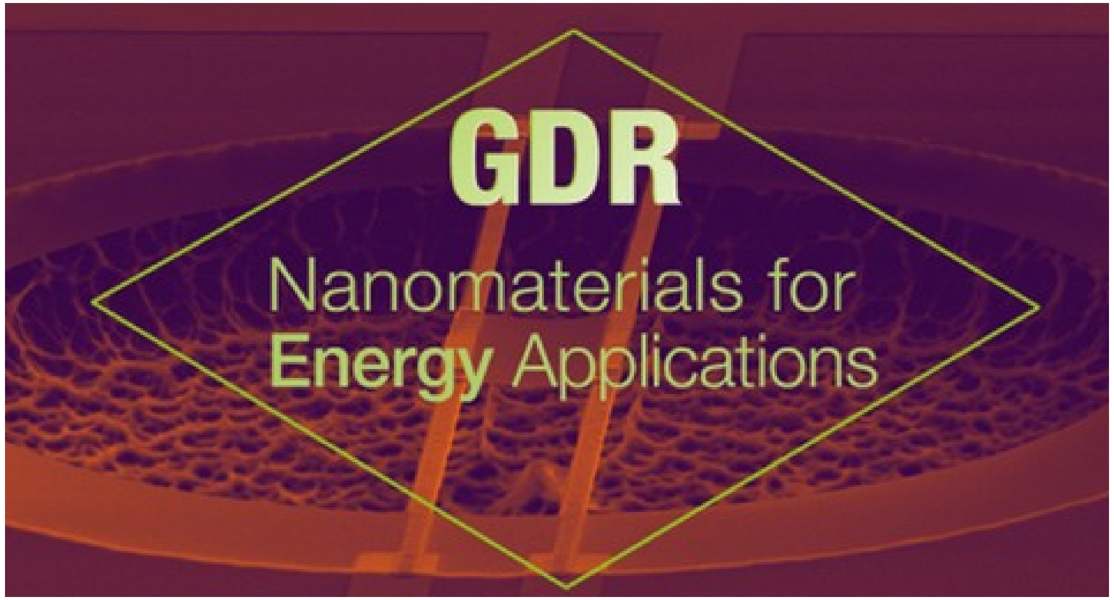
NAMe

GDR Nanomaterials for Energy Applications



Working group 1: Nanomaterials-Nanostructuration

Animators: Séverine Gomès, Fabien Grasset, Samy Merabia, François Piquemal

CETHIL UMR 5008 — Institut des Sciences Chimiques de Rennes UMR CNRS 6226 — iLM Institut Lumière Matière — Laboratoire National de Métrologie et d'Essais LNE

GDR2086

CNRS

Plenaries 19-21 May 2021 - Visioconference

Overview

- **« Nanomaterials for energy application » definition for the GDR**
- **The 3 workshops**
- **The four essential elementary scientific and technological bricks** to produce nanomaterials for Energy applications
- **Conclusion and perspectives**

Nanomaterial Definition

In ISO/TS 80004, nanomaterial is defined as the "*material with any external dimension in the nanoscale or having internal structure or surface structure in the nanoscale*", with nanoscale defined as the "*length range approximately from 1 nm to 100 nm*". PROPOSITION: 100nm ✉ sub-micronic
This includes both nano-objects and nanostructured materials, which have internal or surface structure on the nanoscale.

Nano-objects

nanoparticle
nanofiber
nanoplate
nanorods
nanotubes
nanoribbon
One-dimensional nanostructures
2D materials
nanocristaux

Nanostructured materials

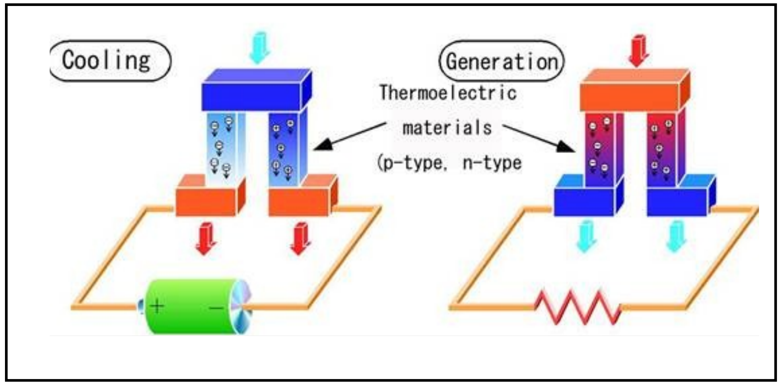
nanocomposite
nanofoam
nanoporous material
nanocrystalline material
3D nanomaterials
...

Energy application

based on energy conversion (analyzed in axis 3):

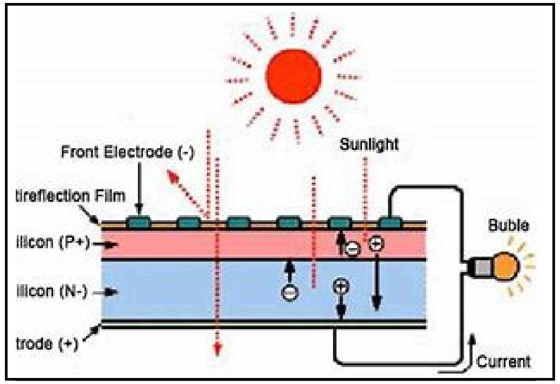
Conversion « Thermal 🔔 Electrical »

