### BOOK OF ABSTRACTS

### **Oral Presentations**



2023

# Parch, 15, 16 and 17

### Friday March 17<sup>th</sup>

### 10.30 am – 12.30 pm

Room 13/14

### **Program of the session**

#### **Chairs: Jérémie DREVILLON & Séverine GOMES**

10:30   Measuring temperature dependent optical indexes by spectroscopic ellipsometry   Simon HURAND • Univ. Poitiers – PPrime, Poitiers – France     11:00   A sensor for manipulation of heat carried by phonons at the nanoscale and very low temperature   Boris BRISUDA • CNRS - Inst. NEEL, France     11:15   Electrothermal measurements on nanolayered structures by means of 3-omega method and Scanning Thermal Microscopy   Carlos ACOSTA • CNRS - CETHIL, France     11:30   Highly sensitive thermal niobium nitride nanoprobe for scanning thermal microscopy   Olivier BOURGEOIS • CNRS - Inst. NEEL, France     11:45   Synthesis of Au-Ag nano-hybrids to investigate heat transfer   Clément VECCO-GARDA • CNRS - ICMCB, France     12:00   Nanostructure thermal measurement: heat conduction within a single nanowire   Séverine GOMÈS • CNRS - CETHIL, France	NANOSCALE HEAT TRANSFER - MEASUREMENT			
A sensor for manipulation of heat carried by phonons at the nanoscale and very low temperature   Boris BRISUDA • CNRS - Inst. NEEL, France     11:00   Electrothermal measurements on nanolayered structures by means of 3-omega method and Scanning Thermal Microscopy   Carlos ACOSTA • CNRS - CETHIL, France     11:10   Highly sensitive thermal niobium nitride nanoprobe for scanning thermal microscopy   Olivier BOURGEOIS • CNRS - Inst. NEEL, France     11:45   Synthesis of Au-Ag nano-hybrids to investigate heat transfer   Clément VECCO-GARDA • CNRS - ICMCB, France     12:00   Nanostructure thermal measurement: heat conduction within a single nanowire   Séverine GOMÈS • CNRS - CETHIL, France	10:30	Measuring temperature dependent optical indexes by spectroscopic ellipsometry	Simon HURAND • Univ. Poitiers – PPrime, Poitiers – France	
Electrothermal measurements on nanolayered structures by means of 3-omega method and Scanning Thermal Microscopy   Carlos ACOSTA • CNRS - CETHIL, France     11:30   Highly sensitive thermal niobium nitride nanoprobe for scanning thermal microscopy   Olivier BOURGEOIS • CNRS - Inst. NEEL, France     11:45   Synthesis of Au-Ag nano-hybrids to investigate heat transfer   Clément VECCO-GARDA • CNRS - ICMCB, France     12:00   Nanostructure thermal measurement: heat conduction within a single nanowire   Séverine GOMÈS • CNRS - CETHIL, France	11:00	A sensor for manipulation of heat carried by phonons at the nanoscale and very low temperature	Boris BRISUDA • CNRS - Inst. NEEL, France	
Highly sensitive thermal niobium nitride nanoprobe for scanning thermal microscopy   Olivier BOURGEOIS • CNRS - Inst. NEEL, France     11:30   Synthesis of Au-Ag nano-hybrids to investigate heat transfer   Clément VECCO-GARDA • CNRS - ICMCB, France     12:00   Nanostructure thermal measurement: heat conduction within a single nanowire   Séverine GOMÈS • CNRS - CETHIL, France	11:15	Electrothermal measurements on nanolayered structures by means of 3-omega method and Scanning Thermal Microscopy	Carlos ACOSTA • CNRS - CETHIL, France	
11:45   Synthesis of Au-Ag nano-hybrids to investigate heat transfer   Clément VECCO-GARDA • CNRS - ICMCB, France     12:00   Nanostructure thermal measurement: heat conduction within a single nanowire   Séverine GOMÈS • CNRS - CETHIL, France	11:30	Highly sensitive thermal niobium nitride nanoprobe for scanning thermal microscopy	Olivier BOURGEOIS • CNRS - Inst. NEEL, France	
12:00 Nanostructure thermal measurement: heat conduction within a single Séverine GOMÈS • CNRS - CETHIL, France nanowire	11:45	Synthesis of Au-Ag nano-hybrids to investigate heat transfer	Clément VECCO-GARDA • CNRS - ICMCB, France	
	12:00	Nanostructure thermal measurement: heat conduction within a single nanowire	Séverine GOMÈS • CNRS - CETHIL, France	
12:15 Elaboration of perovskite thin films with metal-insulator transition for infrared optical modulation Arthur TAUSCH • Univ. Poitiers - Inst. Pprime, France	12:15	Elaboration of perovskite thin films with metal-insulator transition for infrared optical modulation	Arthur TAUSCH • Univ. Poitiers - Inst. Pprime, France	



