Nanoscale heat transfer & Measurement axis

Why is heat transport modelling required for nanometrology?

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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.

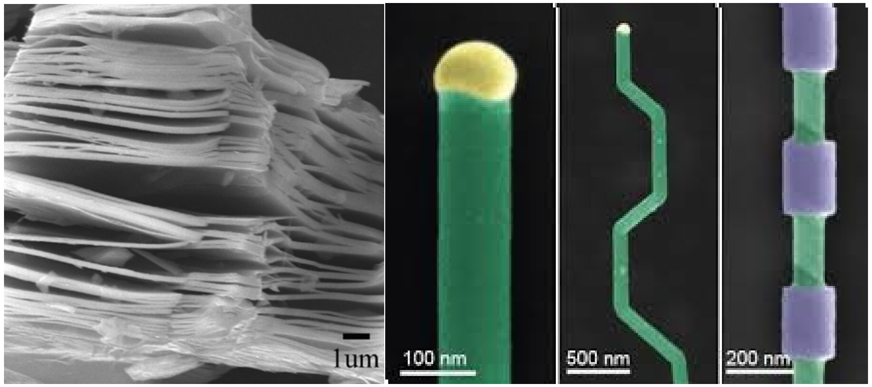
Requirements

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

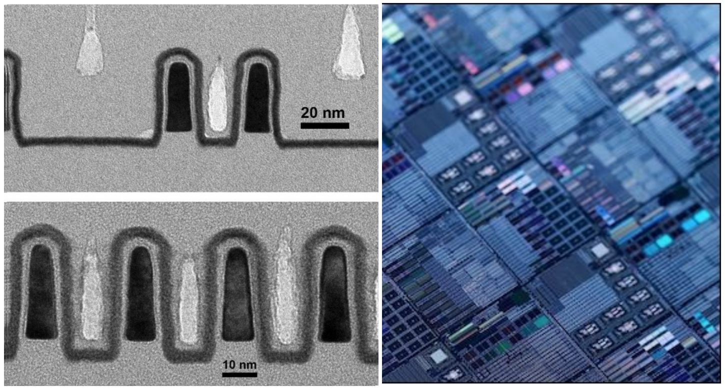
➡ Confidence rate on the measurement

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.

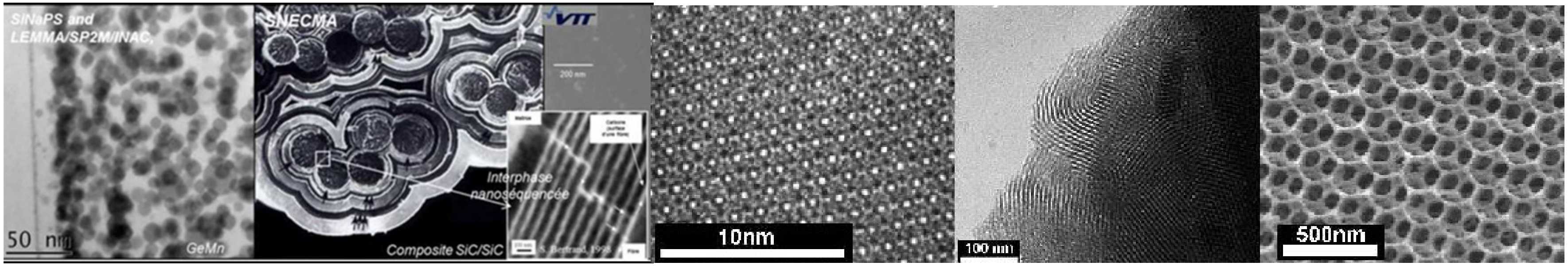
How to measure them ?

