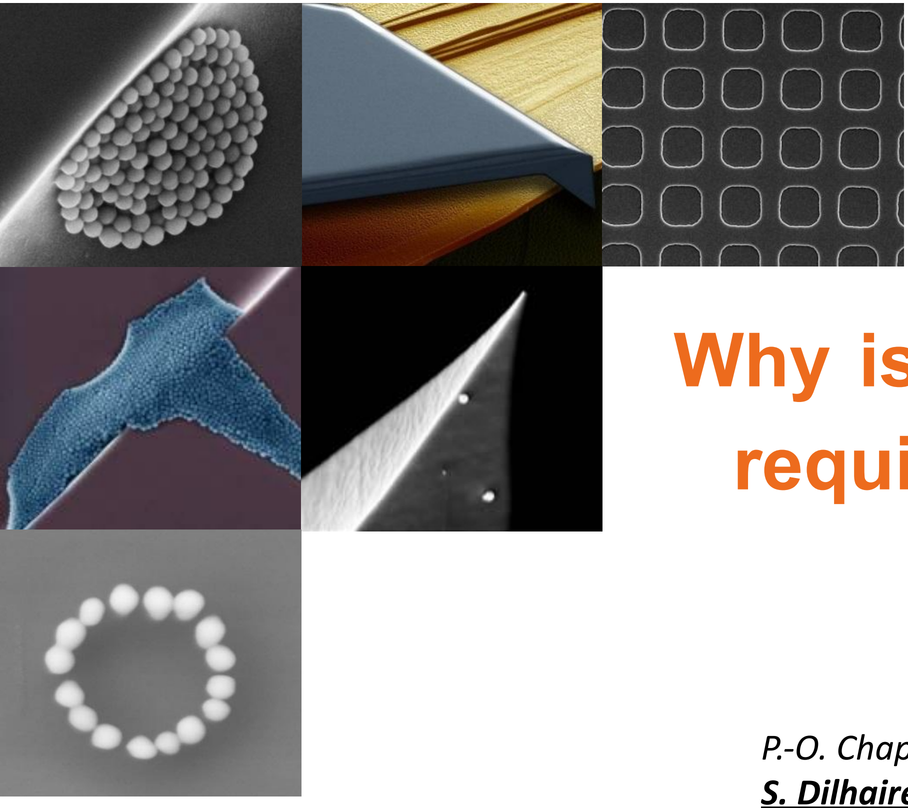
Club nano Métrologie



Nanoscale heat transfer
& Measurement axis

Why is heat transport modelling required for nanometrology?

S. Gomès, CETHIL, Lyon

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LABORATOIRE NATIONAL DE MÉTROLOGIE ET D'ESSAIS LNE cnrs C'NANO NAME

CONTEXT

Why nanometrology?

- Crucial role of instrumentation and measurement techniques in the field of basic research

  by increasing knowledge about the intimate properties of nanomaterials.

- Growing interest in the industrial world

  for better control of manufacturing processes and improvement of quality systems.

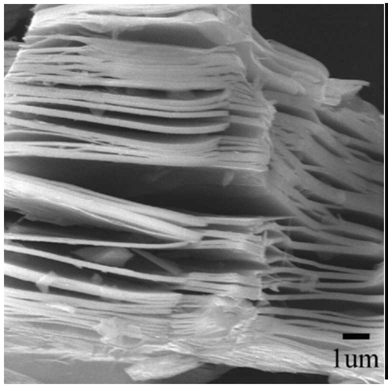
Requirements

Traceability chains to be set up	Reference standards and nanomaterials
Identification & quantification of **<u>all the sources of uncertainty</u>**	Evaluation of uncertainty balance sheets

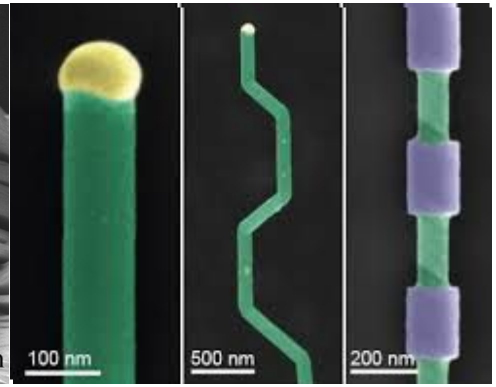
→ Confidence rate on the measurement

CONTEXT

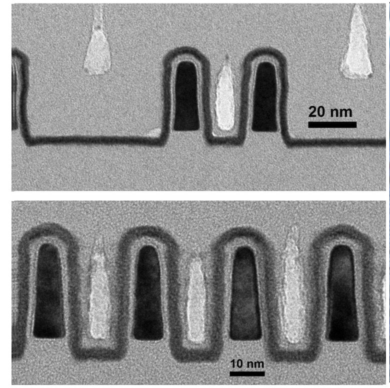
Motivation



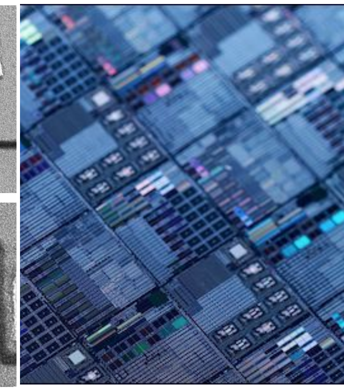
Mxène topological material Ti_3AlC_2



Si nanowires



Intel finFET



Nanocomponents

Nanomaterials

Electronic components

- Multiple interfaces, nanoscale contacts and boundaries
- Plethora of heat generation and transfer phenomena including mixed regimes beyond diffusive transport, i.e., ballisticity, superdiffusion and hydrodynamics.

