“Beyond Fourier” Thematic day

Non-Fourier heat transfer at the nanoscale
Paris │ September 9, 2022

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Program and conference abstracts

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Premise

Dear colllegues,

Welcome to Paris for the thematic day “Beyond Fourier”.

Understanding heat transfer at the nanoscale remains one of the greatest intellectual challenges in the field of thermal dynamics, by far the most relevant under an applicative standpoint. When thermal dynamics is confined to short time and length scales and/or at low temperatures, non-diffusive heat transport regimes set in, ranging from ballistic to hydrodynamic. Depending on the system, different heat carriers may be involved such as electrons, phonons and spins just to mention few of them. Within these regimes, the validity of Fourier’s law, the milestone constitutive relation describing diffusive heat transport, fails, thus calling for novel heat transfer characterization techniques and interpretative schemes. Under an applicative standpoint, managing non-Fourier heat transport is a key-factor for micro- and nano-devices operations and their further downscaling.

This thematic day focuses on recent developments in the general topic of non-Fourier heat transfer at the nanoscale. The scope is to bring together different views on this emerging topic, merging experimental investigations and theoretical studies. This meeting is an opportunity for the community to share ideas and foster new collaborations.

We wish you pleasents scientific discussions in a relaxed and friendly environement.

Francesco Banfi, Paolo Maioli and Konstantinos Termentzidis

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Practical informations

Conference venue
Address: Espace Hamelin, 17 rue Hamelin, Paris 16ème
https://www.espace-hamelin.fr

Public transportation
Subway stations: Boissière (Line6) – Iéna (Line 9)
Bus: 22-30-32-63-82

The restaurant is on site

Invited Speakers

Mauro Antezza

Professor, Département de Physique, Université de Montpellier

Radiative heat transfer between nanostructured objects

Ilaria Zardo

Professor, Departement Physik, University of Basel

Engineering thermal transport in nanowires

Program

09:00 – 09:30	Registration
09:30 – 09:40	Opening by the organizing committee
09:40 – 10:00	Séverine Gomes, CETHIL - INSA Lyon *Why is heat transport modelling required for nanometrology?*
10:00 – 10:20	Jérôme Saint-Martin, C2N - Université Paris Saclay *A Beyond Fourier semi-analytical thermal model based on two-flux approach*
10:20 – 10:40	Yangyu Guo, iLM - Université Lyon 1 *Atomistic simulation of heat transport across nanometer gaps*
10:40 – 11:20	**Invited: Mauro Antezza, Université de Montpellier** *Radiative heat transfer between nanostructured objects*
11:20 – 11:40	Alvarez F. Xavier, Universitat Autonoma de Barcelona *Hydrodynamic experimental observations in bulk semiconductors*
11:40 – 12:00	Marco Gandolfi, Università degli Studi di Brescia *Temperature waves in layered correlated materials and temperonic crystals*
12:00 – 13:30	**Lunch**
13:30 – 14:10	**Invited: Ilario Zardo, University of Basel** *Engineering thermal transport in nanowires*
14:10 – 14:30	Marc Bescond, IM2NP - Université Aix-Marseille *Cooling and Seebeck effects in double-barrier semiconductor heterostructures*
14:30 – 14:50	Raja Sen, LSI - École Polytechnique Palaiseau *Ab initio calculations of the thermoelectric phonon drag effect in semiconductor nanostructures*
14:50 – 15:10	Paul Desmarchelier, CETHIL - INSA Lyon *Parabolic-like heat radial distribution in core-shell nanowires*
15:10 – 15:30	Guéric Etesse, IM2NP - Université Aix-Marseille *A novel structure of cooling nano-devices: the quantum cascade cooler*
15:30 – 16:45	**Coffee Break and Poster Session**
16:45 – 17:00	Closing remarks

Posters

Solène Hoflack and Jérôme Saint-Martin. C2N, Université Paris Saclay *Monte Carlo simulation of static and dynamic thermal properties of nanostructures*
Jelena Sjakste. Laboratoire des Solides Irradiés, École Polytechnique *Electron-phonon coupling and ultrafast dynamics of hot carriers in semiconductors: from interpretation of photoemission experiments to transport simulations*

Abstracts

INVITED

Radiative heat transfer between nanostructured objects

Mauro Antezza (1,2)

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(2) Institut Universitaire de France, Paris, France.

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After a rapid introduction to the basic physical concepts of radiative heat transfer and the presentation of the general theory valid for arbitrary objects [1-2], I will focus on the study of the radiative heat transfer between two identical metallic one-dimensional lamellar gratings. To this aim I will present and exploit a modification to the widely used Fourier modal method, known as adaptive spatial resolution, based on a stretch of the coordinate associated with the periodicity of the grating. I show that this technique dramatically improves the rate of convergence when calculating the heat flux, and that there is a remarkable amplification of the exchanged energy, ascribed to the appearance of spoof-plasmon modes. By comparing our results to recent studies, we find a consistent quantitative disagreement with some previously obtained results going up to 50% [3].

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INVITED

Engineering thermal transport in nanowires

C. Arya (1), D. de Matteis (1), Y. Kaur (1), B. Abad Mayor (1), A. K. Sivan (1), M. De Luca (1), M. Y. Swinkels (1), X. Cartoixà (2), R. Rurali (3), I. Zardo (1)*

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The recently growing research field called "Nanophononics" deals with the investigation and control of vibrations in solids at the nanoscale. Phonon engineering leads to a controlled modification of phonon dispersion, phonon interactions, and transport [1,2]. However, engineering and probing phonons and phonon transport at the nanoscale is a non-trivial problem. In this talk, we discuss how phononic properties and thermal transport can be engineered and measured in nanowires [3] and the challenges and progresses in the measurement of the thermal conductivity of nanostructures and low dimensional systems [4].

The concept of phonon engineering in NWs is exploited in superlattice (SL) NWs. We experimentally show that a controlled design of the NW phononic properties can be decided à la carte by tuning the SL period. Furthermore, Raman thermometry is used to probe the temperature profile along the NWs upon application of a thermal grandient, enabling the differentiation between ballistic and diffusive flow regimes (Figure 1).