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

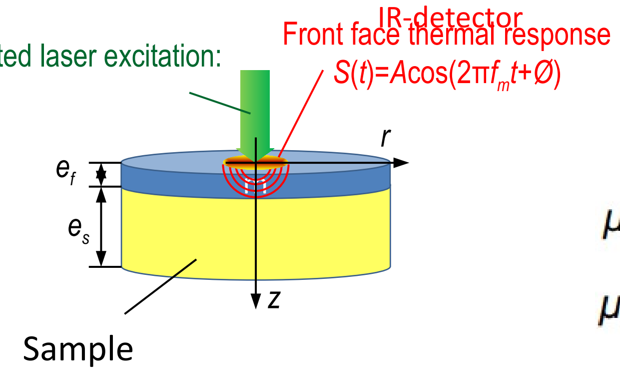
Requirement: method combining ultra-high spatial and temporal resolution

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

OPTICAL METHODS

Performances and application fields

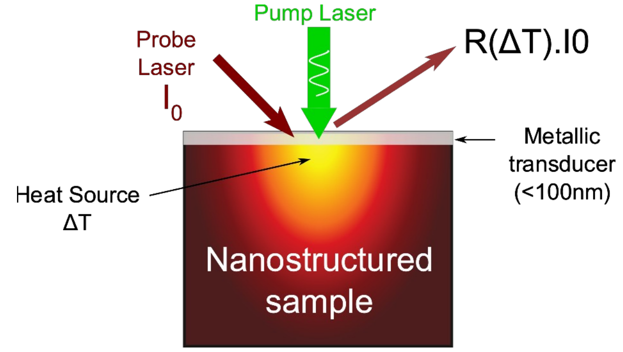
Modulated photothermal radiometry (MPTR): frequency domain



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

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

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

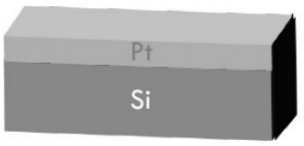
Thermal boundary resistance at metal/SC interface

