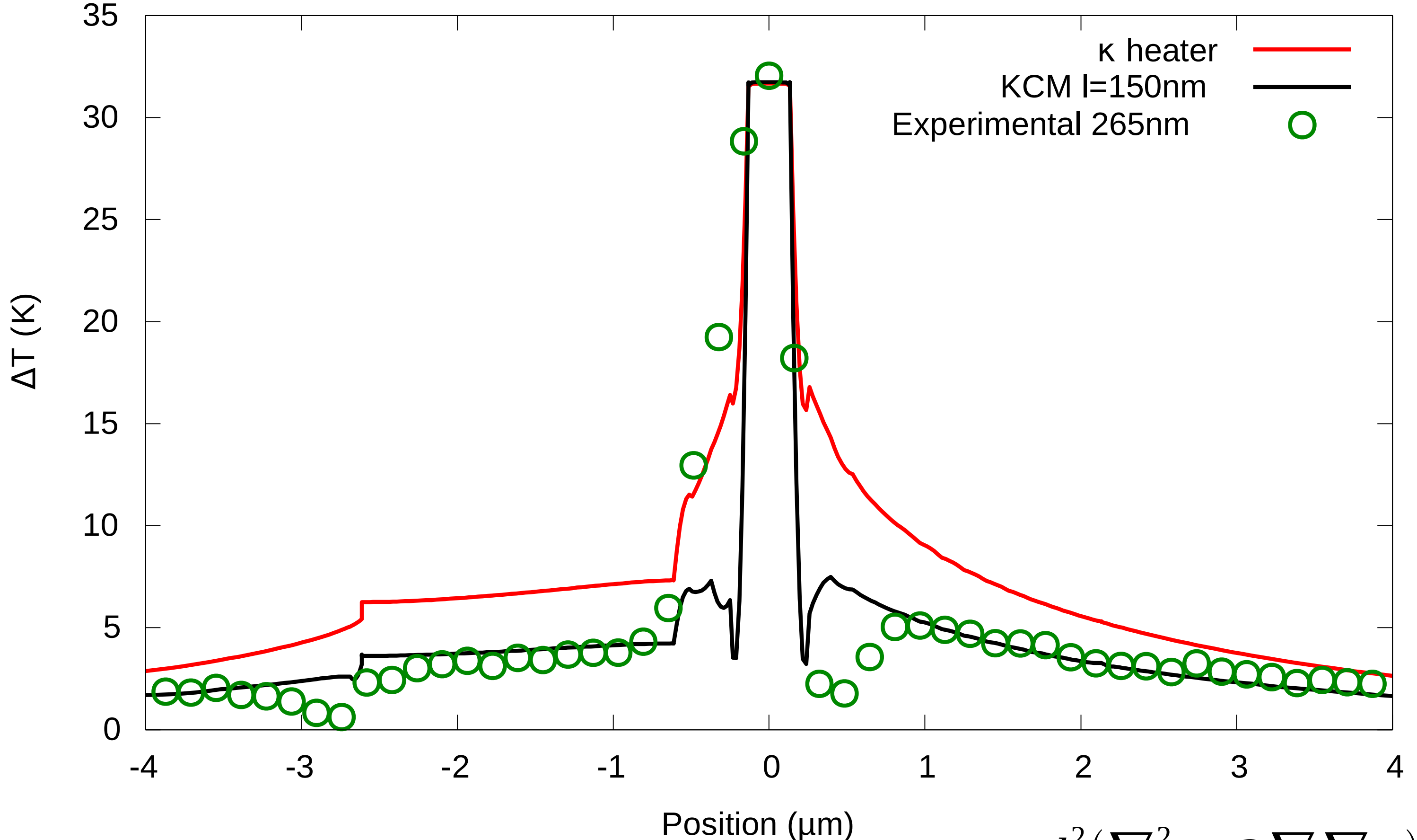
Anisotropic failure of Fourier theory in time-domain thermoreflectance experiments

R.B. Wilson[1] & David G. Cahill[1]