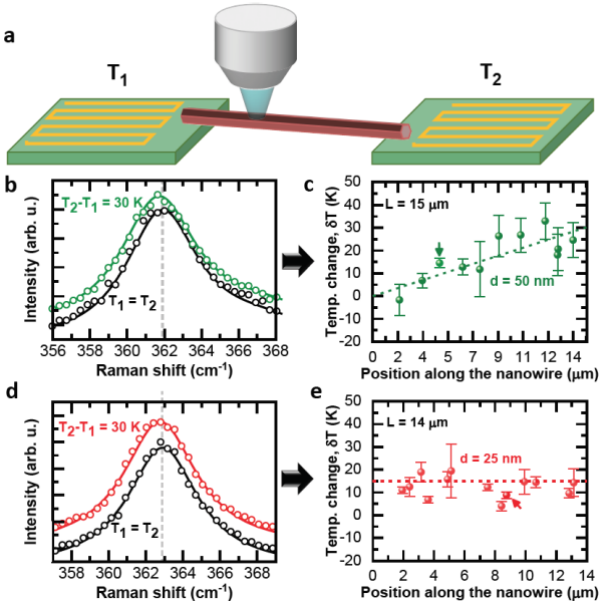

Fig. 1. a) Illustration of the microdevice with NW used for the measurements of the thermal profile. A laser spot is moved along the wire and Raman spectra are acquired for T_1=T_2=300 K and T_1= 300 K, T_2= 300 K +ΔT . b) Spectra measured at the position indicated by the arrow in c for a NW with d = 50 nm and L = 15 µm. Solid lines are Lorentzian fits to the spectra. c) Resulting temperature profile along the NW while applying ΔT = 30 K using the Pt meander heaters. The dashed line is the expected profile for purely diffusive heat flow. d) and e) The same as b) and c) but for a NW with d = 25 nm and L = 14 µm. The dashed line in e is the expected profile for purely ballistic transport.

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Why is heat transport modelling required for nanometrology?

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Nanomaterials and electronic components consist of systems made of multiple interfaces, nanoscale contacts and boundaries, where operate a plethora of heat generation and transfer phenomena including mixed regimes beyond diffusive transport, i.e., ballisticity, superdiffusion and hydrodynamics. Thus, key questions related to the interfacial thermal energy transfer and the heat transport in nanometre-sized contacts need to be addressed. Great challenges still remain although significant progresses have been accomplished in thermal-transport engineering. Heat transport in nanometre-sized materials is still poorly understood owing to in particular the lack of:

- proper modelling of nanoscale heat transport phenomena involved in measurement methodologies, in addition to the current limitations of characterization techniques,
- modelling strategy to fill the gap between the different length scales (atomic and nano-scale, micro and macro-scales) involved in materials and composite systems,
- experimental validation of modelling of heat transport at nanoscale,
- modelling strategy to account for multi-phenomena coupling.

Experimental investigation of nanomaterials (nanowires, nanofilms, nanomembranes, 2D materials suspended or on substrate, 3D nanomaterials, superlattices…) and nanosystems requires characterization techniques with nanometric spatial resolution. Moreover, the highly-localized non-equilibrium thermal processes (heat propagation and scattering processes on nanoscopic length scales, and thermal transport across atomic-layer interfaces) occur at ultrashort time scale. The need of a new generation of sensors combining ultra-high spatial and temporal resolution is now required.

Optical, electrothermal methods and scanning probe techniques (e.g., Fig. 1) have been developed in these directions. Their lateral spatial resolution can reach from a few hundreds of nanometres for far field optical methods (radiometry [1], photoreflectance [2]) to few tens of nanometres for vacuum Scanning Thermal Microscopy (SThM) [3]. These techniques are usually used to determine parameters that require local thermal equilibrium to be reached, such as thermal conductivity, temperature, and thermal properties of nano-objects as well as the thermal conductance of interfaces and contacts. However, the analyses typically use continuum models based on Fourier's law of heat conduction. It is well known that Fourier's law implies a diffusive propagation of the heat carriers and therefore breaks down when considering ballistic transport and when heat sources are comparable to or smaller than the energy carrier mean free path. New models of measurements must be developed to interpret/design experiments improving these approaches of measurements involving phonon ballistic-diffusive regime

that occurs for phonons between electron-phonon thermalisation and thermal diffusion; this regime can start in tens of ps and last up to tens of ns [4], nanoscale heating sources and nanoscale thermal contacts.

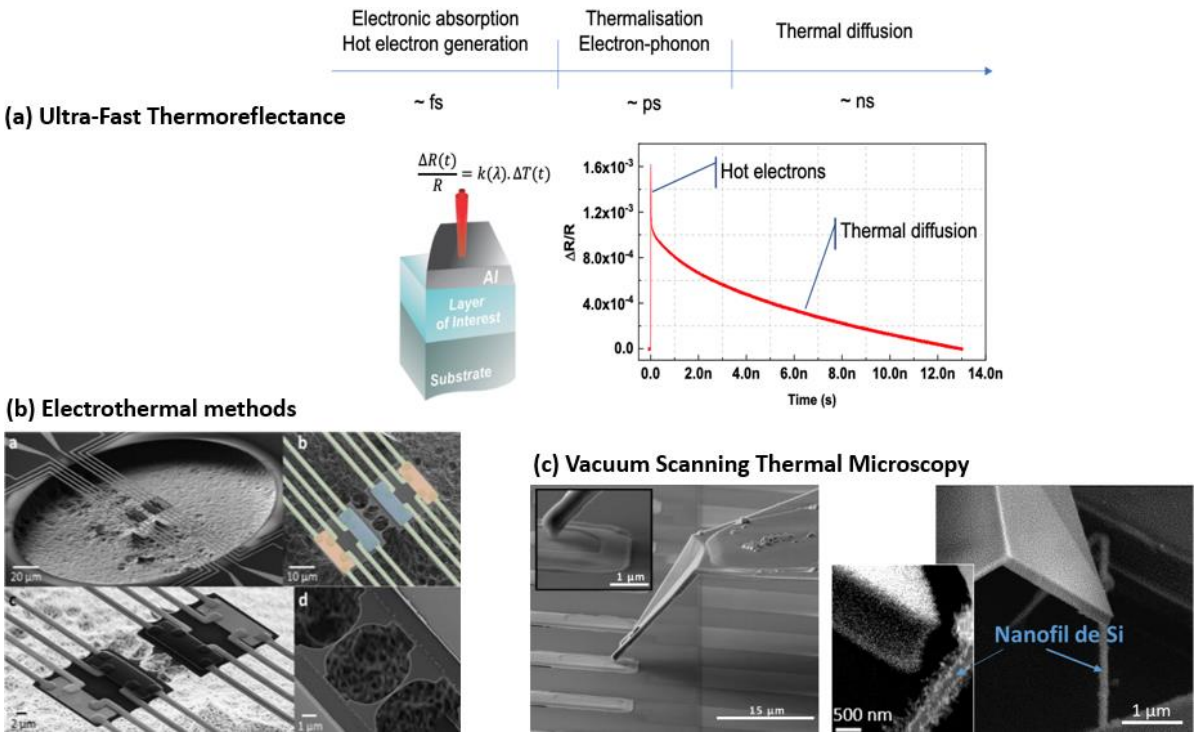

Fig. 1. (a) Time Domain ThermoReflectance (TDTR) [2]: Typical TDTR signal recorded from fs to ns time scales. The wavelength λ is chosen in order to have the best temperature sensitivity $\kappa(\lambda)$ for a given metal transducer. Scanning Electron Microscope images of (b) differential sensors dedicated to very low temperature measurements with nanowires between the membranes [5], (c) a SThM nanotip contacting an electronic component (left) and a suspended nanowire (right) [6].