### Keynote Speakers NANOSCALE HEAT TRANSFER - MEASUREMENT



#### Simon HURAND

**University of Poitiers I Professor** *PPrime Institute https://sfa.univ-poitiers.fr/physique/membres/hurand-simon/* 

#### **BIOGRAPHY**

Simon HURAND is a material scientist with a main focus on the experimental study of the electrical and optical properties of thin films. His PhD work at ESPCI in Paris focused on the study and the control of superconductivity in LaAlO3/SrTiO3 oxides interface through low-temperature electrical measurement. After a Post-doctoral at ICFO in Barcelona on the electro-mechanical properties of freestanding carbon nanotubes, he joined the Université de Poitiers in 2016 as a Maître de conférences (assistant professor). Since then, he developped an expertise on the measurement of the optical properties of bulk materials and thin films through spectroscopic ellipsometry in the visible and infrared ranges, as well as low-temperature electrical measurements. His main research topic now focuses on the electrical and optical properties of a new family of 2D materials called MXenes.

#### MEASURING TEMPERATURE DEPENDENT OPTICAL INDEXES BY SPECTROSCOPIC ELLIPSOMETRY

Spectroscopic Ellipsometry is a powerful tool to unravel the optical properties of materials (bulk or thin films), allowing to extract their optical indexes. It is non destructive, fast, and can be performed in ambient environment or as an in-situ measurement. While reference optical indexes of materials are often available in the litterature for the UV-visible-NIR range, it is often hard to find similar references in the infrared range. Morever, optical indexes available from a reference "ideal" material are often not transposable to a given preparation method (e.g. Physical Vapor Deposition) because it can induce for example porosity, non-stoechiometry, partly amorphisation or multi-grain microstructure, among others. This can induce significant discrepancy in the simulation of the radiation behavior of materials or nanoscale heterostructures. When it comes to temperature dependent optical indexes, the available data base of optical indexes becomes even more sparse. Therefore, there is a need for the measurement of optical indexes of specific materials, in order to correctly represent radiation properties of materials, including spectral variation (up to the infrared range) and temperature dependence. In this presentation, I will introduce the principle of Spectroscopic Ellipsometry, with a focus on the limitations of the measurement and the analysis method to extract the optical indexes, and present some examples of temperature-dependent optical indexes from the UV to the FIR range.

#### **KEYWORDS:**

Spectroscopic Ellipsometry; Optical properties; Infrared; Thin films



# Parch, 15, 16 and 17

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**Keywords:** nanoscale heat transfer, phononic crystal, cryogenic temperatures, thermal rectification

Disciplinary fields involved: Physics

Sustainable Development Goals\* eventually involved in your research: energy recovery

#### A sensor for manipulation of heat carried by phonons at the nanoscale and very low temperature

B. Brisuda<sup>1</sup>, J. Canosa<sup>2</sup>, V. Doebele<sup>1</sup>, C. Polanco Garcia<sup>3</sup>, T. Crozes<sup>1</sup>, N. Mingo<sup>3</sup>, J.-F. Robillard<sup>2</sup>, L. Samidayar<sup>1</sup>, O. Bourgeois<sup>1</sup>

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- 3. CEA LITEN, 16 avenue des Martyrs 38000 Grenoble, France

The manipulation of heat fluxes is possible by acting on the transport of phonons at the nanoscale using advanced nanostructuration in what is currently called thermal metamaterials. This is one of the major challenges of the current small-scale energy management.

In our experiment we are using a suspended double-membrane based sensor functioning at very low temperatures (<100mK) using the state-of-the-art niobium nitride thermometry with attowatt sensitivity [1] [2]. This enables us to demonstrate innovative thermal effects involving large phonon mean-free-paths and long phonon-wavelength (>100nm) in the non-Fourier regime.



**Figure 1**: SEM images of the suspended membranes (left). The plot of the resistance variation with temperature (50 mK to 1K) of different NbN thermometers (right).