Influence of doping level

G. Hamahoui, cientific Report 2018

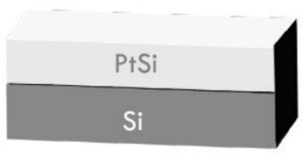
e = 50 nm

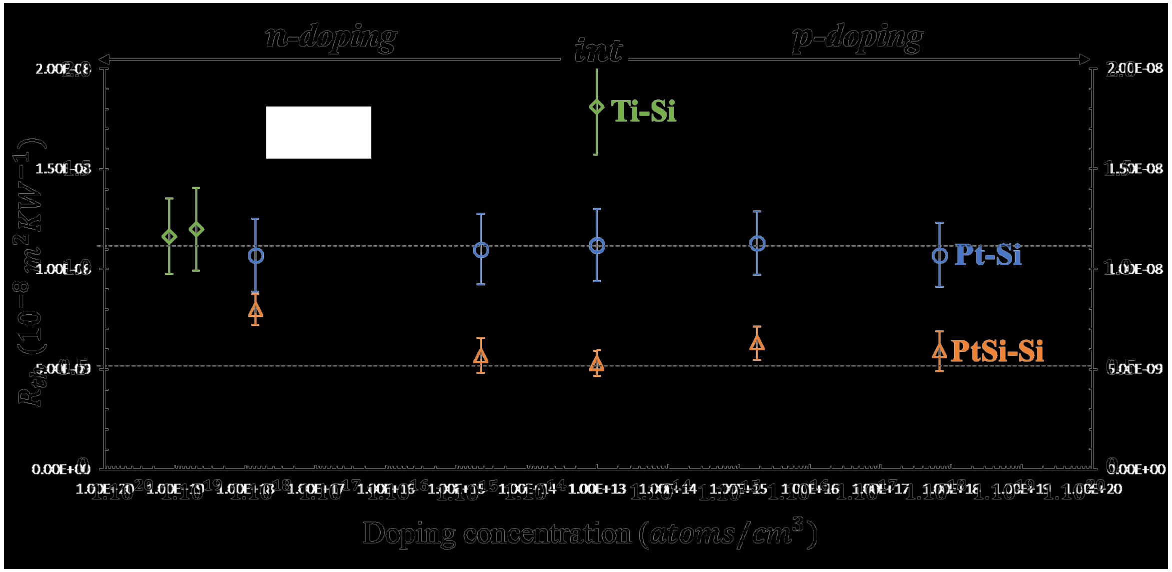
Before annealing



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

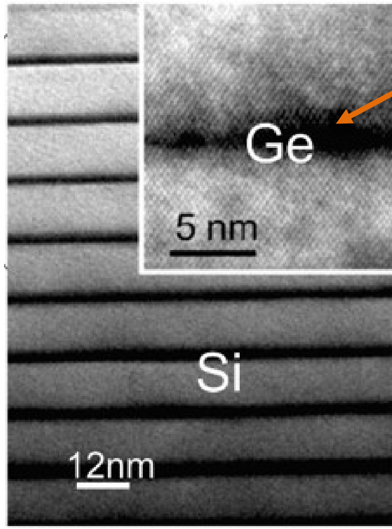
at larger frequencies

- Need of model for ballistic-diffusive transfer with interfaces

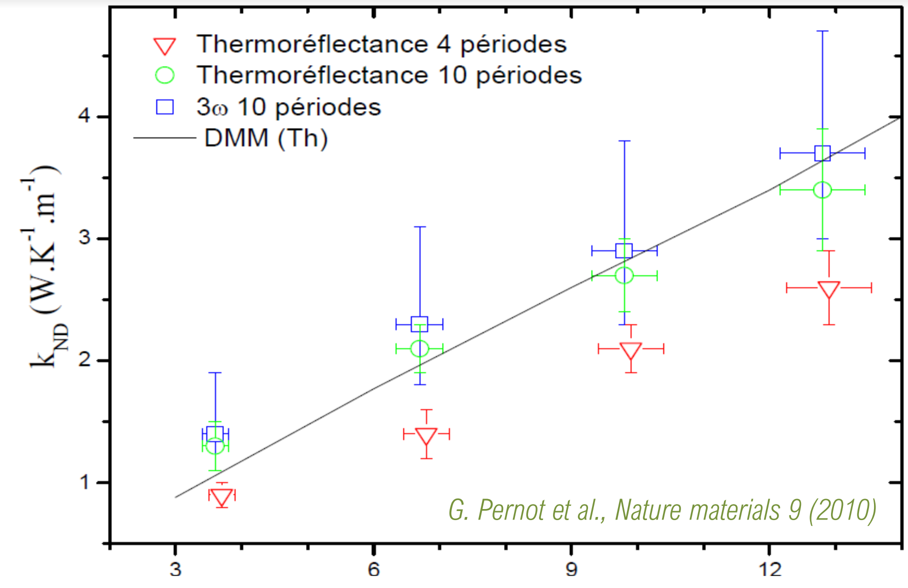
OPTICAL METHODS
FDTR: some results

Thermal conductivity tailoring via non-Fourier transport

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



Ge islets



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

Associated measurement modelling

- Fourier modelling