Ultra-fast laser-based thermoreflectance techniques are the only methods fulfilling the requirement of dynamic effect study in systems far from thermal equilibrium. However, the necessary use of metallic coating (transducer) brings up new issues about hot electron energy decay into phonons and the transmission of these latter across interfaces. Scanning thermal microscopy provides high temperature, which makes it ideal to study heat energy transfer between sub-micrometre layer interfaces but its low temporal resolution complicates the investigation of non-equilibrium effects. SThM may open new avenues for the investigation of physical phenomena in the quantum regime, at least at low temperatures.

Consequently, key questions must be addressed related to the interfacial thermal energy transfer and the heat transport at nanometre-sized contacts especially in the non-Fourier limit. This is true not only for understanding heat dissipation in materials and devices but also for measuring parameters which require local thermal equilibrium and dynamic effects in systems out of thermal equilibrium.

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A beyond Fourier semi-analytical thermal model based on two-flux approach

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In this article, a semi-analytical model based on only three intrinsic parameters able to describe heat transport in heterostructures in all phonons transport regimes (i.e. diffusive, ballistic, and quasi-ballistic regimes) is presented. This formalism considers the phonon dispersion and scattering rates as input parameter and can be used to investigate systems of various sizes from the nano- to the micro-scale. The resulting model agrees well with the thermal conductance and temperature profiles predicted by advanced Monte Carlo simulation even in the presence of interfaces.

The parameters of the thermal model are defined by using the concept of hemispherical temperatures T^+ and T^-. They are defined, even in out-of-equilibrium conditions, as the temperature of phonon sub-populations with a positive/negative velocity (oriented flux toward the cold/hot thermostat, respectively).

Using these hemispherical temperatures, a new comprehensive set of thermal parameters can be defined for the effective thermal conductivity κ_{eff}, the ballistic conductivity $\kappa_{ballistic}$ and he interface conductance G_{int}:

$$Q = \kappa_{eff} \frac{\Delta T_{contact}}{L} \qquad (1)$$

$$Q = \kappa_{ballistic} \frac{\Delta T_{local}}{L} \qquad (2)$$

$$G_{int} = \frac{Q}{\Delta T^I} \qquad (3)$$

where the temperature differences are defined as follows:

$\Delta T_{local}(x) = T^+(x) - T^-(x)$

$\Delta T_{contact} = T_H - T_C$,

$\Delta T^I = T^+(x-\varepsilon) - T^-(x+\varepsilon)$

With a hot thermostat at a hot temperature T_H and a cold one at a cold temperature T_C. Further details on the inner workings of the simulator were given in previous works [1]

Finally, the total thermal conductance G^{total} in a heterostructure made of *N* homogeneous materials (of length L_i, with effective thermal conductivity $\kappa^i_{effective}$. defined in Eq 2) with $G_I^{i,i+1}$ the thermal conductance of the interface between material *i* and material *i+1*, is given by:

$$G^{total} = \frac{Q}{T_{hot} - T_{hold}} = \left[\sum_{i=1}^{N} \frac{L_i}{\kappa^i_{effective}} + \sum_{i=1}^{N-1} \left(-\frac{1}{G^i_{ballistic}} + \frac{1}{G_I^{i,i+1}} - \frac{1}{G^{i+1}_{ballistic}} \right) \right]^{-1} \qquad (1)$$

$$\kappa^{i}_{\text{effective}} = \frac{\Omega}{(2\pi)^3} \sum_{s,\ mat\ i} \hbar\omega_s \left|v_{s,x}\right| \lambda_{\text{mpf}} \frac{\partial f_{\text{BE}}}{\partial T}(\omega_s, \bar{T}) \qquad (2)$$

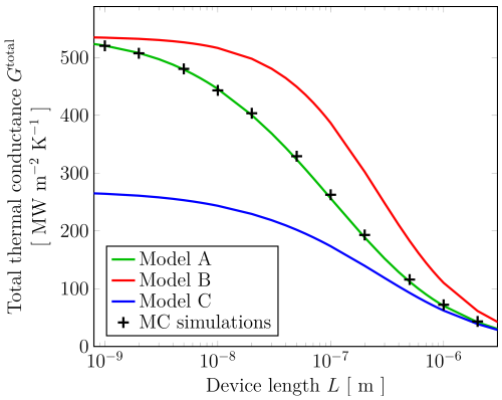

Fig. 1. Total thermal conductance of diffusive Si/Si junctions versus length.

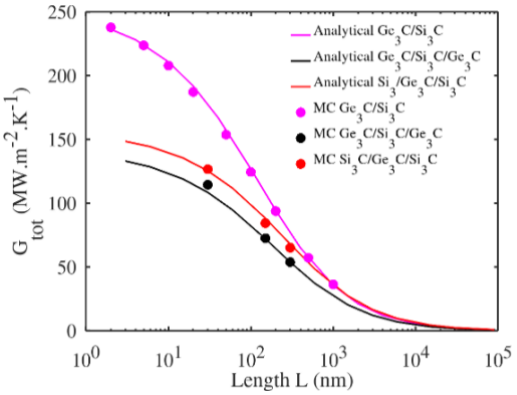

Fig. 2*:* Total thermal conductance of the Si/Ge simple and double heterostructures: Monte Carlo results vs. semi-analytical model. T = 300 K.

It is shown in Figure 1 that our approach provides a significantly better estimation of the thermal conductance than the common approach of thermal resistances in series for systems of length around a few tens of nanometers. The difference with the previous approaches is due to the presence of the ballistic conductance $G^{i}_{ballistic}$ in each side of the interface (which is a material dependent parameter defined in [1]).

As shown in Figure 2, our analytical modeling (Eq. 1) can very well reproduce our results of Monte Carlo simulation [2] of phonon transport in ballistic or quasi-ballistic transport regimes as well as in diffusive regime, even in the presence one or two thermal interfaces.

Finally, our work bridges the gap between the previous thermal model extending Fourier's law into a homogeneous system and the work carried out in the case of non-homogeneous systems with semi-transparent interfaces. Besides, our approach naturally solves the historical paradox called the thermal interface paradox because it is based on two different local temperatures for the two populations of phonons having a positive or negative velocity, respectively. In addition, we rigorously discuss the validity and limitation of the common approach considering three series resistances in the case of heterostructures.

The presented definitions of effective thermal conductivity and interface conductance based on hemispherical temperatures can be applied in many simulation and experimental settings. They provide a very convenient set of parameters clearly separating the influence of materials, geometry and interfaces. The role of ballistic conductance and its contribution in nanostructures is also clarified.

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Atomistic simulation of heat transport across nanometer gaps

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The understanding of extremely near-field heat transport remains an open question. The two recent experimental reports [1, 2] in this regime have shown controversial results. Kloppstech et al. [1] observed giant thermal conductance whereas Cui et al. [2] found much smaller values below the detection resolution. Phonon tunneling across nanogaps has been put forward as an important mechanism explaining the giant heat transfer observed experimentally.