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The nanostructured samples (see Figure 1 left) are installed in between the membranes allowing the measurement of heat flux in both directions. They are nanostructured using microelectronic technology at the length scale of the phonon wavelength which is on the order of 100 nm at 1K in the case of silicon nitride. The length of the sample is inferior to the phonon mean-free path ensuring the ballistic regime of phonon transport. Two types of nanostructured samples are studied in this experiment: one is a periodic system allowing the study of ballistic phononic transport in phononic crystal structures, the other is a non-linear anisotropic lattice meant for the study of thermal rectification.

#### References

[1] A. Tavakoli, K. Lulla, T. Crozes, E. Collin, and O. Bourgeois, Heat conduction in a ballistic 1D phonon waveguide indicate breakdown of the thermal conductance quantization, Nature Commun. 9, 4287 (2018).

[2] Nguyen, T., Tavakoli, A., Triqueneaux, S. et al. Niobium Nitride Thin Films for Very Low Temperature Resistive Thermometry. J Low Temp Phys 197, 348–356 (2019)

Acknowledgment: ANR HANIBAL







NQNO

## 2023

**Keywords:** Nanoscale heat transfer, Thermal conductivity, Thermal boundary resistance, 3omega and Scanning Thermal Microscopy techniques

Disciplinary fields involved: Physics

Sustainable Development Goals eventually involved in your research: Climate Action (Goal 13)

#### Electrothermal measurements on nanolayered structures by means of the 3 $\infty$ method and scanning thermal microscopy

C. Acosta<sup>1</sup>, M. D'Esperonnat<sup>2</sup>, R. Carretero<sup>1</sup>, D. Han<sup>2</sup>, R. Moalla<sup>2</sup>, G. Saint-Girons<sup>2</sup>, R. Bachelet<sup>2</sup>, M. Dewitte, M. Brouillard<sup>3</sup>, J.-F. Robillard<sup>3</sup>, N. Horny<sup>4</sup>, S. Gomes<sup>1</sup>, P. O. Chapuis<sup>1</sup>

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<sup>2</sup> Institut des Nanotechnologies de Lyon (INL), UMR 5270 CNRS, Ecole Centrale de Lyon, 69134 Ecully, France

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<sup>4</sup> Institut de Thermique, Mécanique, Matériaux (ITheMM), Université de Reims Champagne-Ardenne, 51100 Reims, France

Properly managing heat transfer at sub-micrometer scales is an issue of interest in various fields, for instance for thermoelectric devices, in particular those based on oxides, or miniaturized integrated circuits, wich contain metal/semiconductor interfaces or Schottky contacts. Understanding the mechanisms of heat conduction in these systems requires particularly the determination of sample thermal conductance, thin-film effective thermal conductivities and thermal boundary resistances; these are key quantities driving various phenomena at such scales [1]. As the temperature range of use of these devices can be quite varied and/or wide, the study of these quantities as a function of the temperature is crucial in their characterization. In this work, we present experimental results of electrothermal measurements performed on planar nanolayered structures, including a detailed sensitivity analysis, and comparisons with semi-analytical computations [2-3]. Thin-film oxides such as SrTiO<sub>3</sub>/La<sub>0.75</sub>Sr<sub>0.25</sub>CrO<sub>3</sub>/SiO<sub>2</sub> are considered in a first case, and metal-semiconductor Si/Pt structures are analyzed in a second time. The 3-omega method highlighted by Cahill [2] is applied, which is based on the deposition of linear metallic heaters on the surface of the samples and the possible coating of electrically-insulating thin films. For the Si/Pt structure, in addition to thermal conductance measurements, we are also interested in determining the temperature field around the interface by means of scanning thermal microscopy.

#### References:

- [1] D. G. Cahill et al., Appl. Phys. Rev. 93, 793 (2003)
- [2] D. G. Cahill, Rev. Sci. Instrum. Vol. 61, No. 2 (1990)
- [3] T. Borca-Tasciuc, A. R. Kumar and G. Chen, Rev. Sci. Instrum. 72, 2139 (2001)

<u>Aknowledgment</u>: We acknowledge the support of the French RENATECH network and projects MITO (ANR-17-CE05-0018) and EFICACE (ANR-20-CE09-0024)





### P: itiers March, 15, 16 and 17

C'NQNO

## 2023

**Keywords:** Scanning Thermal Microscopy (SThM), Micro-nanoscale heat transfer, NbN nanothermometry, temperature at small length scale **Disciplinary fields involved:** Physics