- Diffuse Mismatch model (D

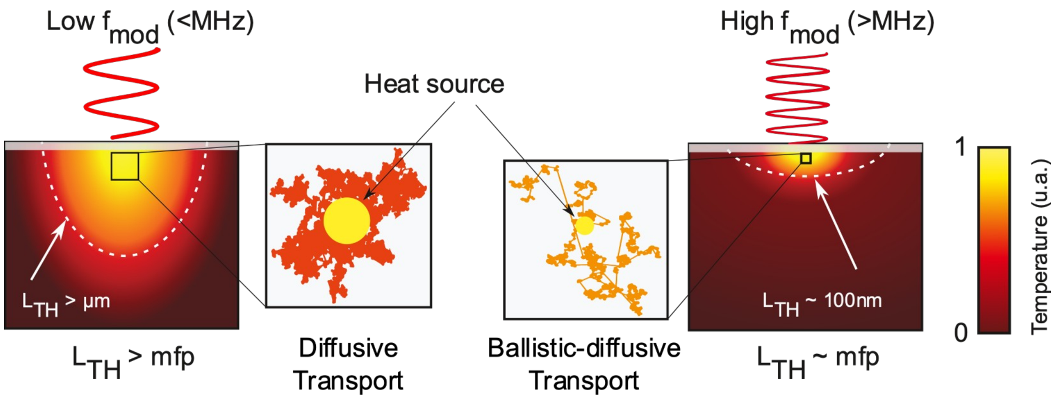
Modelling current limitations

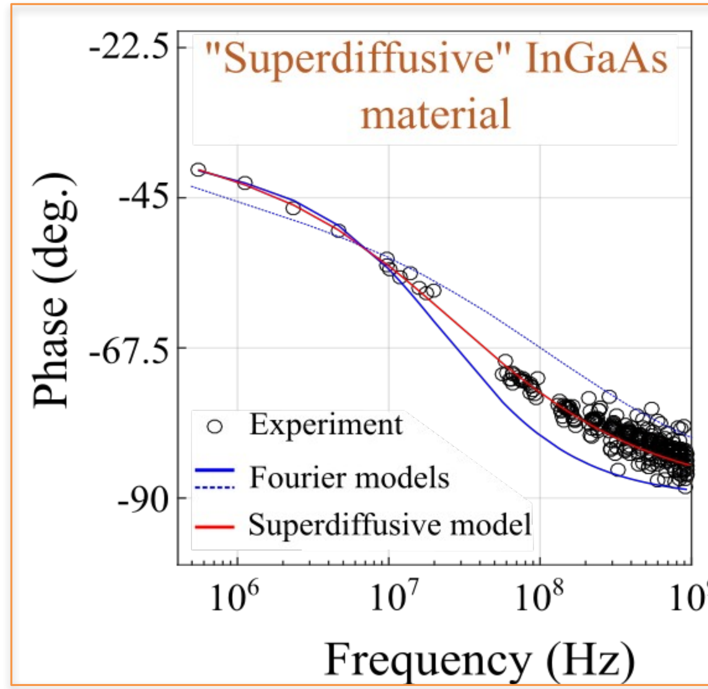
- Fourier modelling does not include ballistic transport in Si layers

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 dat

Error of 30% in thermal conductivity identifica

Error of 300% in thermal interface resistance

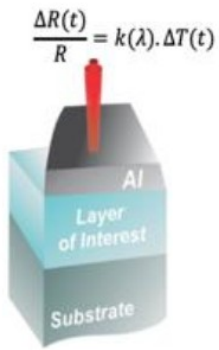
Deviation from Fourier when the heat source dimension becomes comparable to phonon mfp

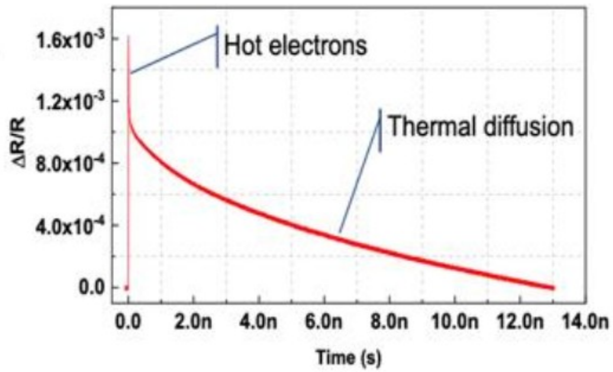
Need for nanometrology

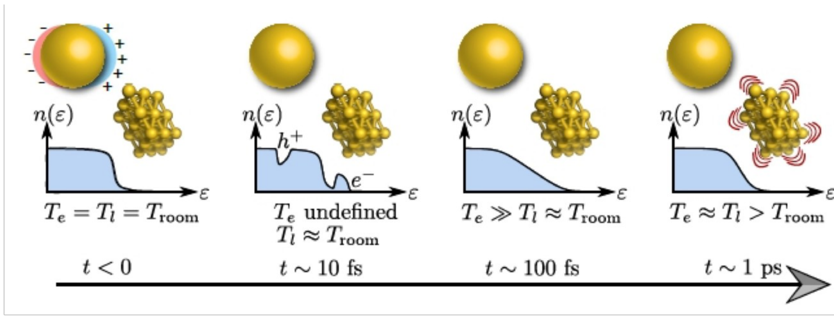
- New model for ballistic-diffusive heat transfer in thin films (Lévy flight modelling)