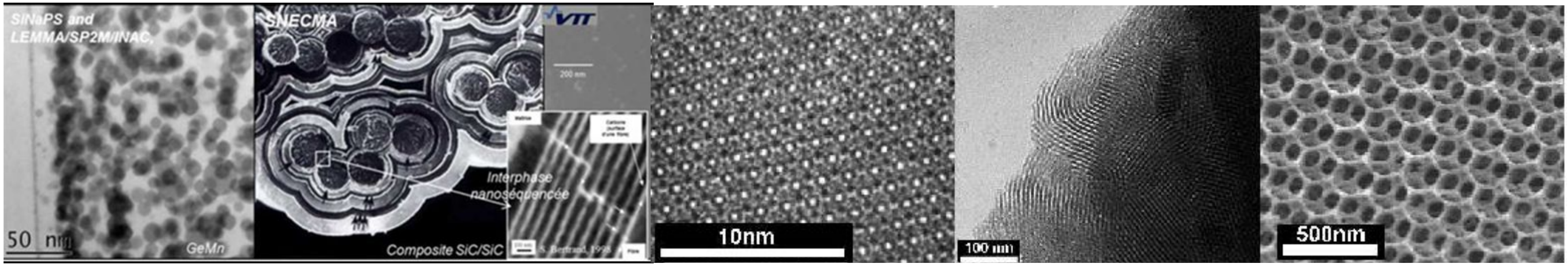
How to measure them ?

Experiment + Modelling □ Measurement

CONTEXT

Scientific issues

- Investigation of nanomaterials



Requirement: characterization techniques with nanometric spatial resolution

- Investigation of highly-localized non-equilibrium thermal processes occurring at ultra-short time scale

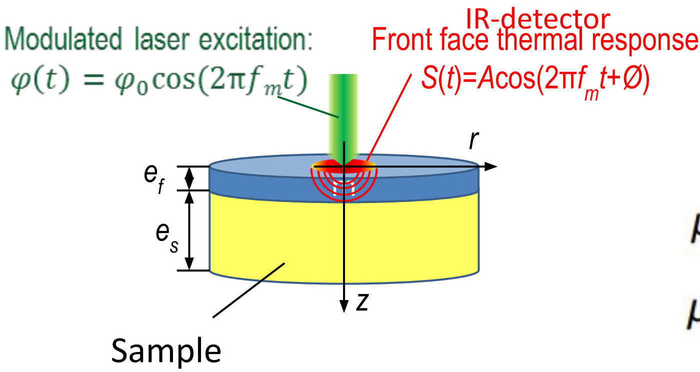
Requirement: method combining ultra-high spatial and temporal resolution

Optical, electrothermal methods and scanning probe techniques developed in these directions

OPTICAL METHODS
Performances and application fields

Club nano Métrologie

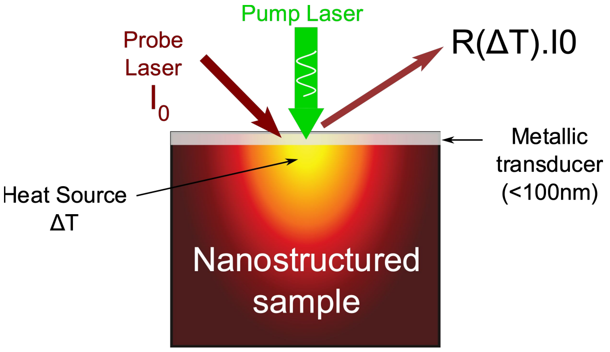
Modulated photothermal radiometry (MPTR): frequency domain



$\mu=(a/\pi f_m)^{1/2}$

$\mu=(a\,\tau_i/\pi)^{1/2}$

Thermoreflectance (FD- or TD- TR): Frequency or Time domain (τ_i)



Technique	MPTR	FDTR and TDTR
Spatial resolutions	• Lateral: 30 µm (diffraction limit) • In depth: 50 nm	• Lateral: µm (diffraction limit) • In depth: 20 nm
Frequency range (f_m)	Up to 50 MHz currently, **goal: up to 100 MHz**	**FDTR: 1 kHZ-300 MHz; TDTR: 100 MHz-1 THz**
Experimental limitation	Need to cap the samples with a thin metallic transducer	
Studied nanomaterials	Thin films, superlattices, embedded nanoparticles	
Thermal properties	Thermal diffusivity (*a*) and conductivity, thermal interfaces resistances	
Explored beyond Fourier heat generation and transfer phenomena	Not yet	Ballistic-diffusive heat transfer, dynamic in systems far from thermal equilibrium ***Associated measured thermal parameters*** Superdiffusivity coefficient α, phonon mean free-path