In this work [3], we present a fully three-dimensional atomistic simulation framework by combining the molecular dynamics (MD) and phonon non-equilibrium Green's function (NEGF) method. The relaxed atomic configuration and interatomic force constants of metallic nanogaps are generated from MD as inputs into harmonic phonon NEGF. Phonon tunneling across gold-gold and copper-copper nanogaps are quantified, and is shown to be a dominant heat transport channel for gap size below 1nm. Through a comparison of the results by MD and NEGF as anharmonic and harmonic approaches respectively, we demonstrate ~20-30% contribution of lattice anharmonicity to phonon tunneling across the nanogap. In addition, the electrostatic interaction turns out to have negligible effect for the small bias voltage typically used in experimental measurements. Our atomistic simulation is consistent with the experiment by Cui et al. [2] while still not able to explain the giant heat transfer in the experiment by Kloppstech et al. [1]. We conclude that phonon tunneling alone can not explain the giant heat transfer seen in the latter experiments.

The present atomistic simulation framework provides a more pertinent modeling of the phonon heat transport channel and hitherto detailed information of the heat current spectrum across metallic nanogaps. Our study contributes to deeper insight into heat transport in the extremely near-field regime, as well as hints for the future experimental investigation.

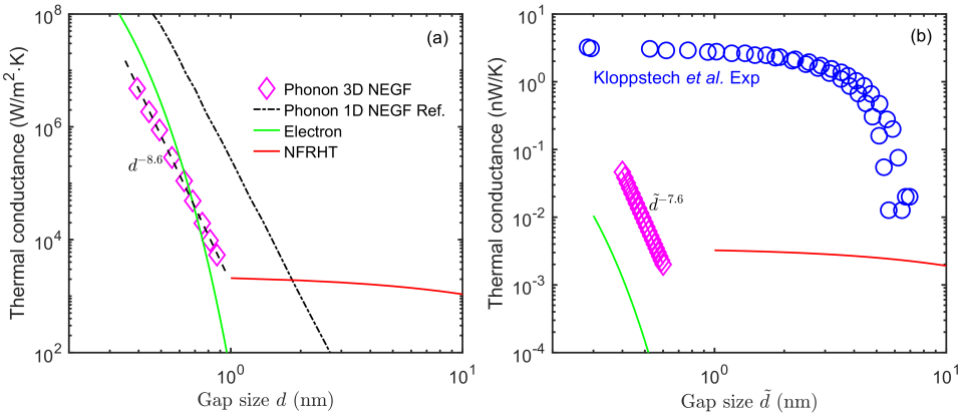

Fig. 1. Thermal conductance of Au-Au nanogap : (a) plate-plate configuration; (b) tip-plate configuration. The 1D phonon NEGF result in (a) is from Ref. [4].

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Hydrodynamic experimental observations in bulk semiconductors

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A large number of experimental observations incompatible with the classical Fourier description of thermal transport at the nanometer and in the picosecond scales has been reported in the last decade [1,2]. Despite the theoretical efforts done in the topic, a model able to describe the gathered data at all length and time scales is still not available.

Two different descriptions have been proposed. Phonon hydrodynamics has been used as a framework to model thermal transport in materials where momentum conservation in phonon-phonon collisions is important. For other situations, a kinetic description based on the propagation of independent phonons, in what is called quasiballistic description, has been developed. The fundamental difference between them is in the number of length or time scales required to describe the observations. While in the hydrodynamic approach, a single scale is enough, in the quasiballistic description, the full set of phonon scales is necessary. For graphene and other 2D materials, the hydrodynamic approach has been the traditional main stream, while the quasiballistic approach has been more used for classical bulk semiconductors.

In the last years, some experiments and theoretical descriptions seems to be challenging this traditional splitting. On the one side, some predictions of the hydrodynamic regime for 2D materials like the second sound velocity have put on doubt the standard approach. On the other side, collective phonon behavior like the use of a single time scale to describe thermal decay in a silicon substrate [3] or the observation of second sound in germanium [4] seem to indicate that the hydrodynamic description could be used in these semiconductors. This could be an indication that a more unified framework could be proposed.

The talk will cover some of the most recent evidences in the theoretical and experimental research on thermal transport and we will analyze them in the framework of the Kinetic/Collective model (KCM) [5], developed to give a more generalized framework to describe thermal experiments.

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Temperature Waves In Layered Correlated Materials And Temperonic Crystals

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Abstract – We demonstrate that layered strongly correlated materials can be tailored to sustain a wide spectrum of electronic heat transport regimes, from ballistic, to hydrodynamic and diffusive. The temperonic crystal, a metamaterial made of correlated materials working in the hydrodynamic regime, is introduced to control the wave-like thermal transport.

The capability to access ultrafast thermal dynamics recently gave access to striking phenomena that take place in materials at the nanoscale before complete local energy equilibration among heat carriers is achieved. For instance, non-Fourier heat transport regimes have been reported for hot spots dimensions inferior to the phonon mean free-path, in which energy is ballistically carried point to point, or have been engineered via nano-patterning of dielectric substrates. As a consequence of the existence of two non-thermal populations, wave-like thermal transport, often referred to as second sound, has been predicted in graphene, both in the frame of microscopic and macroscopic models. Temperature wavelike phenomena have been recently observed at high temperatures in graphene [1] and 2D materials [2] on sub-nanosecond timescales and scheme for their coherent control have been proposed. So far most of the effort has been devoted to phononic non-Fourier heat transport, where, only recently, a theoretical framework, covering on equal footing Fourier diffusion, hydrodynamic propagation, and all regimes in between, has been proposed. On the contrary, electronic non-Fourier heat transport remains relatively unexplored.

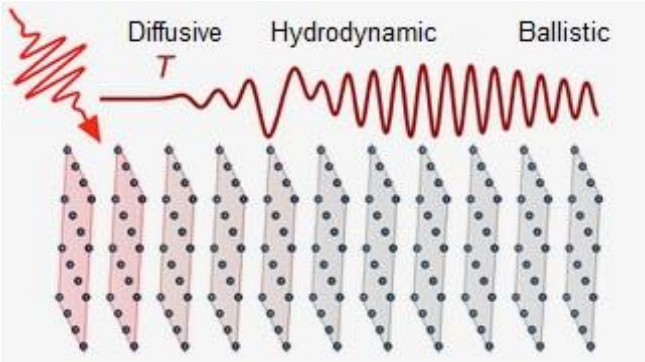

Fig. 1. Sketch of the thermal dynamics occurring in a LCM. Each plane represents a layer and the first layers on the left are excited by a light pulse (the thermal transport occurs from left to right). The red curve on top schematizes the evolution of the temperature in space at a fixed time. On a fixed layer, a ballistic front arrives first, followed by a wave-like temperature oscillation (typical of the hydrodynamic regime) and finally the diffusive regime is restored.