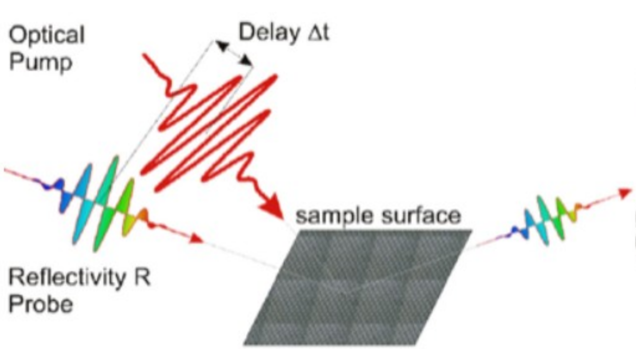
OPTICAL METHODS
TDTR: some results

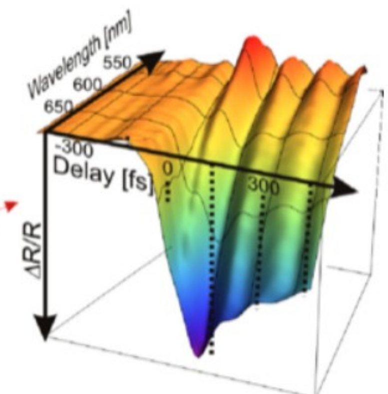
From non equilibrium hot electrons to phonon thermal diffusion