OPTICAL METHODS

MPTR: some results

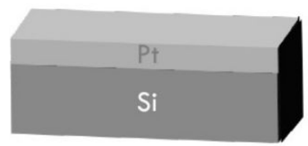
Thermal boundary resistance at metal/SC interface

Influence of doping level

G. Hamahoui, cientific Report 2018

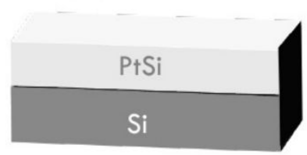
e = 50 nm

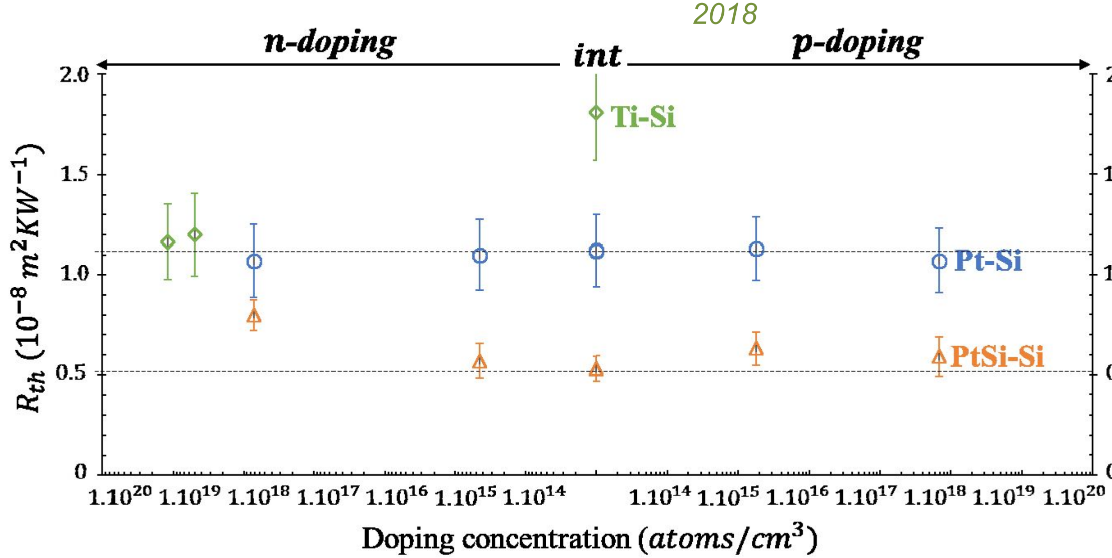
Before annealing



e = 100 nm

After annealing
For T > 338°C





Associated measurement modelling

- Fourier modelling

Current measurement limitation

- Frequency range

Need for nanometrology at 50 MHz

- Samples such as means free path are larger than thermal µ

at larger frequencies

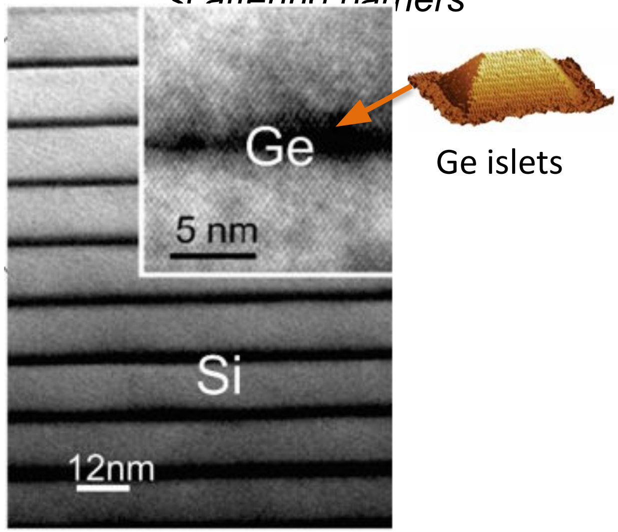
- Need of model for ballistic-diffusive transfer with interfaces