In this work, we demonstrate that layered correlated materials (LCM) can show the entire spectrum of unconventional electronic heat transport regimes [3]. In particular, we find a spatio-temporal range where hydrodynamic regime sets in and the wave-like properties for the electronic temperature may be exploited [4], as schematized in Fig.1. In such a regime we theoretically investigate the temperonic crystal (TC), a superlattice based on a unit cell composed of two slabs sustaining temperature wavelike oscillations on short timescales. The TC allows to control and manipulate the wave-like properties of the electronic temperature [5].

The present results are readily extendible to graphene superlattices, for which it is possible to develop the temperonic crystal [5,6].

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Cooling and Seebeck effects in Double-Barrier Semiconductor Heterostructures

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Based on full quantum-transport simulations, we report a comprehensive study of the evaporative cooling process and thermoelectric Seebeck effect in a double-barrier semiconductor heterostructure thermionic devices. Our model, which self-consistently solves the nonequilibrium Green's function framework and the heat equation, is capable of calculating the electron temperature and electrochemical potential inside the device, in a non-equilibrium regime. By investigating the dependence of those thermodynamic parameters as a function of applied bias and temperature gradient, we give a clear recipe to reach high electron refrigeration and demonstrate a counterintuitive current component in thermoelectric Seebeck conditions.

We consider a double-barrier semiconductor heterostructure thermionic refrigerator (Fig.1a)), since we previously showed that electron bath in the quantum well (QW) is refrigerated thanks to the evaporative cooling effect [1]. When applying a bias, hot electrons are extracted above the thick collector barrier and the remaining low-energy ones rethermalize in the QW at a lower temperature. However, the dependence of the electron temperature on the physical parameters of the device was still not well understood. Our recent simulation results demonstrate that the best electron cooling is obtained when (i) the device operates at the maximum resonant condition (Fig.1b)); (ii) the quantum well state (with the energy E_0) is symmetrically coupled with the contacts [2].

a) b)

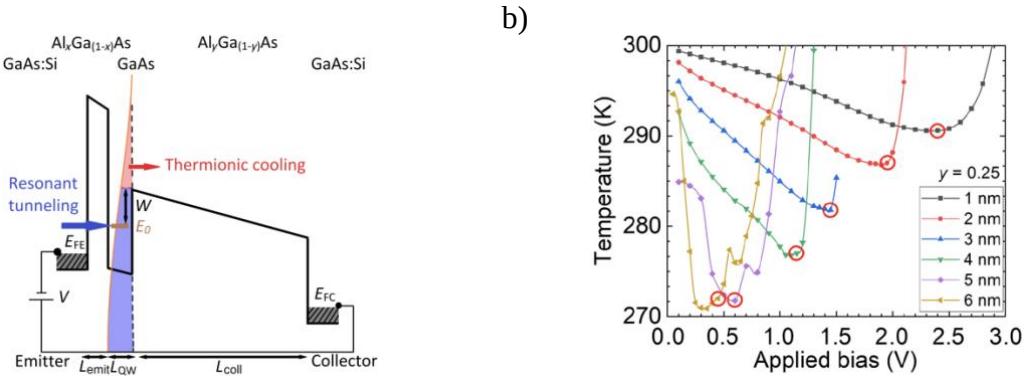

Fig. 1. a) Considered asymmetric double-barrier heterostructure. L_{emit}, L_{QW}, and L_{coll} refer to the thicknesses of the emitter barrier, the quantum well and the collector barrier, respectively. The quantum well of GaAs is cooled by injecting cold electrons (in purple) via resonant tunneling, and by extracting the hot carriers above the thicker barrier (in red); b) L_{emit} dependence as a function of the applied bias V for the electron temperature in the QW. L_{emit} varies from 1 to 6 nm. For each L_{emit}, red circle represents the bias at which the resonance occurs.

We also investigate the thermoelectric Seebeck characteristics by applying a lattice temperature gradient of 1K across the structure (Fig. 2a)) and analysing the electron current spectrum (Fig. 2b)). Interestingly,

a current component (in yellow) is flowing along the reverse direction (*i.e.* from cold contact towards hot contact). The reverse component results from the reflection of the electrons at the left (right) barrier which emit (absorb) phonons and return back to the contact. This phenomenon is explained by calculating the difference of Fermi-Dirac distributions between two consecutive plans using the non-equilibrium electron temperature and electrochemical potential inside the device (Fig.3a) and b)). In the access regions, the Fermi-Dirac distribution difference depicts a sign inversion around 0.85 eV, which corresponds with the energy at which the current spectrum component goes in the reverse direction (Fig.2 b)). This effect could be for instance emphasized by considering an energy filtering analysis.

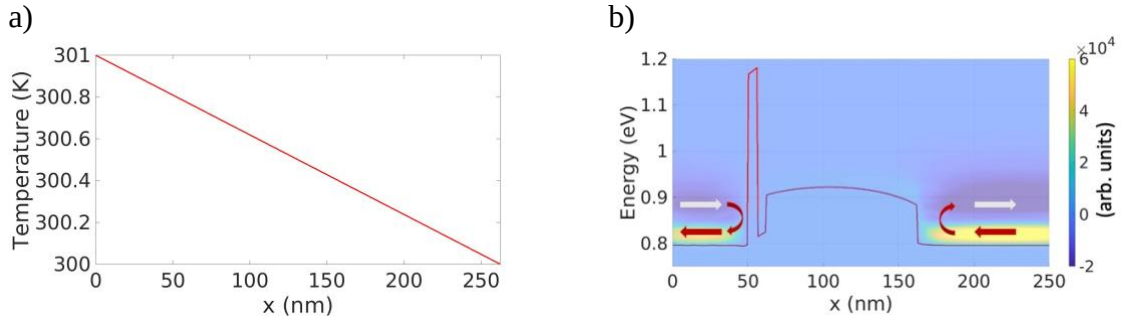

Fig. 2. a) Lattice temperature gradient applied between the two contacts. The applied bias is here equal to 0 V; b) Electron current spectrum in the structure when applying a lattice temperature gradient ($\Delta T = 1$K). We observe an unexpected current component at low energy (in yellow) which goes against the temperature gradient, from the cold toward the hot contact.

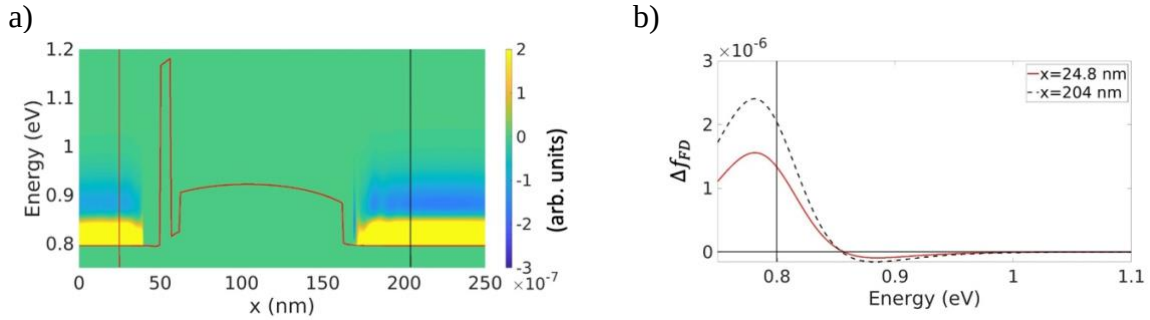

Fig. 3. a) Difference of Fermi-Dirac distributions between two consecutive slices inside the active region, calculated from the non-equilibrium electron temperature and electrochemical potential; b) Difference of the Fermi-Dirac distributions at the positions indicated by vertical lines on Fig. 3.a).