Associated measurement modelling

- 2 temperature model

Current measurement limitation

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

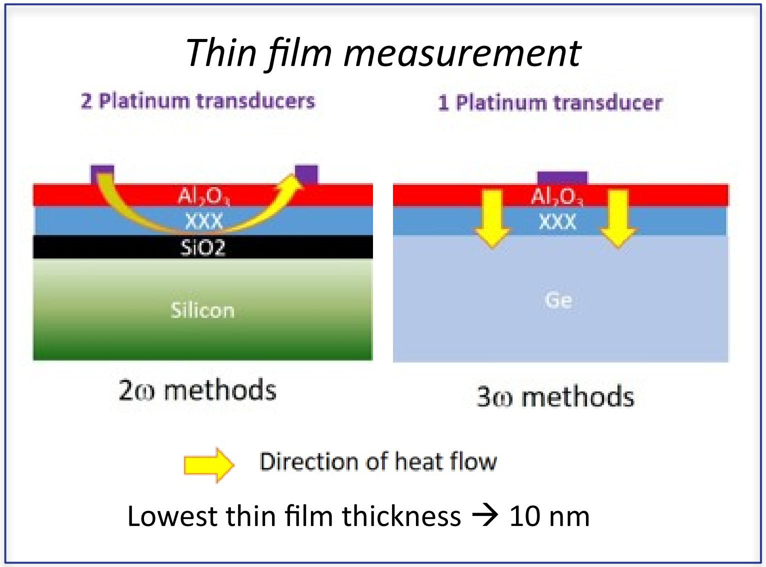
Need for nanometrology

- New model for thermal – optical coupling

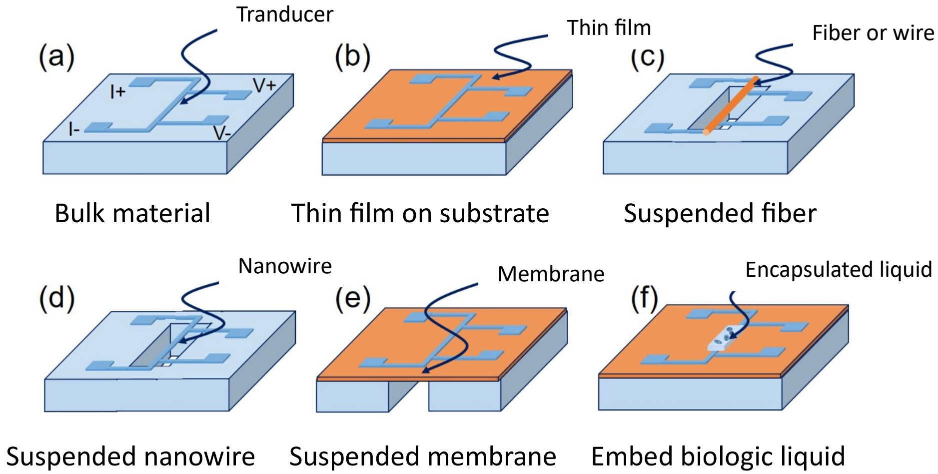
ELECTROTHERMAL METHODS

Performances and application fields

2 and 3ω methods



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)

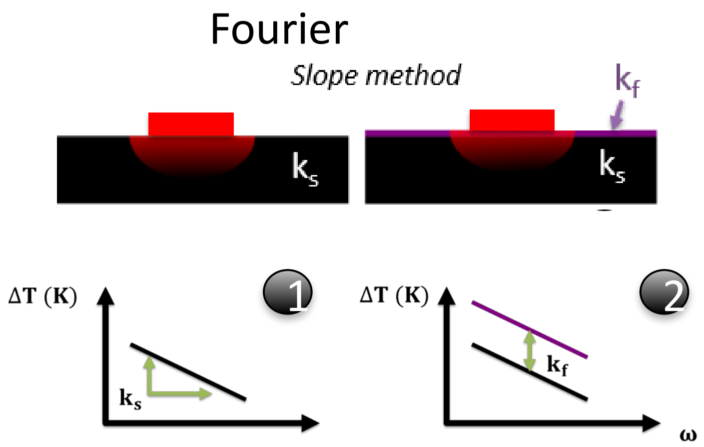
- Possible with playing with the size of the tranduceur, experiment temperature, characteristic dimension of the structure