### Highly sensitive thermal niobium nitride nanoprobe for scanning thermal microscopy

R. Swami<sup>1,2\*</sup>, D. Singhal<sup>1,2</sup>, J. Paterson<sup>1,2</sup>, J. Maire<sup>1,2</sup>, G. Julié<sup>1,2</sup>, S. Le-Denmat<sup>1,2</sup>, J.F. Motte<sup>1,2</sup>, G. Hamaoui<sup>4</sup>, J. Yin<sup>5</sup>, J.F. Robillard<sup>5</sup>, P.-O. Chapuis<sup>3</sup>, S. Gomès<sup>3</sup>, & <u>O. Bourgeois<sup>1,2</sup></u>

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- 5. Institut d'Electronique, de Microélectronique de Nanotechnologie (IEMN), Villeneuve d'Ascq cedex, France

Study of local temperature fields and thermophysical properties in nanometric-scale devices and structures play a crucial role in developing new technologies where thermal management is an issue. Scanning Thermal Microscopy (SThM) is one of the best available techniques to assess temperature fields with a high spatial resolution [1]. However, the growing need for efficient SThM measurements calls for better thermal sensitivity to address current research and development challenges in thermal engineering for nanoelectronics and nanotechnology. In this work, we demonstrate the integration of a highly sensitive thermometer of an alloy of niobium nitride (NbN) on commercial silicon nitride (SiN) AFM probes [2,3]. The electrical resistance of the NbN thermometer on a tip along with its temperature coefficient were characterized. Results highlight the high sensitivity of NbN probe compared to commercial SThM probes. We finally demonstrate thermal measurements of nanostructured samples under vacuum with the new probe using the 3 omega technique. We characterize the thermal resistance of the contact on silicon and sapphire and use it to measure thermal conductivity of various materials like polymer, DNA and dielectric substrate.





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**Figure 1**: SEM of the SThM tip with NbN thermometer (left). Resistance variation with temperature of the NbN thermometers around room temperature (right).

#### **References:**

[1] T. Wagner et al., Beilstein J. Nanotechnol. 9, 129 (2018).

[2] O. Bourgeois et al., Rev. Sci. Intruments, **12**, 126108 (2006).

[3] T. Nguyen et al., J. Low Temp. Phys. 197, 348 (2019).

[4] R. Swami, G. Julié, D. Singhal, J. Paterson, J. Maire, S. Le-Denmat, J.F. Motte, S. Gomes, and O. Bourgeois, Nano Futures **6**, 025005 (2022).





# Parch, 15, 16 and 17

C'NQNO

## 2023

**Keywords:** plasmonic nanoparticles, single nanoparticles detection, heat transfer, nano-hybrids **Disciplinary fields involved:** Chemistry, Physics

#### Synthesis of Au-Ag nano-hybrids to investigate heat transfer

#### C. Vecco-Garda<sup>1\*</sup>, C. Panais<sup>2</sup>, N. Lascoux<sup>2</sup>, N. Del Fatti<sup>2</sup>, A. Crut<sup>2</sup>, S. Mornet<sup>1</sup>, M. Treguer-Delapierre<sup>1</sup>

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2. Institut Lumière Matière, Univ. Claude Bernard, CNRS, Lyon, France

The modalities of energy transfer at the nanoscale strongly differ from those at the macroscopic scales notably because of the increased role played by interfaces. With the development of nanotechnology, understanding and mastering these mechanisms is crucial for fundamental and technological advances in many fields such as electronics, thermoelectricity or sensing <sup>[1]</sup>. In this communication, we will show how with self-assembly approaches, we can construct hybrid nanosystems with well-defined geometry and stability to investigate the modalities of heat transfer in the time domain phonon transport at single particle level <sup>[2]</sup>. Strong coupling and precise positioning between plasmonic nano-units can be achieved via regioselective surface modification. Self-assembly approaches, in particular based on electrostatic interactions, endow the assembly of nanoparticles of different size, shape, composition into desired structures. We will investigate how the internal thermalization and the cooling dynamics within the nano-hybrids are affected by their geometry by exploitation of pump-probe optical spectroscopy.