The present results then shed light on original physical properties of evaporative cooling and Seebeck effect in semiconductor heterostructures. It represents a useful step for the conception, fabrication, and optimization of thermoelectric nanodevices with unprecedented performances.

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Ab initio calculations of the thermoelectric phonon drag effect in semiconductor nanostructures

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With the advance of materials fabrication techniques and increase of computational power during the past two decades, the research aiming to enhance the efficiency of thermoelectric devices, with the search of new materials and manipulation of materials properties at the nanoscale, has attracted significant interest. In general, the efficiency of thermoelectric materials, measured by the figure of merit ZT, directly depends on the Seebeck coefficient of the material. In the present work, we studied, by combining the density functional theory calculations of the electron-phonon [1,2] and phonon-phonon [3] interactions, the enhancement of the Seebeck coefficient due to electron-phonon coupling, known as the "phonon-drag" effect [4]. To account for this effect, we solved the linearized Boltzmann equation for electronic transport in presence of non-equilibrium phonon populations introduced by a temperature gradient. Next, in our aim to understand the phonon drag effect at the nanoscale, we studied the effect of nano-structuring on the Seebeck coefficient of the pristine material. We will present our recent results related to phonon and/or impurity limited carrier mobility, as well as the variation of the Seebeck coefficient of bulk and nano-silicon with temperature and carrier concentrations. Our results for *n*-doped silicon not only show a good agreement with the experimental data [5] but also pave the way to further understand the contribution of phonon-drag in any semiconductor nanostructures, for example Bi_2Te_3 [6], B_4C [7], Bi [8], which still remain largely unexplored. *Acknowledgements.* DFT calculations have been performed using the Quantum ESPRESSO software [9]. We acknowledge access to high performance computing (HPC) resources provided by the French HPC centres of TGCC, CINES and IDRIS (GENCI Project 2210) as well as to the 3L-hpc local computer cluster partly supported by the DIM SIRTEQ (région Île de France) and École Polytechnique.

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Parabolic-Like Heat Radial Distribution in Core-Shell Nanowires

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Since their discovery, in the 60's [1] nanowires (NW) have been widely studied. They offer a quasi one dimensional object, in which the external surfaces plays a major role. This impacts the thermal properties, the most notably it decreases the thermal conductivity compared to the bulk materials due to the very high surface to volume ratio [2]. Moreover, the thermal conductivity of nanowires is size dependent: it is modified by their cross-section and their length [3]. Additionally, the oxide skin formed at the free surface modifies the thermal and vibrational properties of NWs [4]. In this work, the effect of an amorphous layer on the heat flux radial distribution in silicon nanowire is investigated.

For this, 50 nm long nanowires with a crystalline diameter ranging from 5 to 10 nm are modeled using molecular dynamics (MD). On some of these crystalline NWs, an amorphous shell of Si with thickness varying from 1 to 2 nm is added. This amorphous shell is an approximation for the naturally occurring oxide shell [5]. An atomistic visualization of a modeled configuration can be found in figure 1 a.

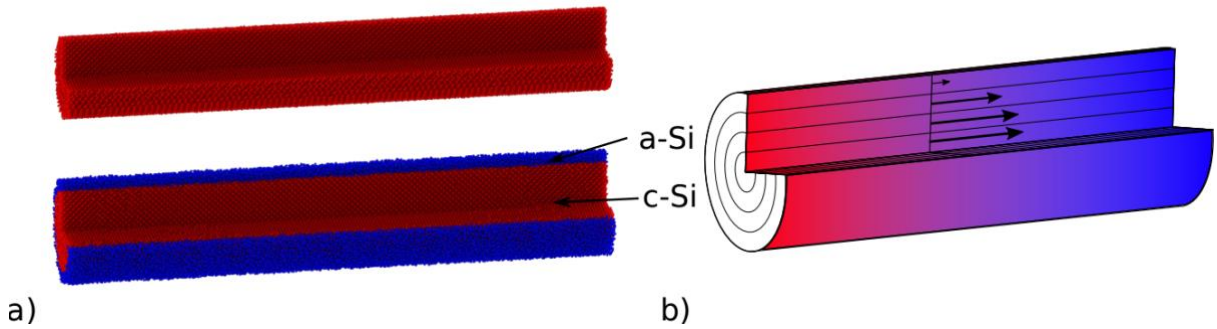

Fig 1: a) Visualization of a crystalline and crystalline-core/amorphous shell NW (a-Si atoms are in blue and c-Si in red) b) schematic NEMD methodology to compute the flux in the concentric hollow cylinders.

To obtain the radial flux distribution, we use the Non Equilibrium Molecular Dynamics (NEMD) method: one extremity of the NW is thermostated at 280K and the other at 320K. The heat flux in different concentric hollow cylinders (as depicted in figure 1 b) is computed through the average heat flux in the direction of the thermal gradient with this formula:

$$j = \frac{1}{V}\left(\sum_i E_i\, v_i + \bar{\bar{\sigma}} \cdot v_i\right)$$

j is the flux, the sum is running over each atom i of the volume V, v the velocity and $\bar{\bar{\sigma}}$ the atomic stress developed by Hardy [6]. To obtain significant statistics, the average is performed over 1 ns for 5 different independent simulations. Additionally, for the larger diameter, we have used the heat flux hydrodynamic equations to fit the results obtained with MD:

$$j + \kappa \nabla T = \ell^2 \nabla^2 j$$

with κ the thermal conductivity ∇T the thermal gradient and ℓ the non-local length [7].