Thermoelectricity



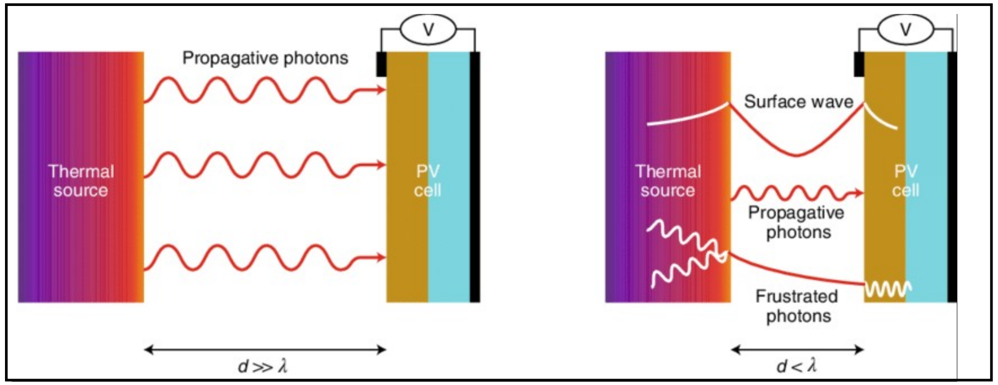
Conversion « Optical 🔔 Electrical »

Photovoltaïc



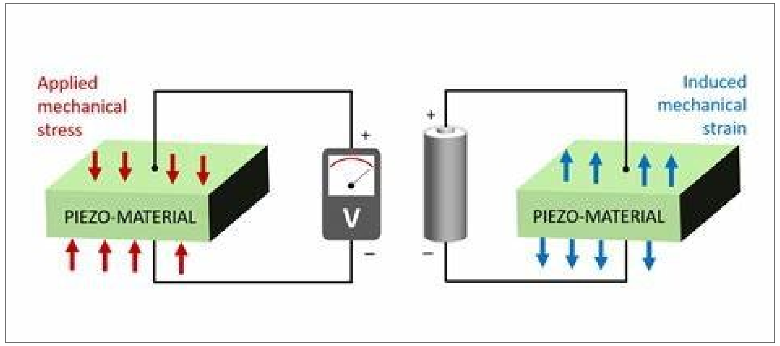
Thermophotovoltaïc

Near-field thermophotovoltaïc



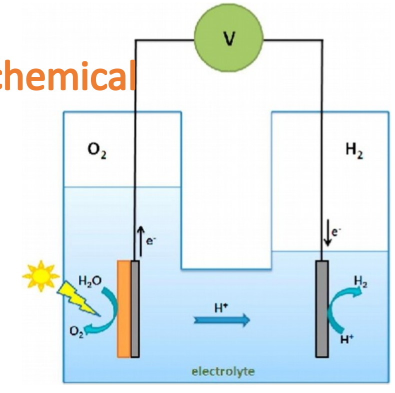
Conversion « Mechanical 🔔 Electrical »

Piezoelectricity

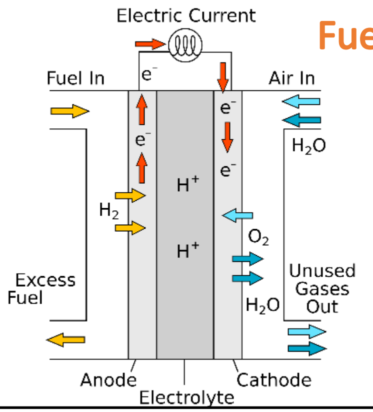


Conversion « Chemical 🔔 Electrical »

Photo-electrochemical effect



Fuel cells



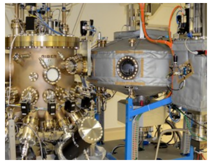
…

Thermal management

required for the actives devices (axes 5&6) based on these principles

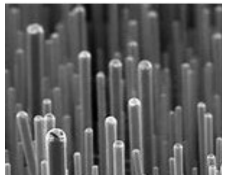
- Contribution of nanomaterials (in axis 4)

Four scientific topics



a. Elaboration-Synthesis

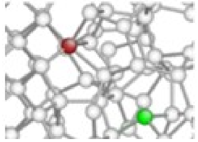
- ➢ Real nanomaterials and synthesis processes



b. Measurements techniques for microstructural definition

- ➢ Characterized nanomaterials and processes

Nanomaterials for Energy applications



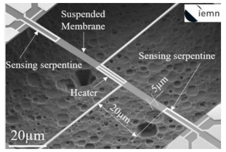
- ➢ Design laws at the nanoscales

c. Simulations of energy transport and conversion properties

- Based on modeling tools and theories available

- ➢ Physical property understanding and prediction

Comparison validation



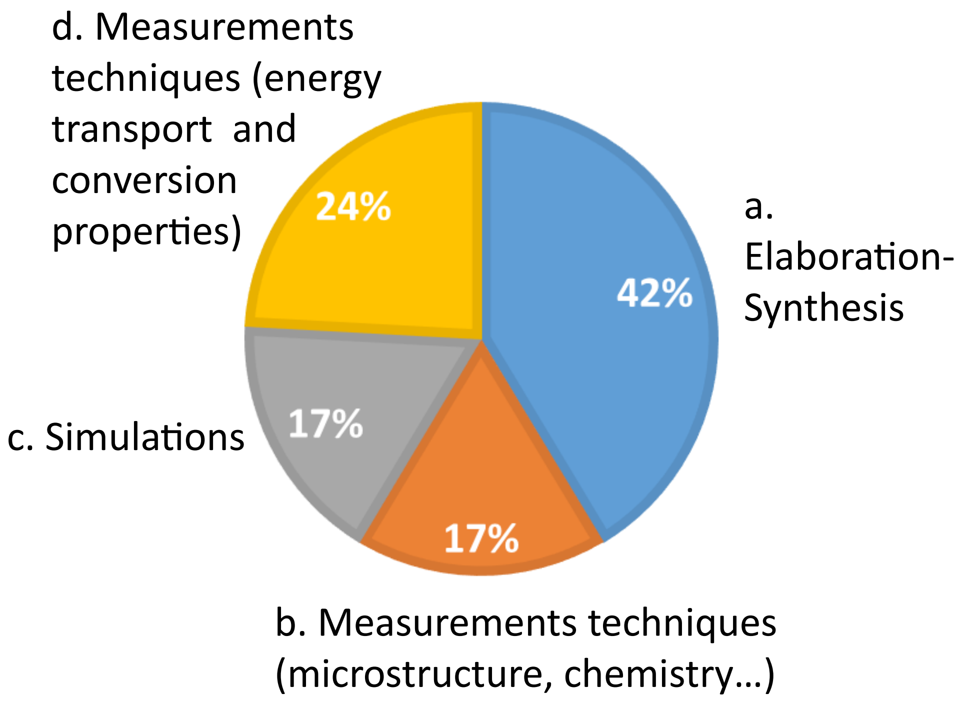
d. Measurements techniques of energy transport and conversion properties