ELECTROTHERMAL METHODS

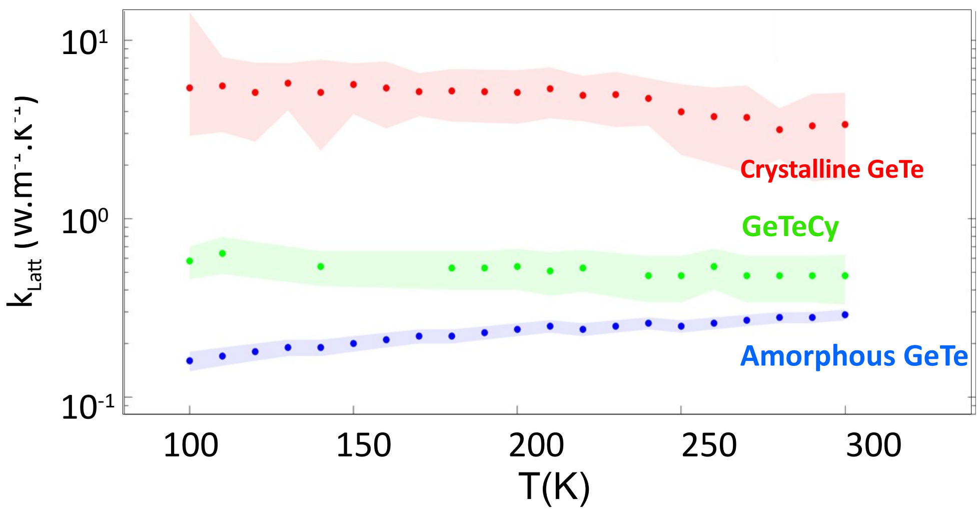
3ω method : some results

GeTe based-phase change materials

Associated measurement modeling



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

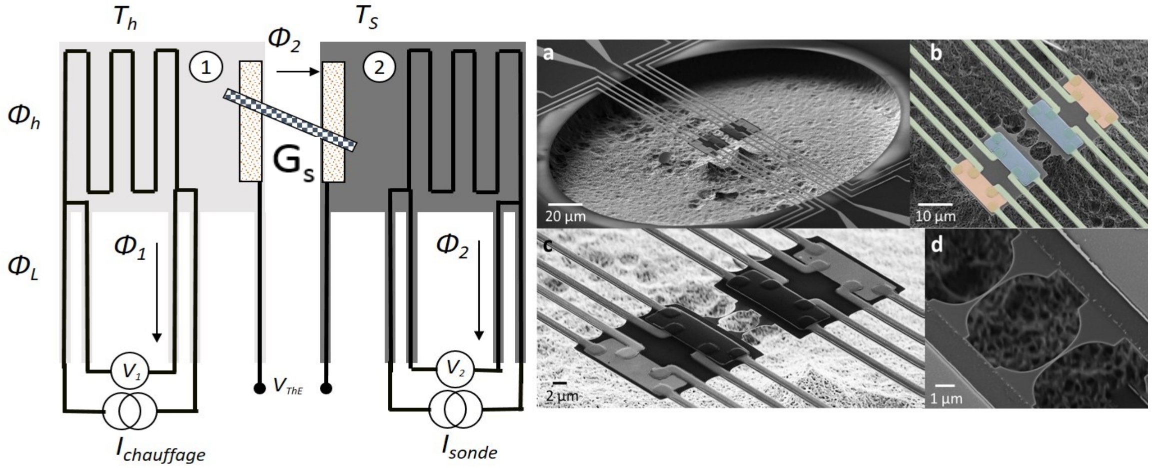
- Reference for thermal boundary resistance between thin films

ELECTROTHERMAL METHODS

Performances and application fields

Thermal bridge method

Temperature gradient across the nanostructures



Power sensitivity
15 attoWatts $\sqrt{\mathrm{Hz}}^{-1}$
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…

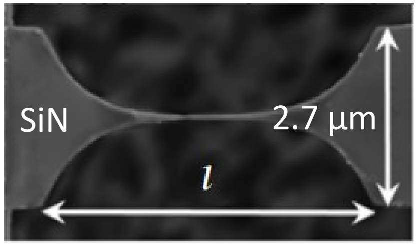
Measured thermal parameters:

- Thermal transport only (heat flux)

ELECTROTHERMAL METHODS

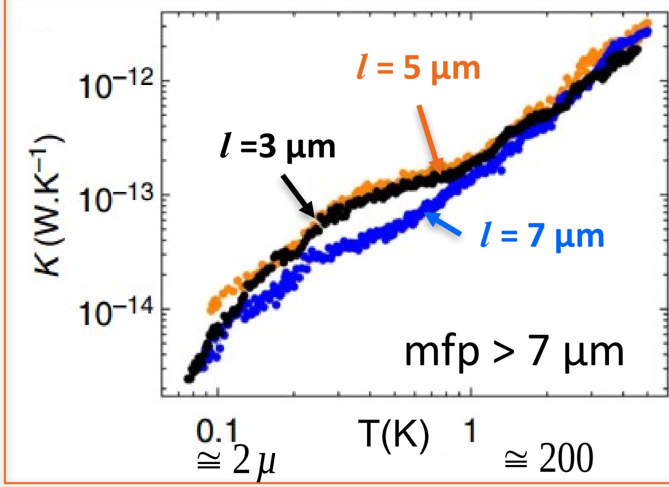
Thermal bridge method: some results

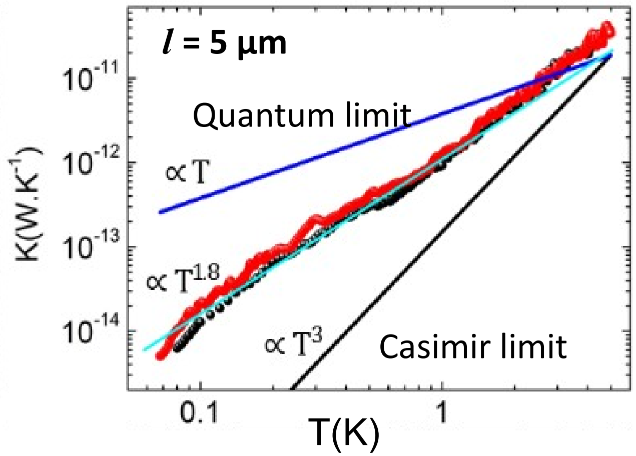
Heat conduction in ballistic 1D phonon waveguide