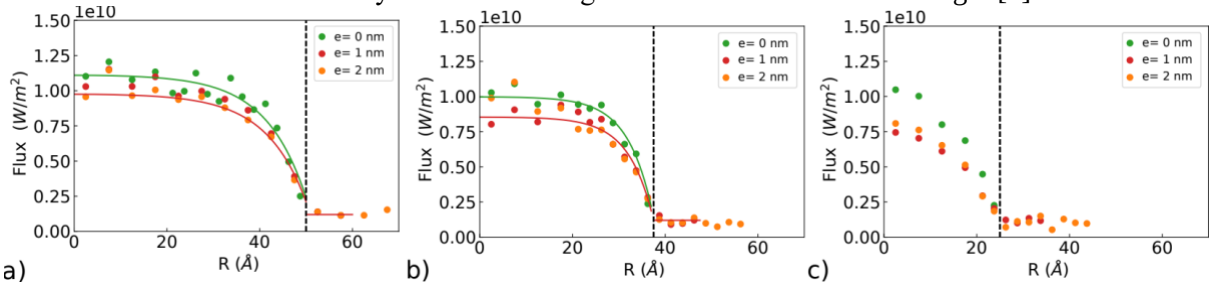

***Fig 2**: Radial heat flux distribution for NWs with a crystalline diameter of a) 10 b) 7.5 c) 5 nm and different thicknesses of amorphous shell (0, 1 and 2 nm). The points are the MD results and the continuous lines the fits with the hydrodynamic equation. The dashed vertical line corresponds to the crystalline diameter*

The results are displayed in figure 2. For all the crystalline diameters and amorphous shell thicknesses the overall shape of the radial distribution is very similar, there is a maximum in the center and the flux decreases close to interfaces. At the interface, the flux is the same for all configurations and very close to what is observed in the amorphous shell. Then, comparing the green curves (e=0nm) with the red (e=1nm) and yellow (e=2nm) one can observe that the addition of the shell does not only affect the interface and the nearby layers. On the contrary, the presence of the shell decreases the maximum flux in the center of the NW. This global effect is reproduced within the hydrodynamic heat equation by decreasing κ rather than changing the boundary conditions at the interface or increasing ℓ.

To conclude, we show that the radial heat flux distribution in a Si NW is Poiseuille like. The flux at the crystalline boundary corresponds to the flux in the amorphous part for all NW diameter and with or without amorphous shell. Finally, these distributions can be fitted with the hydrodynamic heat equation, the impact of the shell on the heat flux being modeled by a decrease of κ.

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A novel structure of Cooling Nano-devices: The Quantum Cascade Cooler

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We propose and study an innovative heterostructure as a cooling nanodevice based on tunneling filtering and thermionic emission. The structure, whose layers are alloys of $Al_xGa_{(1-x)}As$ **(Fig.1)** with varying Al concentration is designed to exhibit successively higher quantized states within quantum wells (QWs). QWs are separated by $Al_xGa_{(1-x)}As$ layers, thick enough to prevent most of the tunnel leakage for energies that are not those of the quantized states. By applying a bias voltage between the two contacts, we induce a net current, and we "force" electrons to "swim upstream" by absorbing phonons before being extracted from the last well by thermionic emission over a thicker AlGaAs layer, acting as a thermal wall to prevent heat backflow.

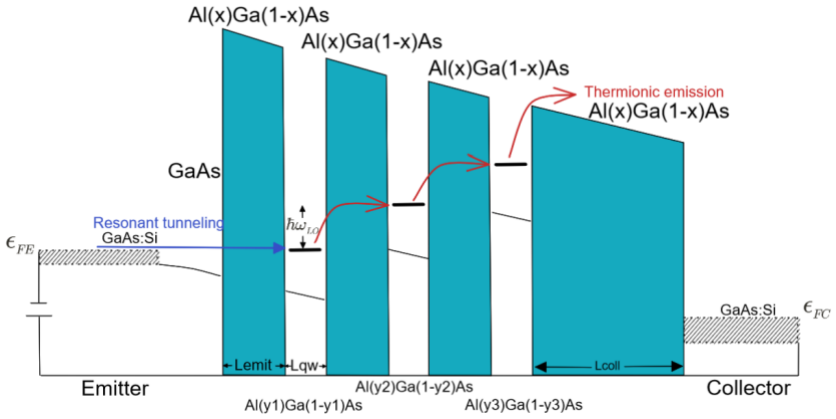

Fig. 1. Schematic band diagram of the studied semiconductor heterostructure. The left and right GaAs contacts are doped at a concentration of $10^{24}m^{-3}$. The concentration of Aluminium is tuned in the active region: The potential barriers (in blue) have the same concentration of aluminium (value?) whilst the white regions in between, representing the quantum wells, have an increasing proportion of Al ($y_1<y_2<y_3$).

In order to investigate the properties of such structure, we use an in-house code which couples self-consistently non-equilibrium Green's functions formalism for electron, heat equation and Poisson equation [1]. We include the interactions between the electrons and both acoustic phonons (elastic) and polar optical phonons (inelastic) [2] through the use of self-energies.

This self-consistent approach yields important electronic properties to understand the underlying physics in such device. For instance, figure 2 shows the current density spectrum across the device at V=0.2 V. **(Fig.2)**. This device is constituted of 7 layers of AlGaAs (9 with the GaAs contacts) with 0, 15 and 30% Aluminium respectively in the successive quantum wells and 40% in the barriers.

We subsequently determine the temperature of electrons (which is usually very different from the lattice's in out of equilibrium system like the one described here) by using the virtual Büttiker probes [3,4]. The principle of the latter is to weakly couple a probe to the active region of the structure of interest. We then cancel the carrier and heat current between the probe and the system by modifying the

electron temperature and electrochemical potential of the probe. The probe will then be in local equilibrium with the structure, even though the device operates far from equilibrium.

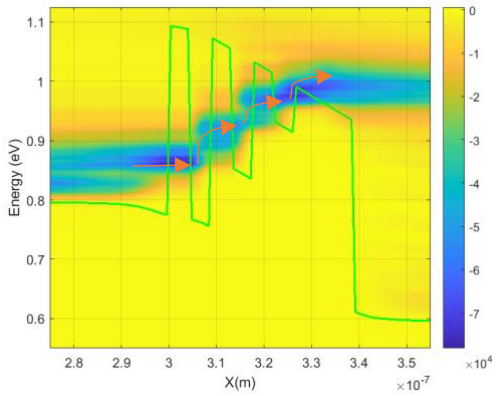

Fig. 2. Current density spectrum (arb. unit) obtained with a bias of 0.2V. Arrows highlight the physical process involved. Potential profile is plotted in solid green line

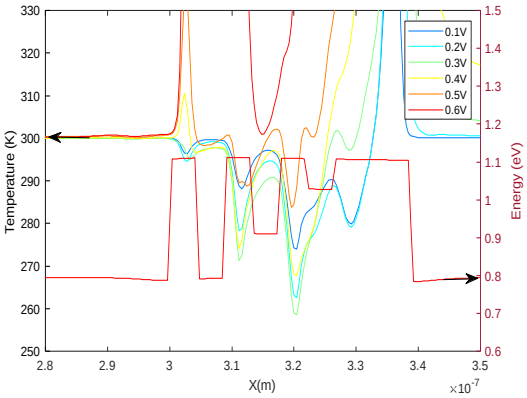

Fig. 3. Electron temperature profiles for different applied biases. Potential profile is also represented with a red solid line

With this method we calculated the temperature profiles **(Fig.3)** for the structure considered in Figure 2. From the obtained data we have found that the structure we proposed successfully cooled down the electrons up to 20K inside the quantum wells. We also drew the hypothesis that the minimum of temperature in the quantum wells is closely related to the energy of one longitudinal optical phonon.