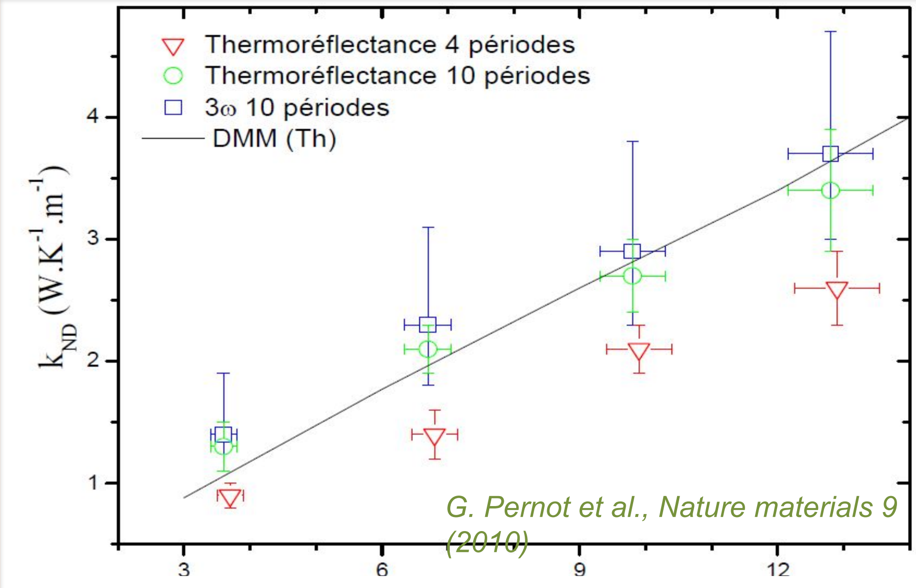
OPTICAL METHODS

FDTR: some results

Thermal conductivity tailoring via non-Fourier transport

Precise control of thermal conductivity at the nanoscale via individual phonon scattering barriers





- Ballistic transport in Si layers
- Crystalline thermal insulator
  k = 0.8 W.m-1.K-1

Associated measurement modelling

- Fourier modelling
- Diffuse Mismatch model (DMM)

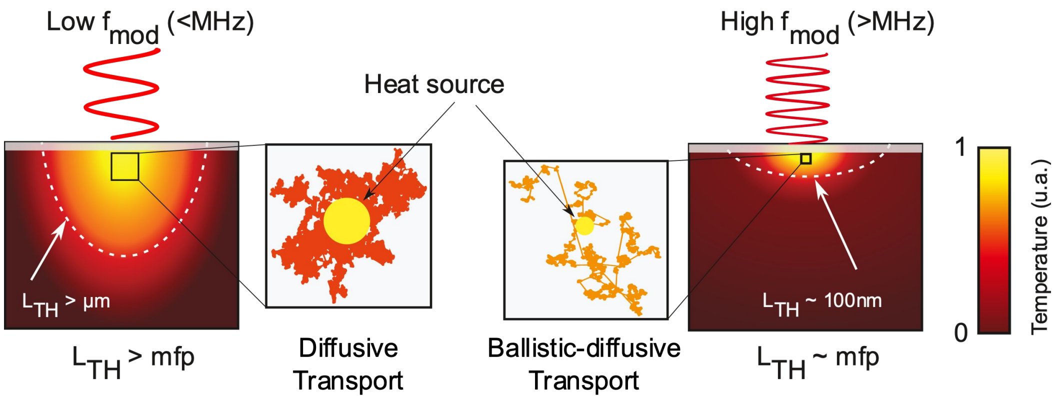
Modelling current limitations

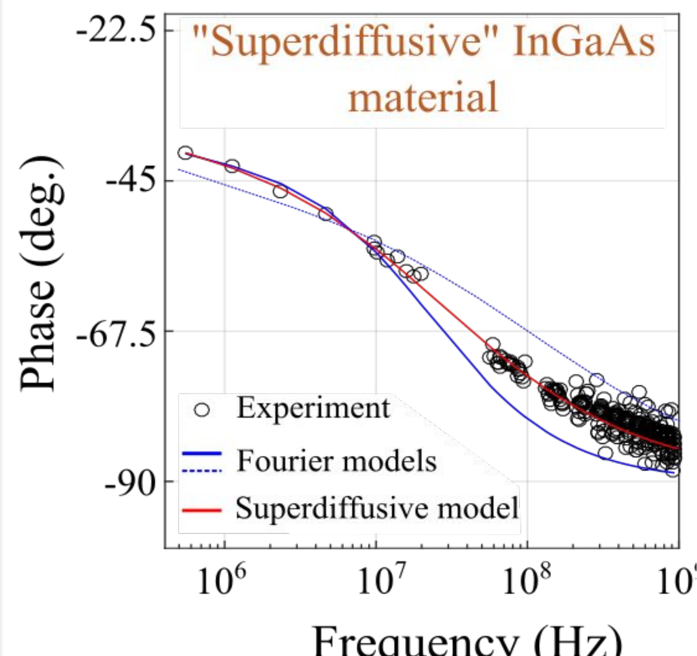
- Fourier modelling does not include ballistic transport in Si layers

OPTICAL METHODS

FDTR: some results

Seeking for super-diffusivity





Associated measurement modelling for comparison

- Fourier heat model
- "Superdiffusive" Lévy model for ballistic-diffusive heat transport

Modelling current limitations

Fourier model CANNOT reproduce experimental data

Error of 30% in thermal conductivity identification

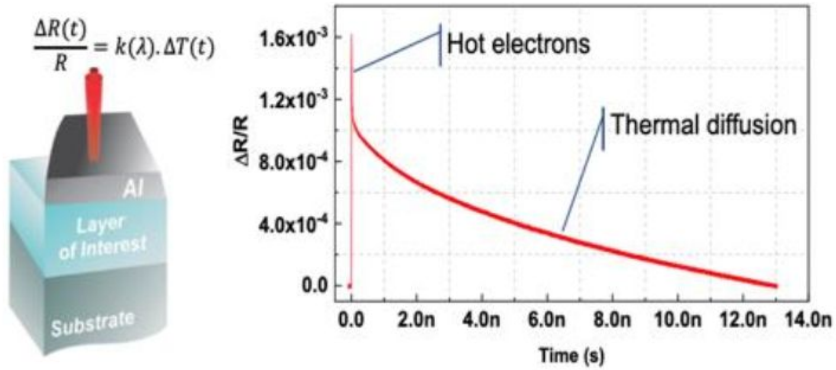
Error of 300% in thermal interface resistance