- ➢ Physical property understanding and measurement

Three half-day workshops

March 31 14:00-17:00	April 01 09:00-12:00	April 06 14:00-17:00
Nanoparticles, Nanorods, Nanocomposites, Thin films	Materials 2D, 1D, 0D	Silicon and semiconductors and other materials

28 contributions



Objectives

To take stock of:

- the **international state of the art**
- the **skills available within the GDR**
- our **needs and perspectives on nanomaterials for energy**

Three half-day workshops

Contributions from 14 laboratories/organisms

a. Elaboration-Synthesis

Animator: Fabien Grasset

STATE of the ART

Keywords: “nanomaterials” and “energy”
WoS (2015-2021): 14258 references
02/04/21

Keywords: “thin film” and “energy” and “transport”
WoS (2015-2021): 16883 references
02/04/21

First indication:

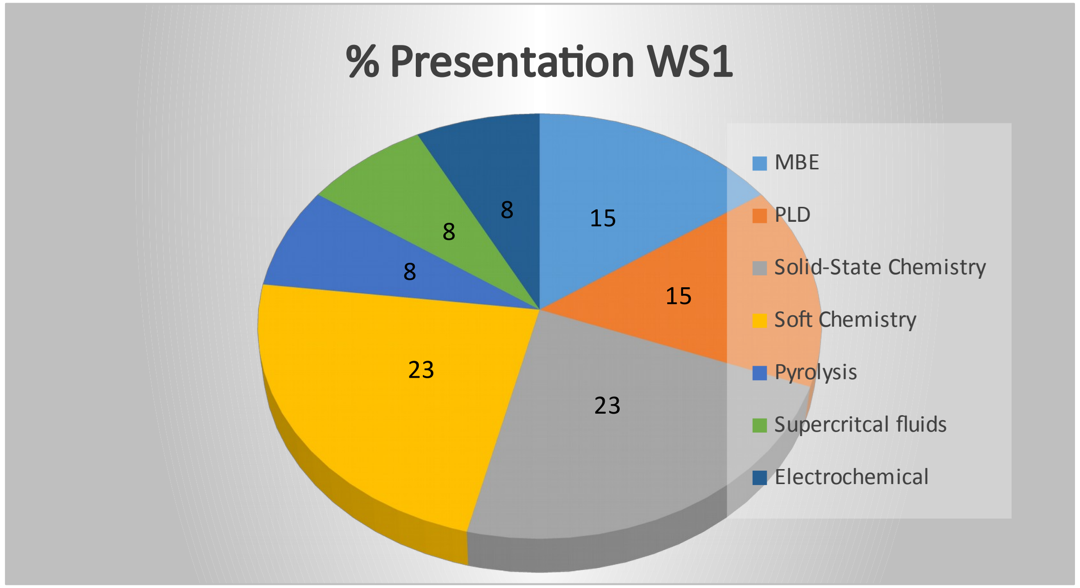
A full review is quite complicated and highly time consuming
Imagination seems to be without limit

ELABORATION PROCESSES

The "Elaboration-synthesis" processes could be divided in two main parts:

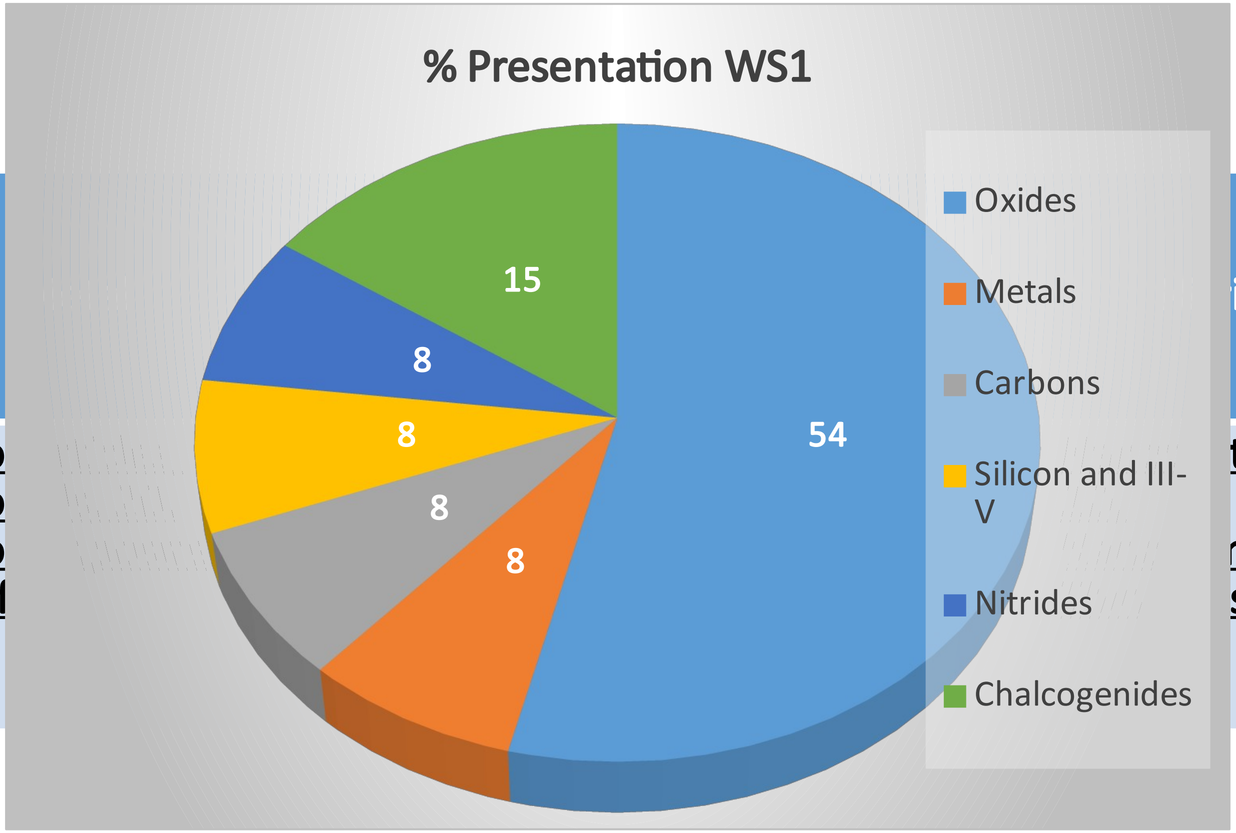
Vacuum (or low partial pressure control) and non-vacuum processes.

- Vacuum processes = **MBE, PLD, CVD,** Sputtering, ALD, Plasma…
- Non-vacuum processes = **Chimie « douce », solid-state chemistry**, **supercritical fluids, chemical deposition process, electrochemistry, pyrolysis,** organometallic chemistry, coordination chemistry, microwave, solvothermal, pulsed laser irradiation in solution, high pressure …



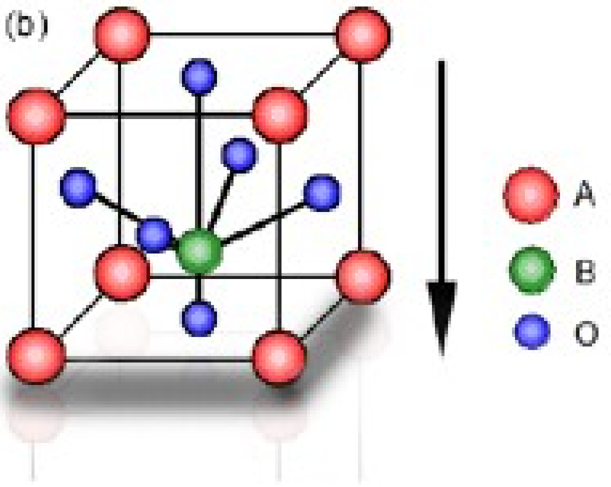
MAIN COMPOUND FAMILIES

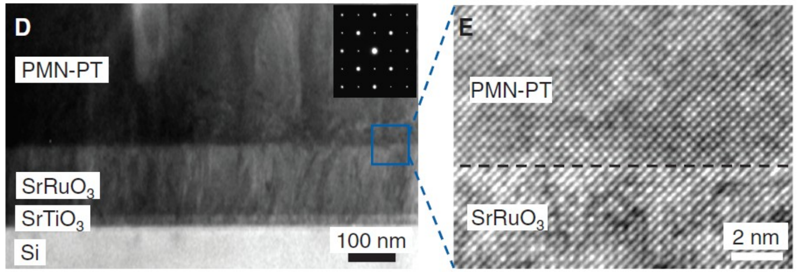
Oxides		ides	Chalcogenides
Nanoparticles, Nanorods, 2D, Nanocomposites, Thin films	Nano Nano Nano Thin f	ticles, nposites, s	1D

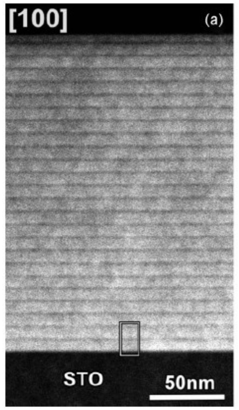


OXIDES

Perovskite

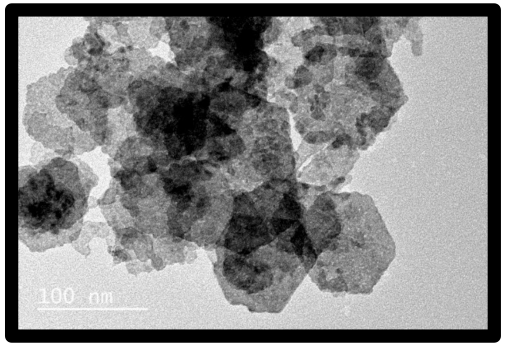




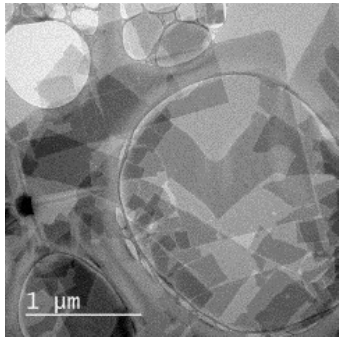


inl RISM GREMAN matériaux microélectronique acoustique nanotechnologies UMR 7347 - Université de Tours / CNRS