Figure 1 : Example of nanohybrid cluster made from assembly of different colloidal building blocks

#### **References**:

- 1. Snyder G. J., Toberer E. S. *Nat. Mater*. Vol. 7, (2008), 105-114.
- 2. Rouxel R., Diego M., Medeghini F., Maioli P., Rossella F., Vallée F., Banf F., Crut A., Del Fatti N. J. Phys. Chem. C, Vol. 124, (2020), 15625-15633





### P: itiers March, 15, 16 and 17

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## 2023

**Keywords:** thermal conduction, nanowire, scanning thermal microscopy, nanostructure, measurement

Disciplinary fields involved: physics and engineering

#### Nanostructure thermal measurement: heat conduction within a single nanowire

#### S. Gomès<sup>1</sup>, J. M. Sojo Gordillo<sup>2</sup>, P. Vincent<sup>3</sup>, D. Renahy<sup>1</sup>, P.-O. Chapuis<sup>1</sup>, A. Morata<sup>3</sup>, A. Tarancon<sup>2,4</sup>

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- 4. IMB-CNM (CSIC), Campus UAB, 08193, Bellaterra, Barcelona, Spain

Despite the interest for nanowire application in thermoelectric generation and microelectronics after recent successful implementation in miniaturized devices, a proper evaluation of the thermal conductivity in such nanostructures still represents a great challenge. In this work, we demonstrate a spatially resolved technique based on a combined scanning thermal microscope (SThM) [1] - scanning electron microscope (SEM) instrument [2] for the assessment of

the thermal conductivity of a single suspended silicon nanowire.

Figure 1: SEM images of the self-heated resistive SThM nanotip (on the left) approaching the measured nanowire and (on the right) in contact with the measured nanowire at different locations along the nanowire.



#### **References:**

- [1] S. Gomès, A. Assy and P.-O. Chapuis, Phys Stat Solidi A, 2015, 212:477–94.
- [2] D. Renahy, A. Assy and S. Gomès, THERMINIC, 2015.

**Acknowledgment:** The research leading to these results has received funding from the European Union Seventh Framework Programme (grant agreement n°604668), the ANR through the project ATTSEM ANR-10-LABX-0064 (LabEx iMUST).





### P: itiers March, 15, 16 and 17

C'NQNO

2023

**Keywords:** Thin films, thermochromism, infrared, heat radiation, metaheuristic **Disciplinary fields involved:** Chemistry, Physics

### Elaboration of perovskite thin films with metal-insulator transition for infrared optical modulation

#### Arthur Tausch<sup>1</sup>, Fabien Capon<sup>2</sup>, Jérémie Drévillon<sup>1</sup>, Simon Hurand<sup>1</sup>, Karl Joulain<sup>1</sup>,

- 1. Institut Pprime, (UMR 3346 CNRS), Departement FTC, Université de Poitiers, Poitiers, France
- 2. Institut Jean Lamour, (UMR 7198 CNRS), Departement CP2S, Université de Lorraine, Nancy, France

Mixed valence manganites present a metal-insulator transition that is not only described by a strong variation in the material's resistivity but also by an optical contrast between the conductor and the insulator state [1]. Such variations in complex optical indexes with temperature characterized using infrared variable angle spectroscopic ellipsometry paired with meta-heuristic methods allows the materials to be a good candidate for multilayer coatings for infrared optical modulation applications. In this work we demonstrate that  $Sm_{0.5}Ca_{0.5}MnO_3$  thin films deposited by magnetron co-sputtering exhibit a thermochromic effect associated with variations of the complex refractive index around room temperature Using scattering matrix method for semi-infinite thin films and an Improved Grey Wolf Optimization meta-heuristic algorithm [2], it is possible to optimize the emissivity variation of a multi-layered material with temperature in the transparency bands of earth atmosphere [3]. Such tendency can allow the control of the material's spectral radiance and therefore it's detectability with thermography.



#### **References:**

[1] P. Laffez, M. Zaghrioui, L. Reversat and P. Ruello. Thermal emittance changes at the charge ordering transition of  $Sm_{0.35}Ca_{0.65} MnO_3$ , Appl. Phys. Lett 93 (2008).

[2] M. H. Nadimi-Shahraki, S. Taghian and S. Mirjalili. An improved grey wolf optimizer for solving engineering problems, Expert Systems With Applications 166 (2021) 113917

[3] A. Hervé, J. Drévillon, Y. Ezzahri, K. Joulain, Radiative cooling by tailoring surfaces with microstructures: Association of a grating and a multi-layer structure, Journal of Quantitative Spectroscopy and Radiative Transfer, 221 (2018).