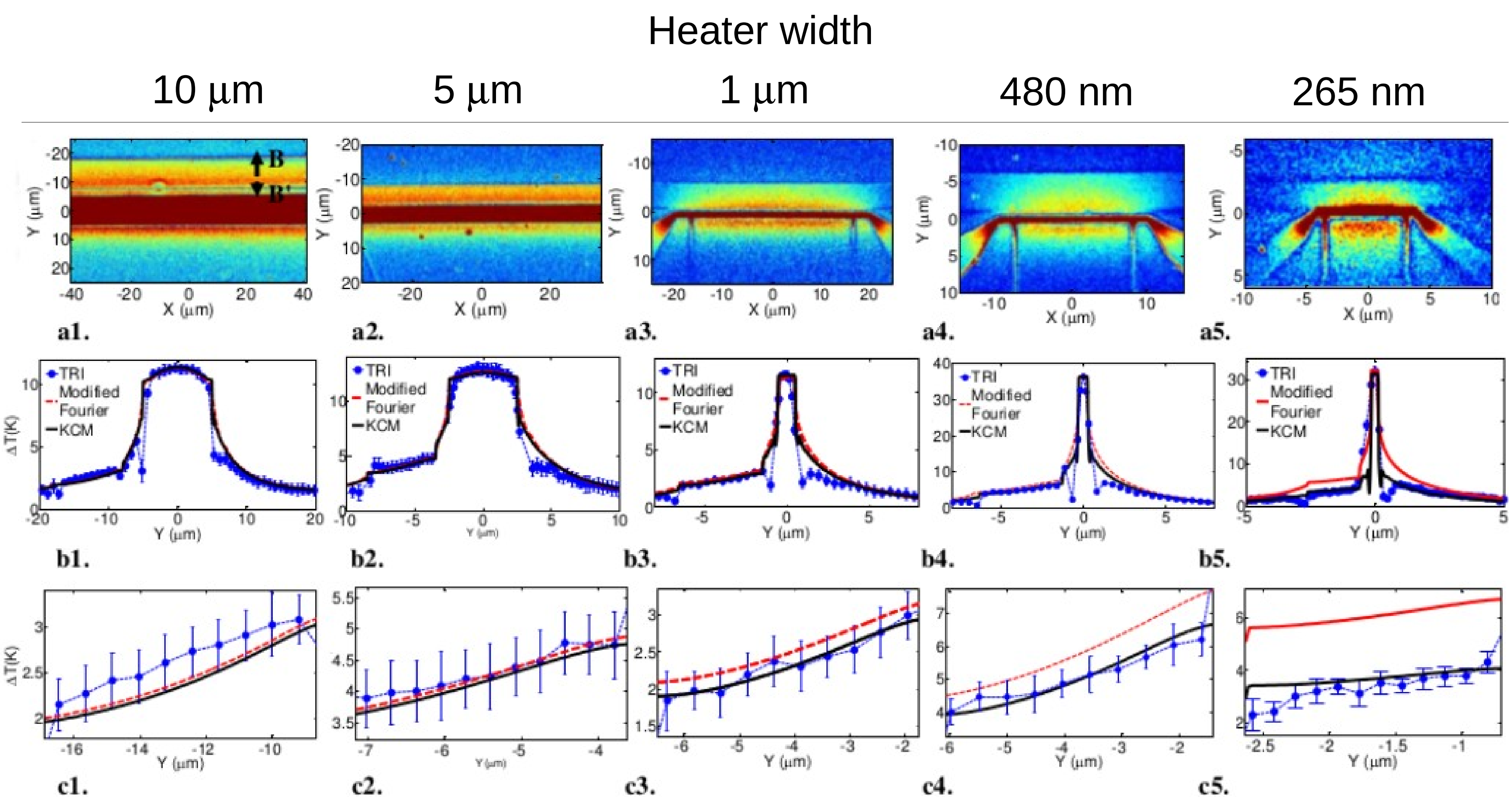
KCM modelization of TRI experiment

KCM allows the prediction of heater and thermometer
with the same values of κ and l