2D: Lamellar compounds, nanosheets



H_xCoO_2



$[Ca_2Nb_3O_{10}]^-$

icmcb

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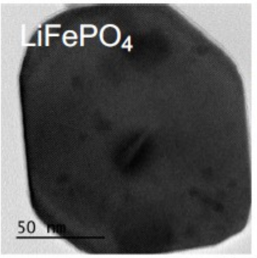
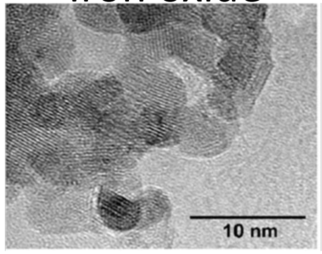
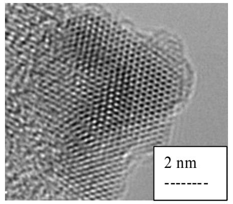
Nanoparticles



Iron oxide



Zinc oxide

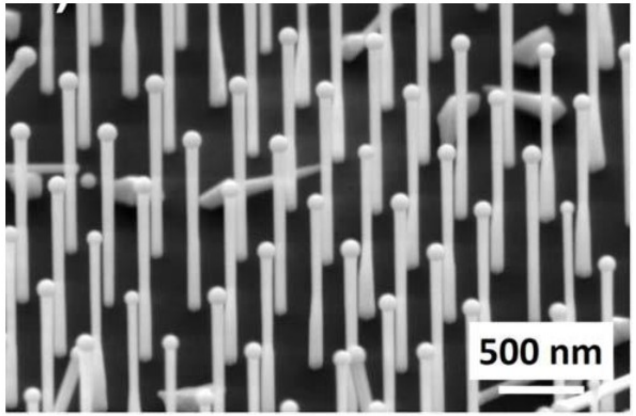


nanosciences & innovation nimbe

Piezoelectrics, Pyroelectrics, Thermolectrics, Electrochromism, Catalysis_…

Others Materials

Si and III-V 1D



Carbon

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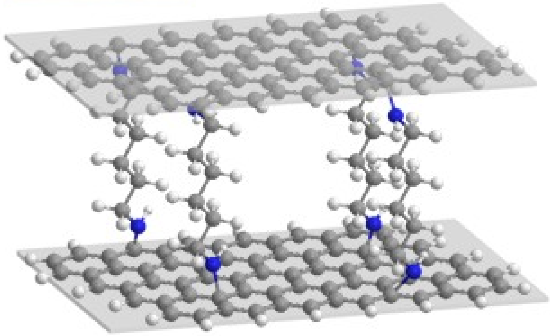
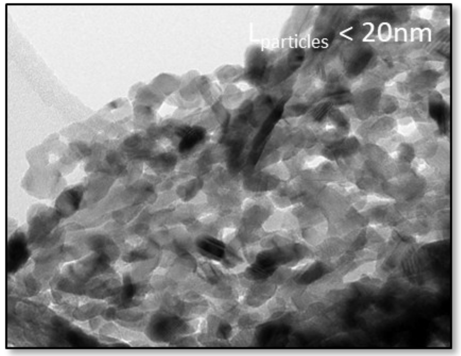
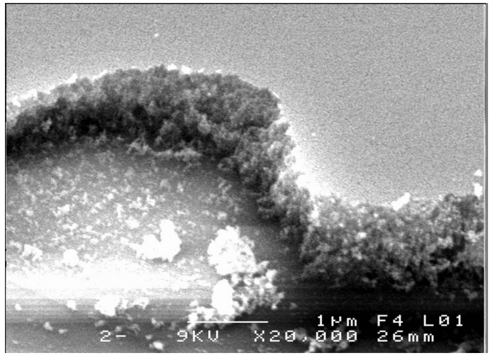


Graphene

Nitrides and oxynitrides (nanoparticles and thin films)





Mo_5N_6

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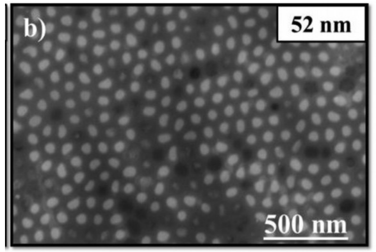
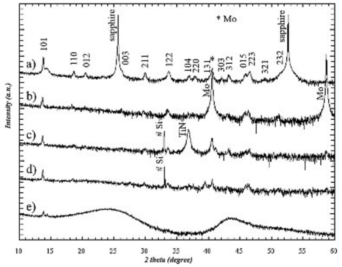
"TiON"

Chalcogenides (1D, nanoparticles, thin films)





Bi$_2$Te$_3$ nanowires

Institut Jean Lamour

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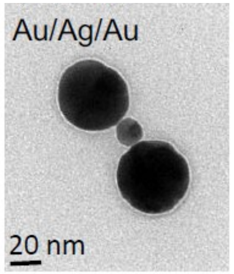
Chevrel Phases

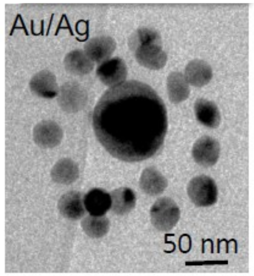
« $M_xMo_6X_8$ »

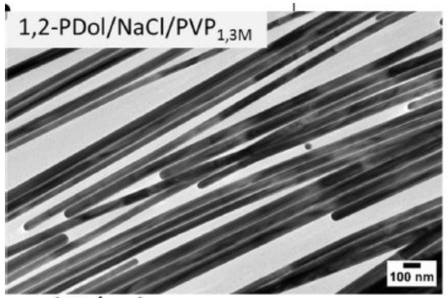
(X = S, Se)