Conclusion – By numerically investigating the cooling properties of an AlGaAs based heterostructure, we manage to provide a proof of concept for the Quantum Cascade Cooler whose optimization may lead towards highly efficient cooling nano-devices.

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Monte Carlo simulation of static and dynamic thermal properties of nanostructures

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In this work, an in-house full-band Monte Carlo code [1] has been used to simulate the thermal response in different nanostructures at a short time scale in order to highlight the characteristics of the non-equilibrium transport i.e., beyond the Fourier regime.

The nanodevices studied are both nanowires and nanofilms, as shown in Fig. 1. For nanofilms (e.g., Fig. 1.a) and nanowires (e.g., Fig. 1.b), the external interfaces are assumed to be specular and diffusive, respectively. 3 different kinds of nanostructures are simulated:

- Si3C straight nanofilms
- Si3C L-shaped nanowires
- Si3C/Ge3C heterojunctions

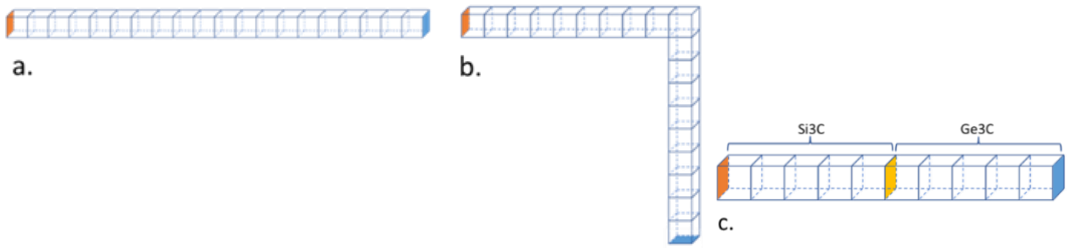

Fig 3: a. Straight specular nanofilm at echelon b. L-shaped specular nanowire at echelon c. Heterojunction at echelon.

The lengths of the studied nanostructures are 100 nm and 200 nm. For the nanowires, 2 cross sections of 10x10 nm and 5x5 nm are considered. The devices are divided into uniform cells, usually 20 cells are used. Each of these systems has a changeable thermostat at each end, and the temperature of the cells within it can also be changed. For example, a stepwise simulation was performed with one thermostat changing from 300K to 400K at t=0s and the other remaining at 300K (see Figure 1).

In each device, both heat flux density and temperature are studied as a function of time and length, as shown in Figure 2 for the 200x10x10 nm straight nanofilm. To characterize the transient and stationary thermal response of each cell, they are identified to a linear system.

In general, first-order approximations with a time delay are sufficient, but for the flow in cells near the hot thermostat where the transport is strongly out of equilibrium, higher order approximations are required.

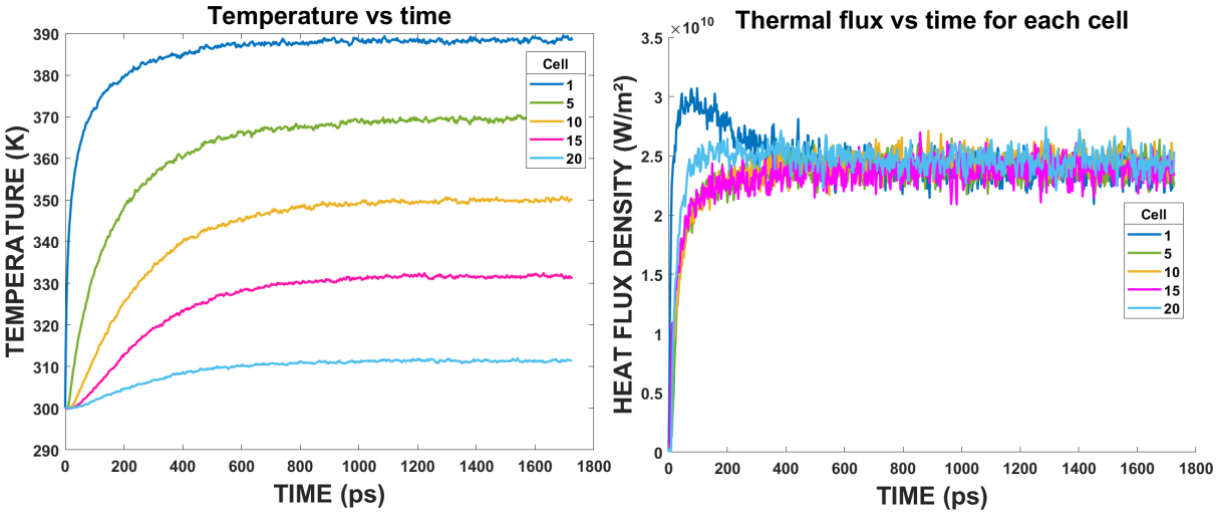

Fig.4: Heat flux density and temperature as a function of time – Straight 200nm long nanofilm

The gain and the time response for different nanostructures are shown in Table 1.

	Dimension 200x10x10 nm - Straight		Dimension 190x10x10 nm - L-shaped	
	Temperature	Heat flux density	Temperature	Heat flux density
	Specular nanofilms			
Gain [K] [E10 W/m²]	388	2.37		
Response time at 5% (ps)	81.0	481		
	Diffusive nanowires			
Gain [K] [E10 W/m²]	397	0.60	397	0.51
Response time at 5% (ps)	92.0	1190	99.0	1560

Table 1: Extracted parameters for straight nanofilms and L-shaped nanowires for the first cell

Table 1 highlights the difference between specular and diffusive devices. Diffusive (nanowire) systems evolve more slowly than specular systems. This is because phonons are randomly reflected at the external interface, which increases the time required to reach the steady state. In diffusive devices, the temperature gain is higher than in specular devices while the heat flux density gain is lower (higher thermal resistance per unit area).

Further simulations were also performed for a 400 K perturbation in the central meshes of the nanowires and the heterojunction.

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Electron-phonon coupling and ultrafast dynamics of hot carriers in semiconductors: from interpretation of photoemission experiments to transport simulations in devices

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Electron-phonon coupling determines the charge transport properties of materials as well as the relaxation dynamics of photoexcited carriers. Computational methods based on density functional theory, on the one hand, and time-energy- and momentum- resolved spectroscopy, on the other hand, allow today an unprecedently detailed insight into the role of the electron-phonon coupling [1]. At the same time, hot carriers start to attract attention in the context of emerging concepts for energy conversion.

In this work, we will present our results for relaxation dynamics of photoexcited electrons in InSe, in presence of the two-dimensional electron gas on the surface, which was studied by photoemission spectroscopy and by ab initio calculations. We will also discuss photoexcited electron relaxation in several other semiconducting materials [2-5]. More generally, we will discuss the necessity of time-resolved simulations as well as the problematics related to the coupling of ab initio data with device-oriented simulation methods [6].

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