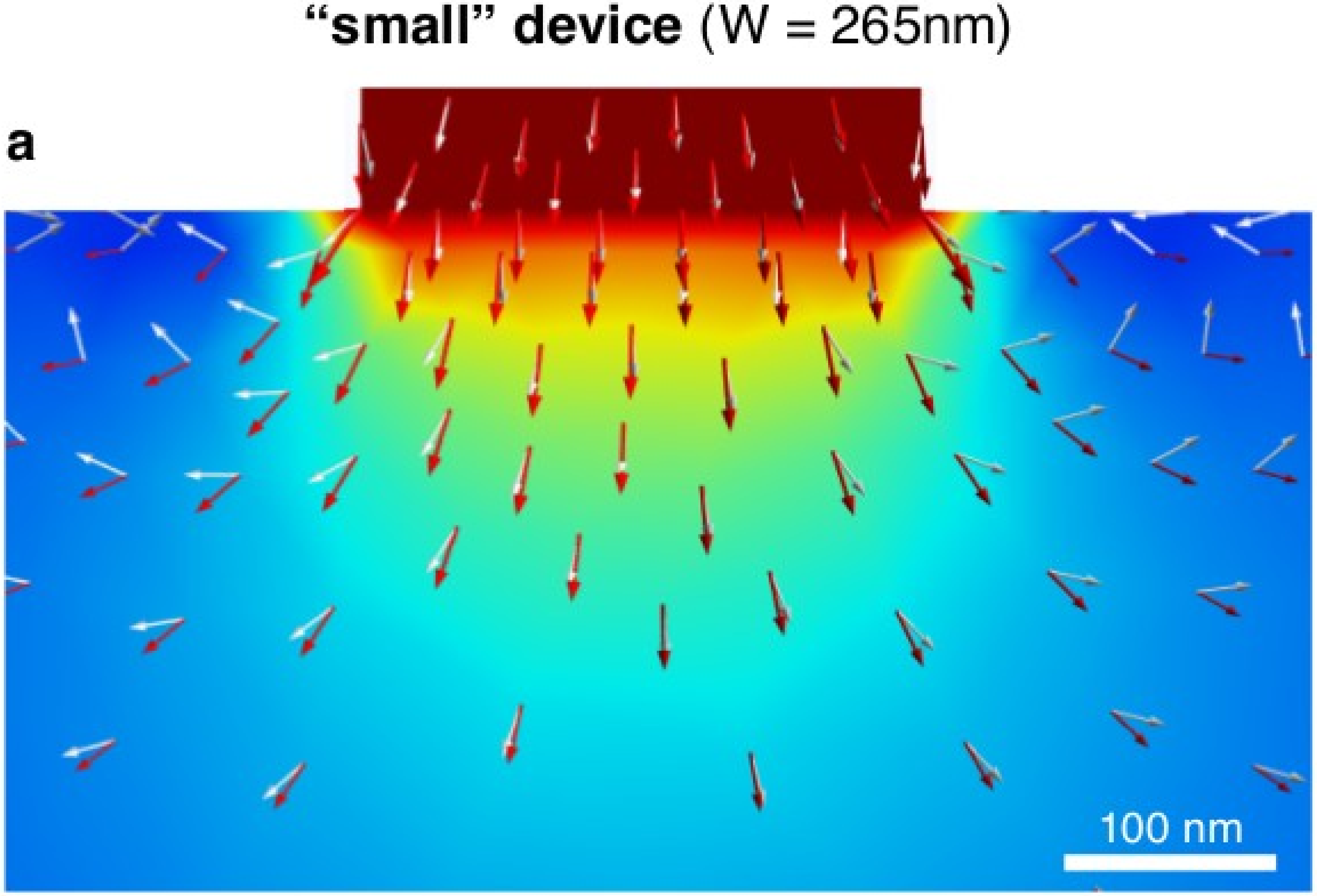


$$q - l^2(\nabla^2 q + 2\nabla\nabla q) = -\kappa \nabla T$$

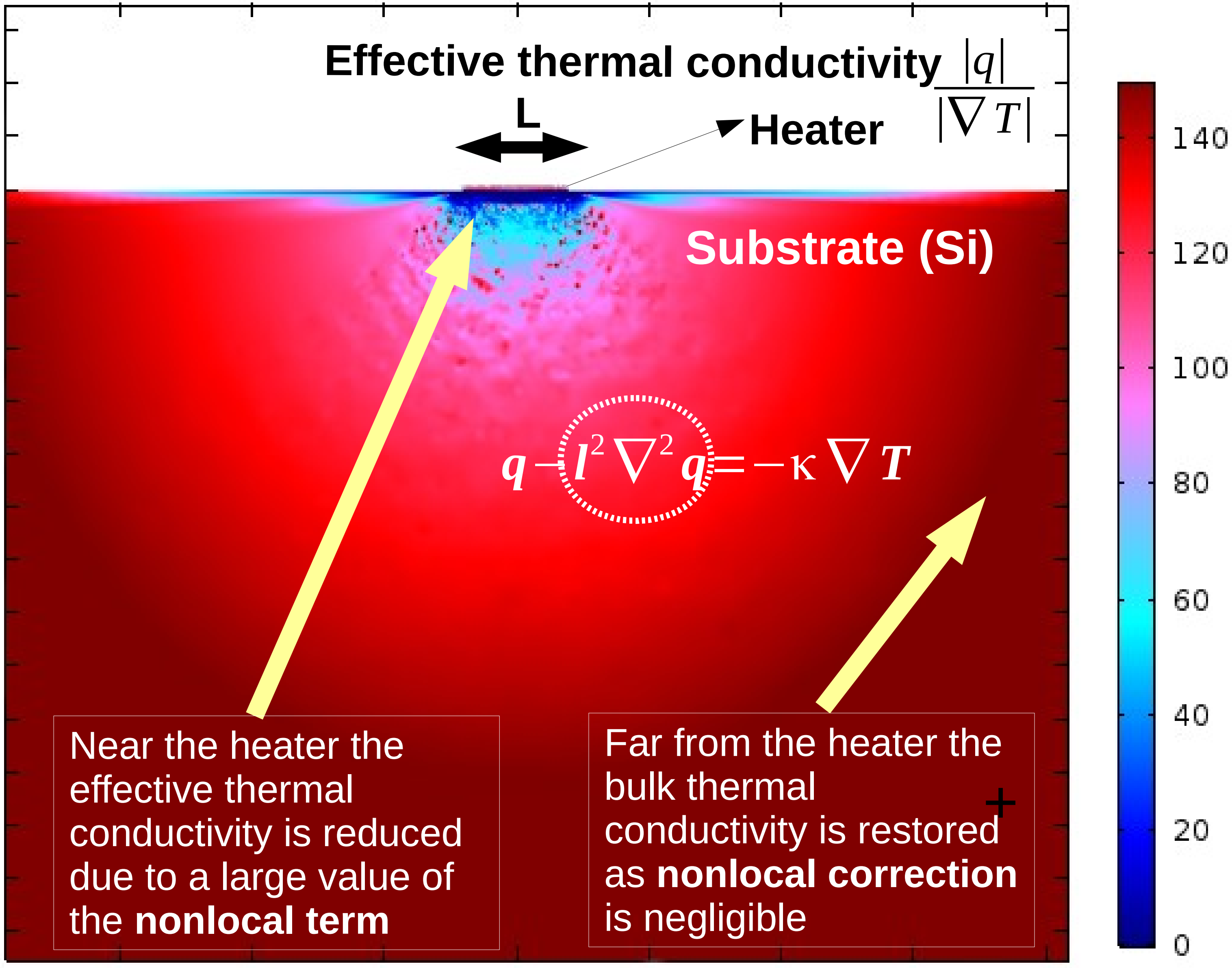
KCM predictions for different lines



Vorticity effects



KCM as a boundary



Conclusions

EIT allows the treatment of far from equilibrium situations by the inclusion om nonlocal and memory effects

The number of terms to describe an experiment depend on the complexity of the nonequilibrium excitation

The hydrodynamic model (second order approach) allows the prediction of a large number of experimental results at the nanoscale

KCM is a method to treat anharmonicities in the phonon collision term in a simple way