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### Friday March 17<sup>th</sup>

### 2.00 pm – 3.45 pm

Room 13/14

### **Program of the session**

### **Chairs: Nolwenn FLEURENCE & Raphaël SOMMET**

#### NANOSCALE HEAT TRANSFER - MEASUREMENT

14:00	Monte Carlo simulations of heat transport in nano-devices, a brief overview and recent developements	<b>David LACROIX</b> • Univ. Lorraine – LEMTA, Nancy – France
14:30	Micro and nanoscale heat transfer investigation by 3D FEM for Scanning Thermal Microscopy	Sarah DOURI • LNE - CETHIL, France
14:45	Combination of thermal measurements and simulation to extract the hotspot temperature of GaN HEMT transistors	Khalil KARRAME • Univ. Limoges - XLIM, France
15:00	Full Band Ab-initio Monte Carlo simulation of phonon transport in GaAs nanostructures	Junbum PARK • Paris-Saclay Univ C2N, France
15:15	Passive nighttime radiative cooling with Black Silicon	<b>Armande HERVE</b> • Univ. Gustave Eiffel - ESYCOM, France
15:30	Investigation of nanostructured materials of topography free surface by Scanning Thermal microscopy	Nathaly CHAARAOUI • Univ. Reims Champagne Ardennes - iTheMM, France



### evnot NANOSCALE HEAT TRANSFER - MEASUREMENT



#### David LACROIX

**University of Lorraine I Professor** Energy & theoretical and applied mechanics laboratory https://lemta.univ-lorraine.fr

#### **BIOGRAPHY**

David LACROIX is Professor at the Université de Lorraine in Nancy. Within the LEMTA (Laboratoire Energies & Mécanique Théorique et Appliquée) his group is interested in the study of thermal transport at the nanoscale by both experimental (Scannig Thermal Microscopy, Thermoreflectance, Raman spectroscopy, ...) and theroretical (DFT, MD, ...) approaches. His research activities are mostly related to the modelling of thermal transport in nanostructured semiconductors using Monte Carlo techniques through the development of numerical tools dedicated to the resolution of the Boltzmann Trasport Equation for phonons. The applications of his research concerns thermal

management and thermoelectricity.

#### MONTE CARLO SIMULATIONS OF HEAT TRANSPORT IN NANO-DEVICES, A BRIEF OVERVIEW AND **RECENT DEVELOPEMENTS**

Models and numerical tools devoted to the simulation of thermal material properties as well as heat transport in nano and micro-structures have been more and more popularized during the two last decades along with the rapid development of computing ressources. Atomistic scale modeling, which includes Density Functional Theory (DFT) and Molecular Dynamics (MD) based methods, is now very popular to predict with few or no assumption material transport properties allowing to explore in-silico lot of different pure or not compounds. However, even if those approaches are powerfull and increasingly accurate they inhently suffer of a major drawback, namely the computational resources required to perform simulations on devices whose size exceeds hundreds of nanometers. Yet the latter, such as nanowire, nanofilms, nanoporous structures, superlattices, etc., are often the ones which are produced in clean room and that are valuable for a lot of applications. In addition, for these nanosystems, the classical numerical approaches based on the assumption of a continuous medium (bulk-like) are often inadequate to describe the physics of transfers and effects such as ballistic transport or interface resistance. For semiconductors, what we call the "mesoscopic" scale (10nm~10µm) needs alternative tools to model and simulate heat exchange and thermal transport properties. To tackle this issue, we have developped in the group for many years, a simulation environment dedicated to the resolution of the Boltzmann Transport Equation for phonons using stochastic approaches known as Monte Carlo (MC) methods. With such methodology semiconductor devices with lengthscale that falls into the mesoscopic range can be accurately modelled in a broad range of temperatures; taking into account complex geometrical features and/or interface occurrence. In addition, recent developments shows that such calculations can be performed at fixed temperature and take advantage of Green-Kubo formalism to derive from heat flux autocorrelation thermal conductivity tensor in complex systems such as phononic membranes. In this talk, we will give a brief review of these MC models from non-equilibrium to equilibrium approaches and their application to the calculation of heat transport properties in nano-devices.

#### **KEYWORDS:**

Nanoscale heat transfer; Boltzmann Transport Equation; Monte Carlo Method; Thermal properties; Green-Kubo

### Keynote Speakers NANOSCALE HEAT TRANSFER - MEASUREMENT



#### David LACROIX

University of Lorraine I Professor Energy & theoretical and applied mechanics laboratory <u>https://lemta.univ-lorraine.fr</u>

#### **REFERENCES (THE FOLLOWING)**

[1] Lacroix, David and Joulain, Karl and Lemonnier, Denis, "Monte Carlo transient phonon transport in silicon and germanium at nanoscales", Phys. Rev. B, 72 (6), 064305, 2005.

[2] Chaput, Laurent and Larroque, Jérôme and Dollfus, Philippe and Saint-Martin, Jérôme and Lacroix, David, "Ab initio based calculations of the thermal conductivity at the micron scale", Appl. Phys. Lett. 112, 033104, 2018.