Metal (nanoparticles, 1D)

icmcb







Piezoelectrics, Pyroelectrics, Thermolectrics, Electrochromism, Catalysis…

Partial conclusion

- **A very broad variety of compounds and nanomaterials seems to be available in the GDR Name.**
- **Necessity to be in relation and connected with others workshops.**

b. Measurement techniques for microstructural definition

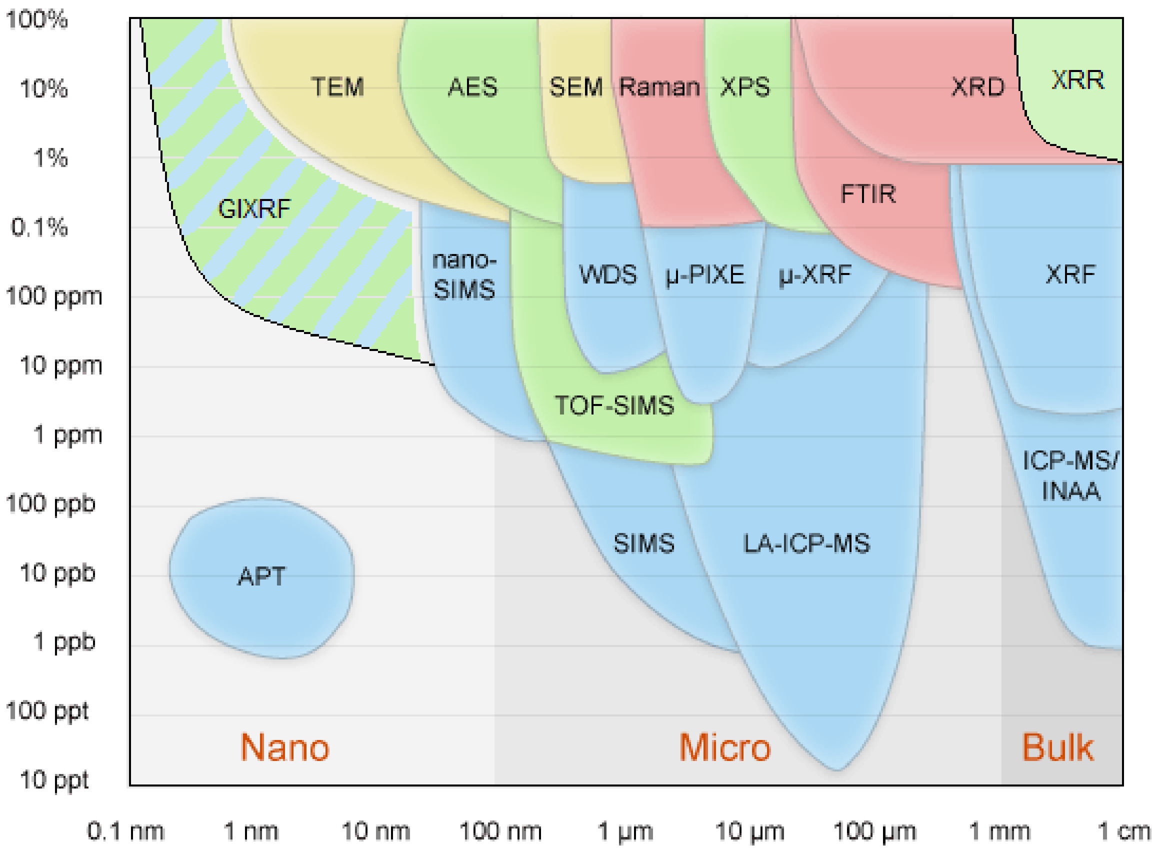
Animator: François Piquemal

Starting an Overview on characterization techniques of structural and chemical properties

- ✓ X-ray analysis (GIXRF, SIMS etc)
- ✓ Zeta potential measurements
- ✓ Dimensional nanometrology (AFM, SEM …)

What about novel or hybrid techniques ?

e.g. mixing SEM and eSPM techniques



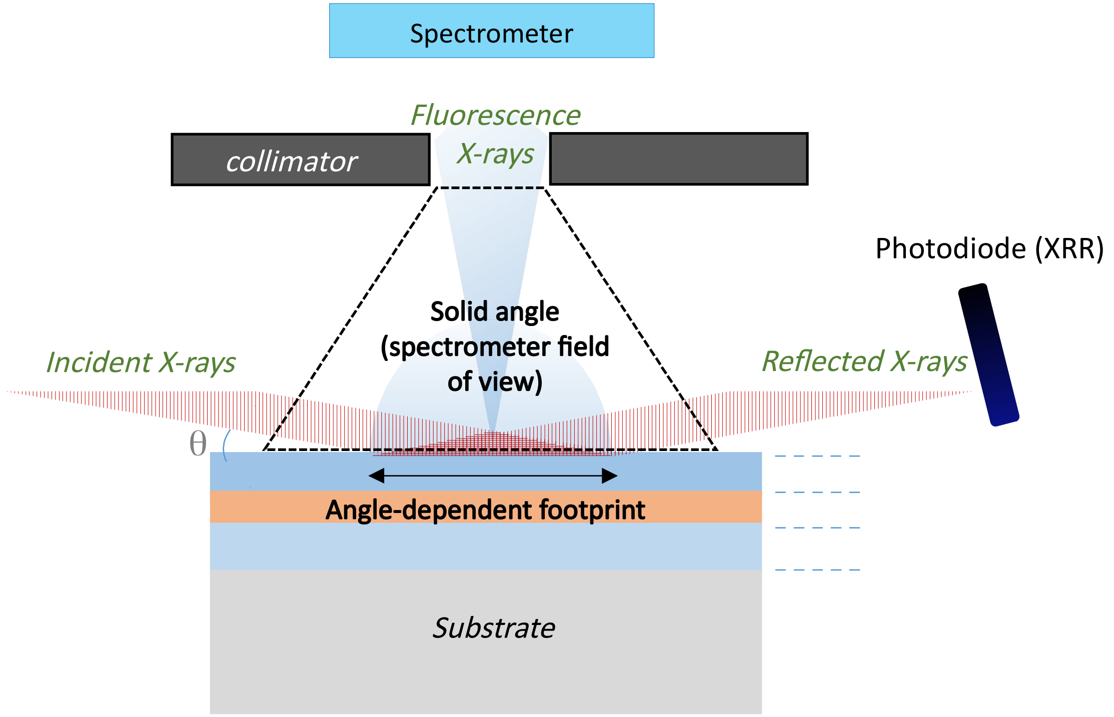
- Elemental composition
- Structural information
- Surface and thin films analysis
- Multiple electron microscopy techniques