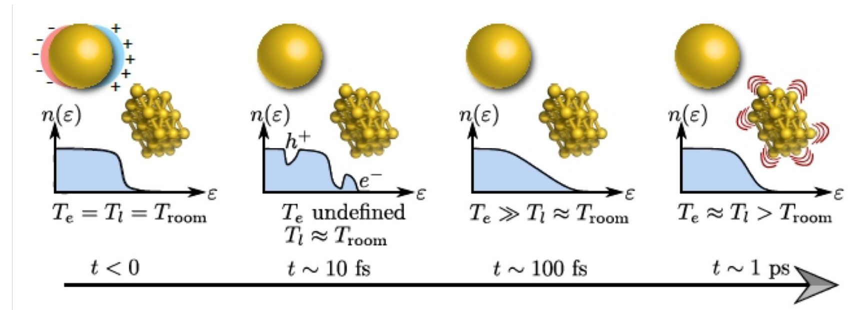
Deviation from Fourier when the heat source dimension becomes comparable to phonon mfp

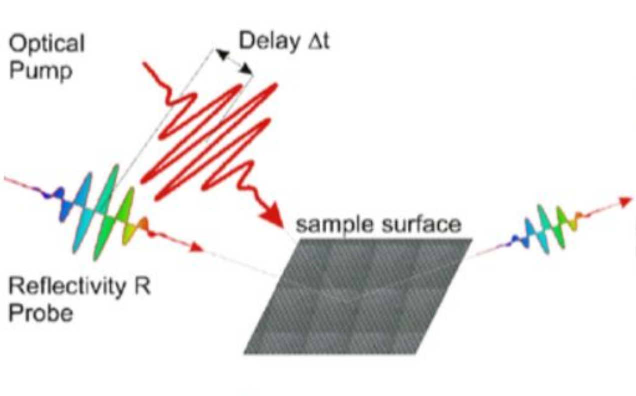
Need for nanometrology

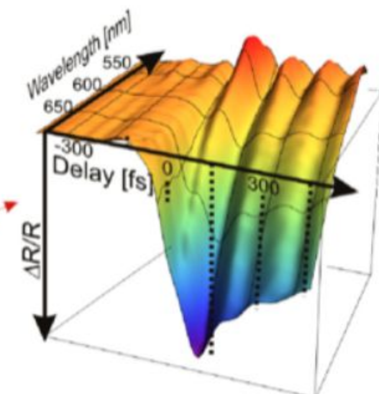
- New model for ballistic-diffusive heat transfer in thin films (Lévy flight modelling)

From non equilibrium hot electrons to phonon thermal diffusion









Associated measurement modelling

- 2 temperature model

Current measurement limitation

- Temperature measurement?
- Non linerarities
- Thermal effect? Optical effect?

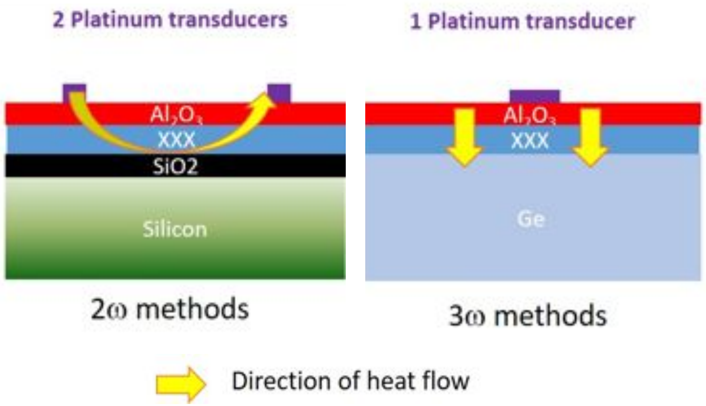
Need for nanometrology

- New model for thermal – optical coupling

ELECTROTHERMAL METHODS
Performances and application fields

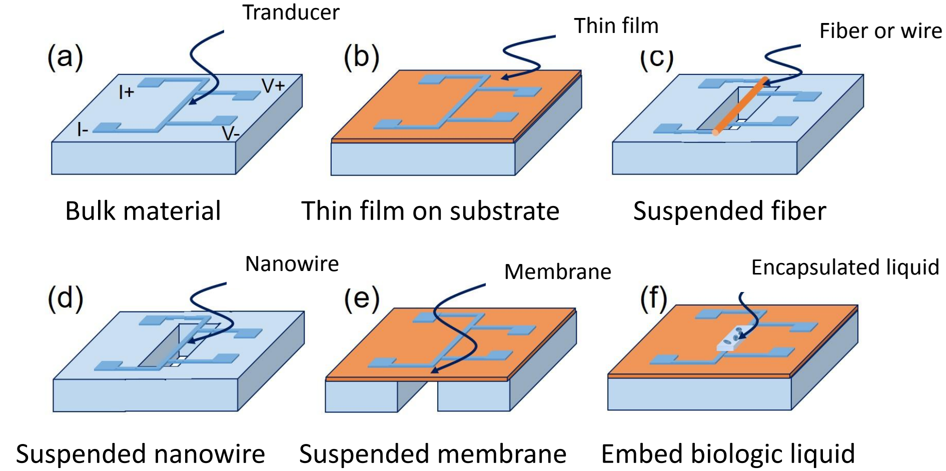
2 and 3ω methods

Thin film measurement



Lowest thin film thickness □ 10 nm

3ω method



Measured thermal properties

- Thermal conductivity and diffusivity, specific heat if thick enough, interface thermal resistance