[3] Lacroix, David and Isaiev, Mykola and Pernot, Gilles, "Thermal transport in semiconductors studied by Monte Carlo simulations combined with the Green-Kubo formalism", Phys. Rev. B, 104 (16), 165202, 2021.

[4] This work was performed in the framework of the ANR MESOPHON (ANR-15-CE30-0019) and the ANR SPIDERMAN (No. ANR-18-CE42-0006) projects funded by the French Agence Nationale de la Recherche.

[5] This work was performed using HPC resources from GENCI-TGCC and GENCI-IDRIS (Grant No. 2020-A0080907186), in addition HPC resources at EXPLOR mesocentre were partially provided by the FEDER thanks to "STOCK NRJ" that is co-financed by the European Union within the framework of the Program FEDER-FSE Lorraine and Massif des Vosges 2014-2020





C'NQNO

## 2023

**Keywords** SThM, nanoscale heat transfer, nanoscale interfacial transport phenomena, modelling

Disciplinary fields involved: Physics

Sustainable Development Goals\* eventually involved in your research:

#### Micro and nanoscale heat transfer investigation by 3D FEM for Scanning Thermal Microscopy

#### Sarah DOURI<sup>1, 2</sup>, Nolwenn FLEURENCE<sup>1</sup>, Jacques HAMEURY<sup>1</sup>, Séverine GOMES<sup>2</sup>

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With the development of micro and nanotechnologies, traceable techniques for physical property characterization at micro and nanoscales are required. To investigate the thermal properties at these scales, the Scanning Thermal Microscopy (SThM) technique is promising [1]. In the frame of thermal conductivity (k) analysis, the experimental calibration of SThM probes is based on the measurement of a set of bulk materials with well-known thermal conductivities. The resulting calibration curve represents a measurand linked to the probe electrical resistance variation, as a function of k. For the determination of an unknown thermal conductivity, an electrothermal model describing the heat dissipation within the probe-sample-environment system is required. Previous works have demonstrated that the simple analytical model proposed by Fischer [2] for microprobes still needs to be improved for nanoprobes [1]. In order to better reproduce the measurements with the KNT nanoprobe we have developed a 3D numerical electrothermal model of the sample-probeenvironment system for the second generation of KNT probes using the finite element method. The probe response (variation of the electrical probe resistance) in vacuum and in air out of and in contact with a sample were investigated. We find that the resistive element dimensions and room temperature are the most influencing model parameters on the probe. Considering the contact thermal resistance Rc and the ballistic regime due to the nanosize of the probe-sample thermal contact in our model we also demonstrate through simulations that parameters such as Rc and the amorphous or crystalline nature of the sample have an impact on the k sensitivity range of the technique. These results give new paths to improve the calibration methodology. The probe response in air is also investigated as a function of the probe-sample distance taking into account ballistic heat transfer through air.

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2023

Pitiers March, 15, 16 and 17

C'NQNO

**Keywords:** GaN HEMT, Gate Resistance Thermometry, Thermoreflectance, FEM thermal Simulation

Disciplinary fields involved !: Physics

### Combination of thermal measurements and simulation to extract the hotspot temperature of GaN HEMT transistors

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Two electrical methods and one optical method are used to measure the temperature as close as possible to the hotspot of a 150nm gate length GaN HEMT. One of the electrical methods is based on Gate Resistance Thermometry (GTR) [1] and the other one is based on the On State resistance Ron obtained from I(Vgs, Vds) characterizations [2]. Both electrical methods involve the variation of an electrical resistance versus temperature as sensitive parameter but in different direction. The optical one, based on CCD-thermoreflectance test bench [3], uses the reflectivity variation principle with temperature to measure the surface temperature.

The use of the GTR electrical method allows the characterization of the temperature along the gate close to the hotspot region and averages the temperature over the gate width. This method demonstrates a relative linearity in the variation of thermal resistance as function of the applied dissipated power and notably a higher thermal resistance value compared to the conventional way of R<sub>ON</sub> extraction. We may notice that with the On-State resistance, the average is realized over the Source-Drain length. The optical method based on ThermoReflectance (TR) allows the measurement of a "surface temperature" few nanometers above the hotspot. As the channel is physically inaccessible, access to the hotspot is impossible. In order to extract the temperature of the hotspot, the different measurement methods are combined with simulation. Measurement and simulation results demonstrated that the temperature of the hotspot is 25% higher than the temperature of the outer surface closest to the hotspot