from Y. Ménesguen's contribution

Combined XRR-GIXRF analysis for nanolayers

Combining XRR (X-Ray Reflectivity) with GIXRF (Grazing Incidence X-Ray Fluorescence) is a powerful and non-destructive technique to control the accuracy of thin film deposition giving access to the layer parameters: **thickness, roughness, composition, density, depth profile**

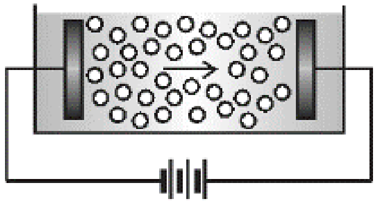
GIXRF (Grazing Incidence X-Ray Fluorescence) is a technique belonging to the XRF family (confocal XRF, TXRF, GEXRF…), sensitive to the nature of elements

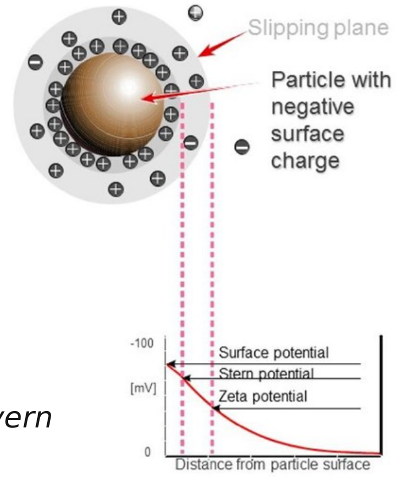


- The XRR-GIXRF combined analysis is performed with a specific goniometer at SOLEIL synchrotron
- The LNHB develops its own softwares for data acquisition, XRF spectra processing and multilayer modeling
- The reference-free approach uses only fundamental atomic quantities to derive the multilayer parameters: no standards needed

Zetametry for caracterisation of nanoparticles and thin layers

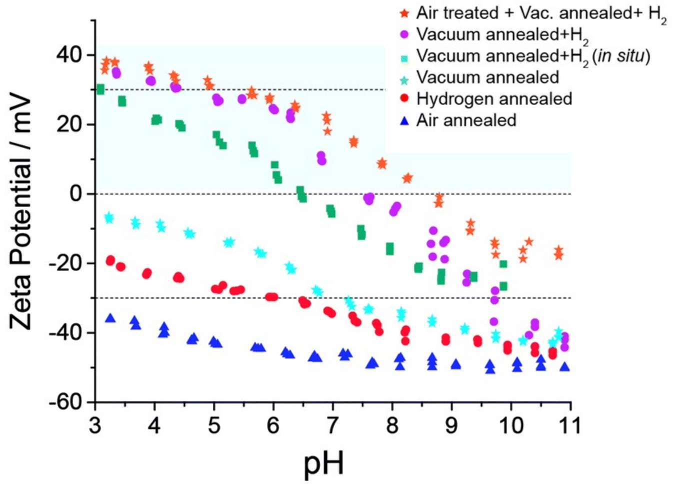
Electrophoresis (nanoparticles)





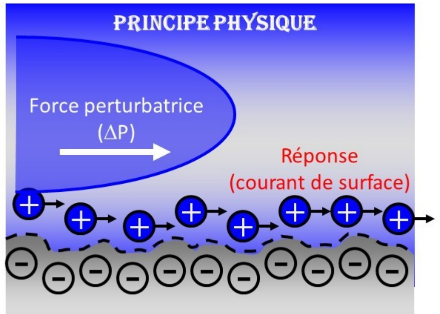
Courtesy of Malvern Panalytical.

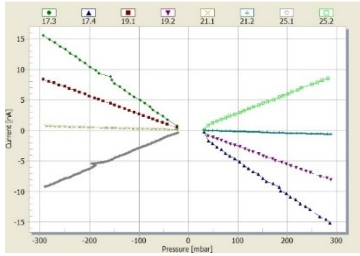
Heat treatment of nanodiamonds



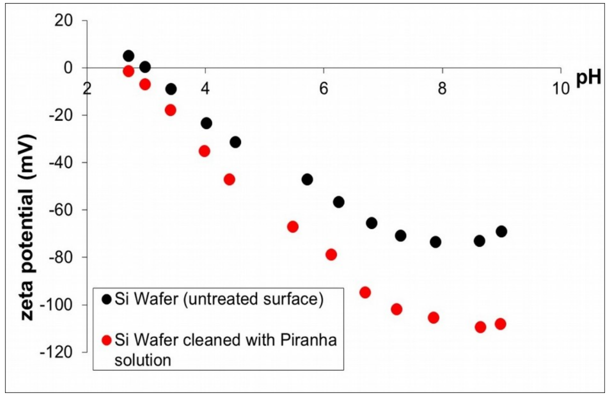
Nanoscale 9 (2017) 12549.