Explored heat generation and transfer phenomena (beyond Fourier)

- Possible with playing with the size of the tranduceur, experiment temperature, characteristic dimension of the structure

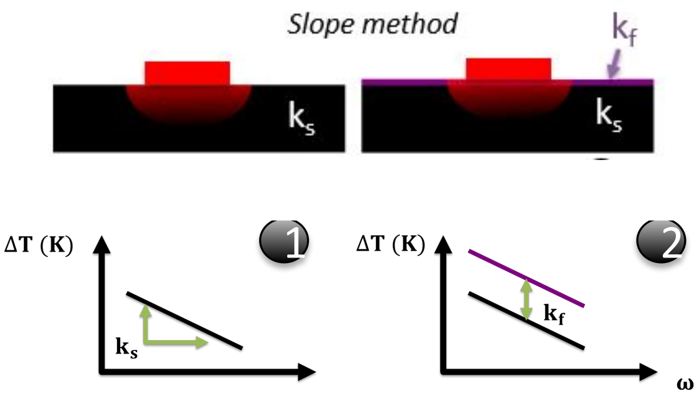
ELECTROTHERMAL METHODS

3ω method : some results

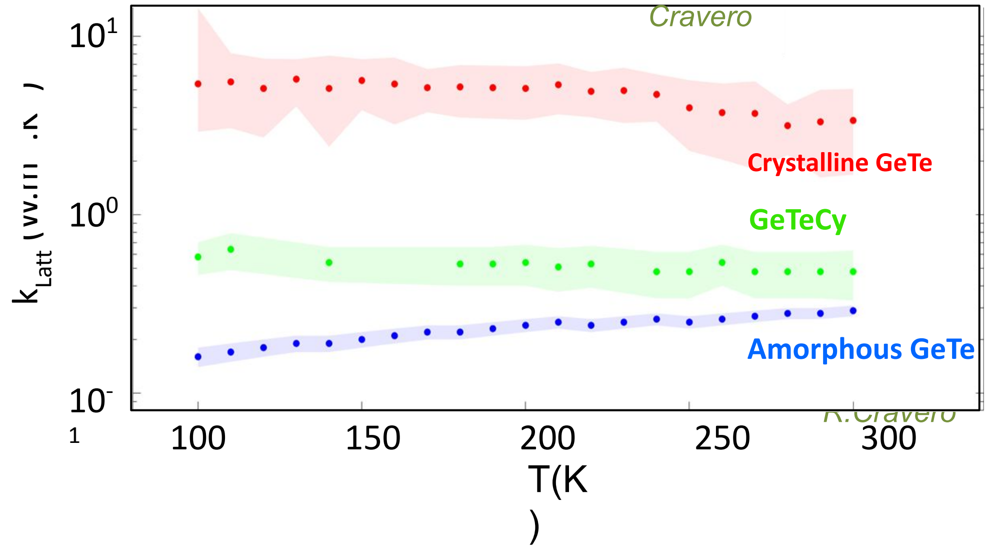
GeTe based-phase change materials

Associated measurement modeling

Fourier



Credits: PhD thesis R. Cravero



Modelling current limitations

- Thermal model with multilayers/multi-interface

Current measurement limitation

- Measuring thermal conductivity of highly conductive very thin films by 3ω
  (can be easier by 2ω).

Need for nanometrology

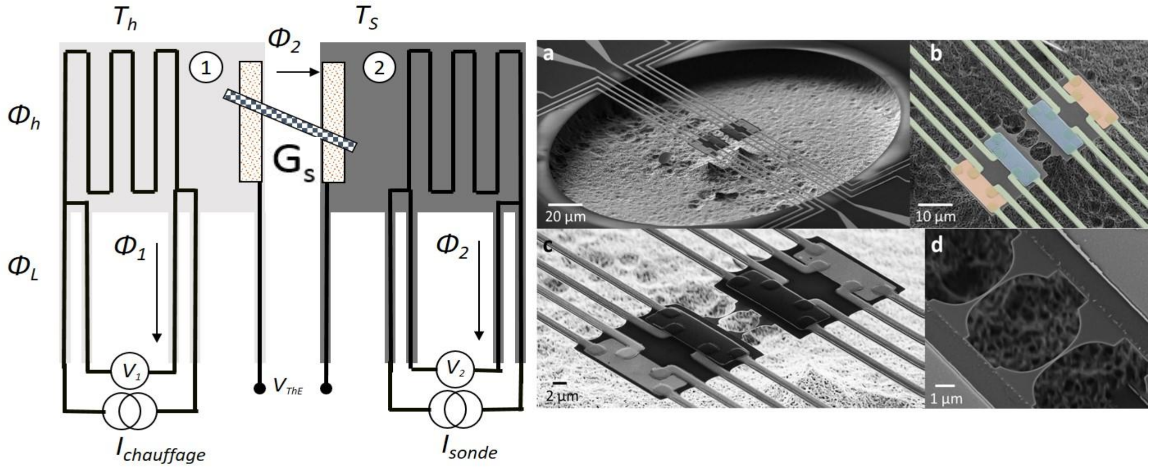
- Reference for thermal boundary resistance between thin films