Nanowire .diameter < 100 nm

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





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

Current measurement limitations

- Thermal link to the heat bath not controlled

Modelling current limitations

- Full thermal model of the double membrane s

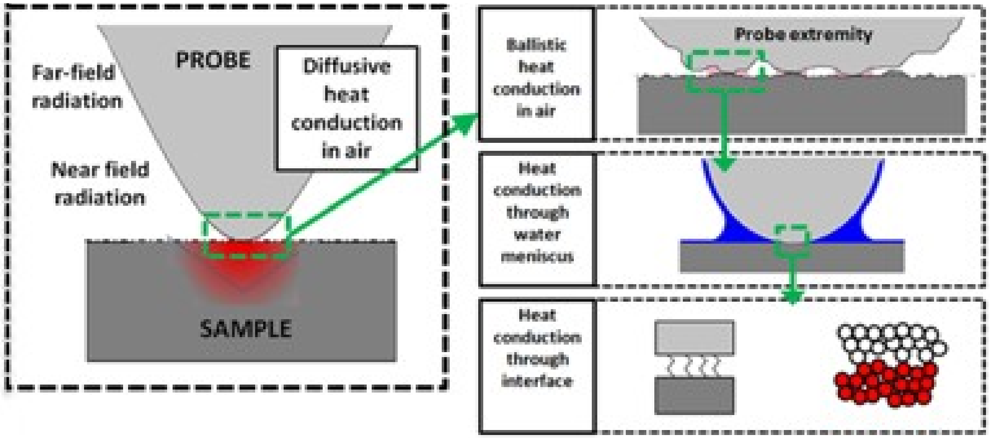
Need for nanometrology

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

Club nanoMétrologie

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

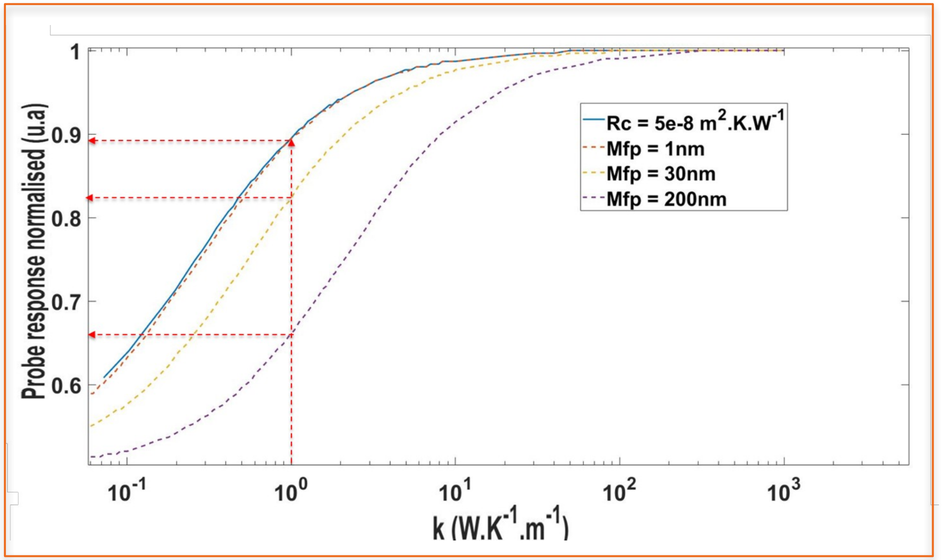
SThM: some results

Calibration with bulk samples

Credits: PhD thesis S. Douri

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



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**
- **heat transport in nanometre-sized contacts**

especially in the non-Fourier limit

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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Other animators and contributors

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Matériaux

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