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**Keywords:** Monte Carlo method, Density functional theory, Phonon transport, Nanostructure **Disciplinary fields involved:** Physics

**Sustainable Development Goals\* eventually involved in your research:** Affordable and clean energy (Goal 7)

#### Full Band Ab-initio Monte Carlo simulation of phonon transport in GaAs nanostructures

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In view of effective thermal management, nanostructures based on thermoelectric (TE) semiconducting materials such as Si and GaAs are a key technology for increasing the energy efficiency of electronic devices [1]. Despite significant progress in thermal transport modeling beyond Fourier's law, analysis of the nanostructures that fully capture their properties are still scarce [2]. In this work, we present a Full-Band Monte Carlo approach based on the Boltzmann's transport equation for phonons using ab initio parameters [3]. All necessary material parameters are calculated by ab initio method in the framework of the density functional theory (DFT), e.g. the



Fig 1. (a) Thermal conductivity of GaAs nanostructures nd (b) modal contribution as function

phonon frequency, group velocity and phonon-phonon scattering rates in the temperature range from 0 and 1000 K. Thermal conductivity and phononic properties of GaAs cross/in-plane nanofilms and nanowires are analyzed in all phonon transport regimes with different device lengths, widths, temperatures and porosities.

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Keywords: Metamaterials, Radiative cooling, Thermal emission Disciplinary fields involved: Physics Sustainable Development Goals\* eventually involved in your research: Affordable and Clean Energy (Goal 7)

#### Passive nighttime radiative cooling with Black Silicon

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Black Silicon (BSi) is a nanostructured material. It demonstrates high absorptivity and emissivity on a large spectrum [1]. These specific properties make it useful for numerous applications [2-3]. Here, we study BSi for a night-time passive radiative cooling application. Atmospheric transmittivity is maximum between 8 and 13  $\mu$ m [4-5], but it also shows some transmission for other wavelengths, so a wideband large absorptivity could be promising.

We consider different BSi samples we fabricated using cryogenic plasma etching and characterized using FTIR spectroscopy to obtain their emissivity. We then compute the radiative cooling power of the considered samples as a function of their temperature given by the difference between the power radiated by the samples and the power they absorb from the atmospheric thermal radiation. We assume in a first approximation that our samples are insulated from the surroundings through conduction and convection. We compare High (HD) and Low doping (LD) BSi (doping levels up to  $5 \times 10^{19}$  cm<sup>-3</sup>) with flat silicon substrates (High and Low Doping) used as a reference. We observe that passive cooling occurs when the cooling power is positive when the sample temperature is equal to the ambient temperature. When the sample temperature decreases below ambient temperature, the cooling power decreases gradually. We show that BSi cooling power is significantly larger (up to a factor 2) than its flat silicon counterpart while HD BSi shows slightly better results than LD BSi.

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**Keywords:** SThM, inverse techniques, local thermal conductivity **Disciplinary fields involved:** Physics

#### Investigation of nanostructured materials of topography free surface by Scanning Thermal microscopy

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Nanotechnology requires characterization technics for nanosystems and nanomaterials. Scanning thermal microscopy based on Atomic Force Microscopy technique is a tool for investigating material's thermal measurements and heat transfer mechanisms at the micro/nanoscale. This project aims to investigate local thermal properties of nanostructured materials. For that, a buried nanostructured sample was specially designed and fabricate. The sample consists of SiO<sub>2</sub> step of triangular shape deposited on Silicon substrate and covered by polished CVD SiO<sub>2</sub>. The interface of SiO<sub>2</sub>/Si layer is linear, and its thickness is upgradable between 400 to 2150 nm. Obtaining thermal information about nanostructured materials using Scanning Thermal properties requires the use of probe with thermal sensor at the tip. Our study deals with Wollaston resistive probe. For a comprehensive interpretation of experimental results obtained by SThM, we developed a physically consistent and numerically solved heat transfer model of the probe-sample system in order to characterize/estimate the effect of probe volume on thermal conductivity measurements. From the numerical model and the experimental results, we applied an inverse technique allowing us the investigation of thermal conductivity of SiO<sub>2</sub> layer that has variable thickness deposited on Silicon substrate. The results verified that the thermal conductivity decreases with respect to the layer thickness of the material. As the layer thickness of SiO<sub>2</sub> decreases the thermal conductivity decrease and we found a value of 1.023 W/m.K for 576 nm layer thickness of SiO<sub>2</sub>. The material acts like a bulk sample from 1400 nm thickness with a local thermal conductivity of 1.378 W/m.K