ELECTROTHERMAL METHODS

Performances and application fields

Thermal bridge method

Temperature gradient across the nanostructures



Power sensitivity
15 attoWatts $\sqrt{\text{Hz}}^{-1}$
around 100 mK

Studied nanomaterials or nanosystems

- Nanowires, nanostructured membrane

Measured thermal properties

- Thermal conductivity or conductance

Explored heat generation and transfer phenomena (beyond Fourier)

- ballistic limit, quantum limit etc…

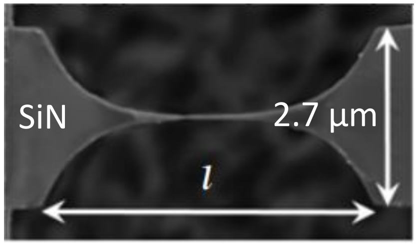
Measured thermal parameters:

- Thermal transport only (heat flux)

ELECTROTHERMAL METHODS

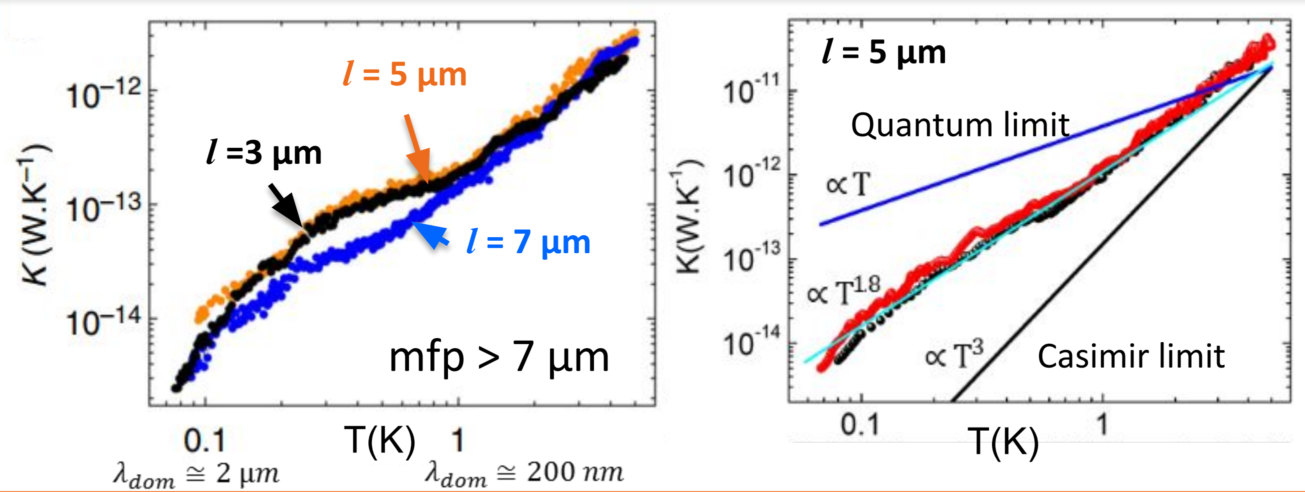
Thermal bridge method: some results

Heat conduction in ballistic 1D phonon waveguide



Nanowire .diameter < 100 nm

G. Tavakoli et al., Nature Communications (2018)
G. Tavakoli et al., Scientific Reports (2022)



Current measurement limitations

- Thermal link to the heat bath not controlled

Modelling current limitations

- Full thermal model of the double membrane sensor

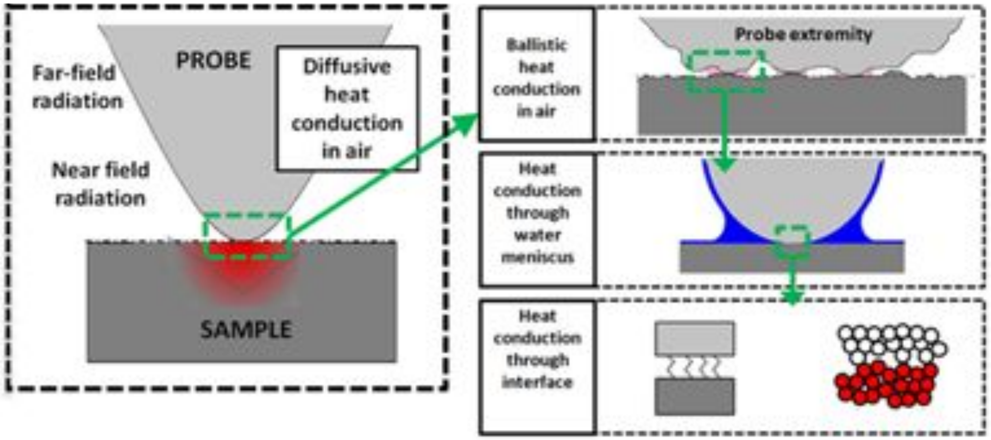
Ballistic phonon transport dominated by non-ideal transmission coefficients, not by the quantized thermal conductance of the nanowire itself