KCM gives a remarkable agreement with experimental results with a considerable reduction in the calculation requirements respect other ab initio approaches

KCM + Hydrodynamic model allows the prediction of complex geometries due to its simplicity

Thank You!

Financial Support: MINECO-FEDER ELEPHONT PROJECT

ELEPHONT

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MINISTERIO DE ECONOMIA Y COMPETITIVIDAD

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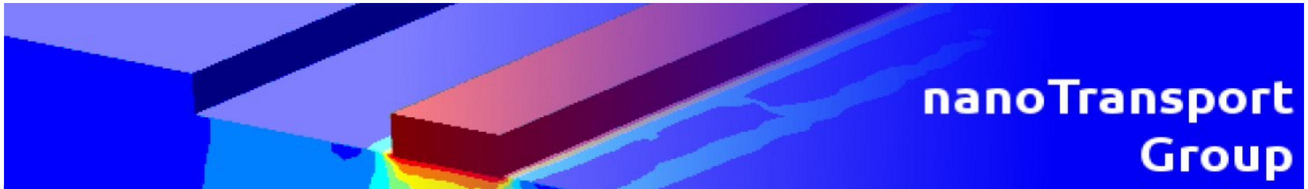

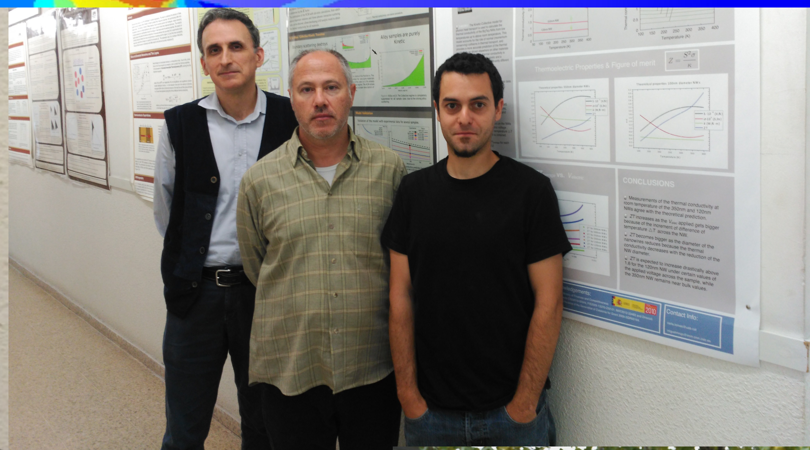

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