Need for nanometrology

- Measurement of transmission coefficient (1D<->3D or 1D<->2D)
- Reference needed for the quantum of thermal conductance

SCANNING THERMAL MICROSCOPY

Performances and application fields



S. Gomès et al., Pss.a (2015)

Spatial resolution

10 nm (vacuum conditions)

Time resolution

1 ms

Current experimental limitations

Complex probe –sample interaction

Probe sensivity and time resolution

Probe calibration

Studied nanomaterials or nanosystems

- Nanostructured materials, thin films, suspended membranes, Matrix or suspended nanowires, interfaces and nanocontacts

Measured thermal properties

- Effective thermal conductivity, thermal conductance of contact and sample

Explored heat generation and transfer phenomena (beyond Fourier)

- Thermal transport through nanocontact, nanomeniscus…

Measured thermal parameters

- Thermal transport estimated using thermal conductance

SCANNING THERMAL MICROSCOPY

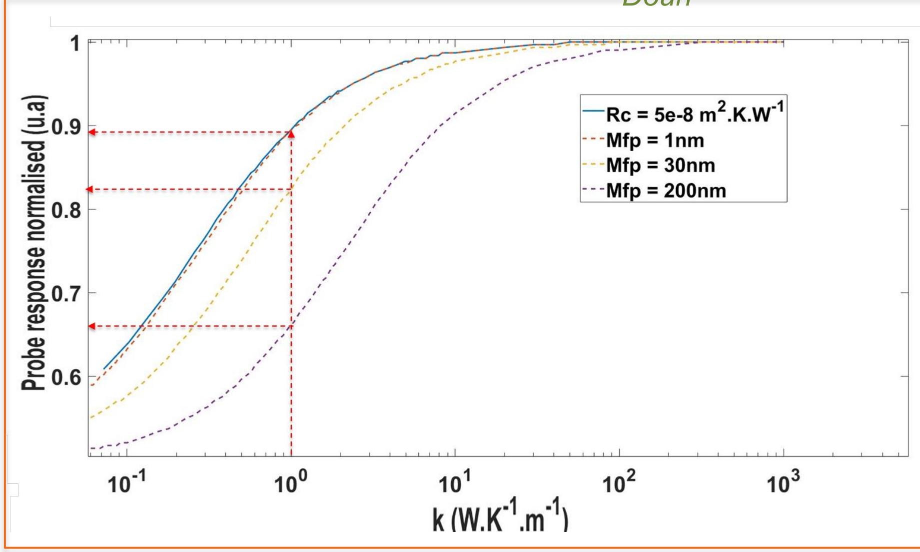
SThM: some results

Calibration with bulk samples

Associated measurement modelling

- 3D numerical simulation, Fourier for the probe description
- Fourier
- Heuristic model of the thermal nanocontact
- Boundary thermal resistance from large heat sources

Credits: PhD thesis S. Douri



Current measurement limitations

- Probe sensitivity
- Description of the thermal contact and probe-sample interface

Strong impact on sensitivity of the nanocontact thermal resistance

Need for nanometrology

- Modelling of nanoconstriction and thermal boundary resistance for limited source
- Improved calibration methodology

CONCLUSION

Current experimental techniques

- Effective thermal conductivity and diffusivity of nanostructured materials and nanocomposites
- Equivalent thermal conductivity of nanostructures
- Thermal conductance of interfaces

Local thermal equilibrium

- Heat flux through a nanostructure and nanomaterial
  - *Adjusting the size of nanostructure (wire, film, contact) and temperature*
  - *Adjusting the time (when possible)*

Ballistic transport within sample

Ballistic-Diffusive transport within sample
(alloys or nanostructured materials)

But some instrument and modelling limitations

Need of modelling for nanometrology

- New models of measurements to interpret/design experiments involving non-local equilibrium

CONCLUSION

Requirements

- Adaptation or development of instruments

+

- Reference samples

+

- **Proper modelling of nanoscale heat transport phenomena involved in measurement methodologies**
- **Modelling strategy to fill the gap between the different length scales**
- **Experimental validation of modelling of heat transport at nanoscale**
- **Modelling strategy to account for multi-phenomena coupling**

Key remaining questions

- **interfacial thermal energy** *especially in the non-Fourier limit*
- **heat transport in nanometre-sized contacts**

PERSPECTIVES

Our goal

- Network for thermal nanometrology
- Initiate collaboative projects

Invitation

- Next meeting in early 2023 with invited members from the modelling community
- You are welcome to join the « nanocale heat transfer » WG of the Club nanoMétrologie for discussing of these challenges!

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Thanks!

Acknowledgement

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Caractérisation

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Matériaux

Métrologie

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