Streaming current / potential (thin films)





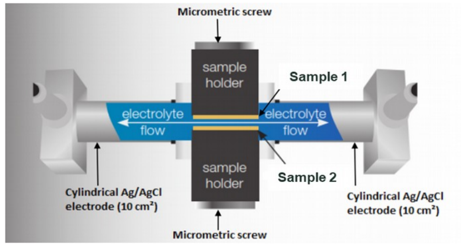
Courtesy of Anton Paar.

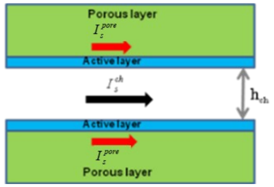


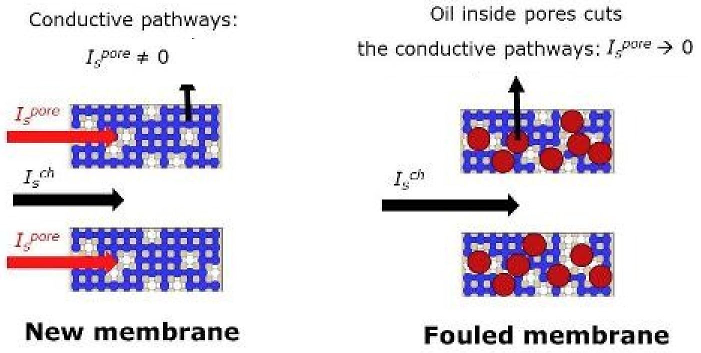
T. Luxbacher – The zeta guide, 2014

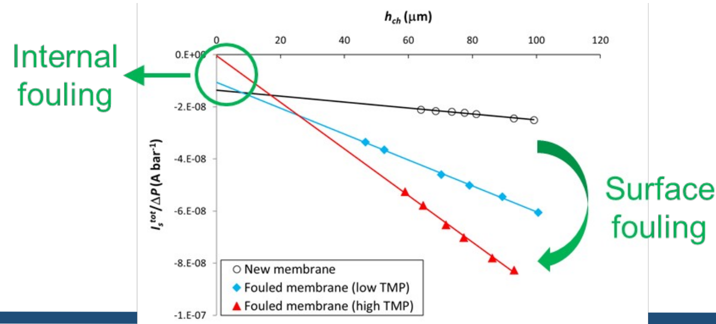
Chemical treatment of Si wafers

Electrokinetic leakage as a probe







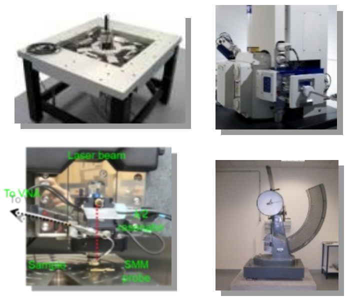


LABORATOIRE NATIONAL DE MÉTROLOGIE ET D'ESSAIS

Nanometrology for the characterisation of graphene-related 2D materials

*"Development and provision of **reliable and accurate measurement methods** for graphene-based materials and products for **characterisation, quality control, performance evaluation** and **risk assessment**"*

- Structural (AFM, SEM, BET, …)
- Chemical (EDS, ICPMS, …)
- Electrical (SMM, e-AFM, 4pp)
- Thermal (MPTR, SThM)
- Mechanical (impact Charpy tests,…)
- …

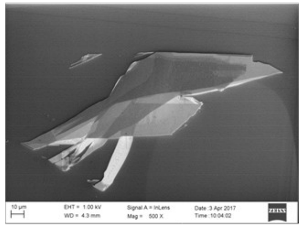


+ Hybrid metrology

"Combining complementary techniques for reliable measurements of complex materials"

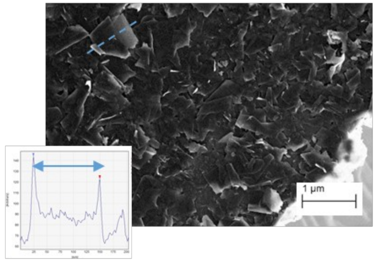
Scanning Electron Microscopy (SEM)*

Exfoliated graphene on SiO_2/Si



At low voltage: Contrast related to the **number of layer**

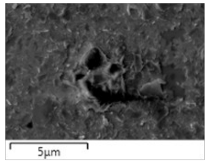
FLG flakes on Si

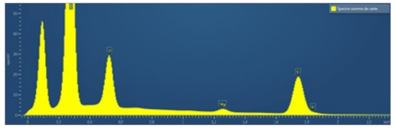


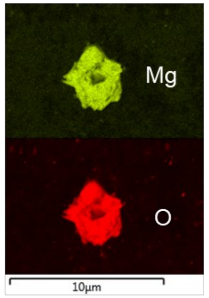
Lateral size + morphology

+ Energy Dispersive X-ray Spectroscopy (EDS)

FLG flakes on Si



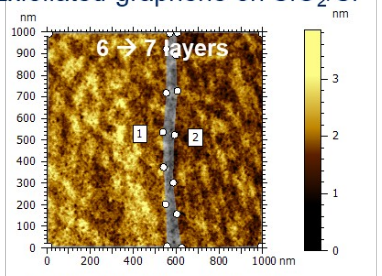




Elemental composition

Atomic Force Microscopy (AFM)*

Exfoliated graphene on SiO_2/Si



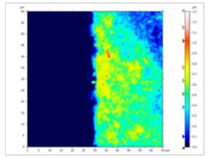
Paramètres différentiels	P2 - P1	Unité
Zmean(higher) - Zmean(lower)	-0.321	nm
Différence d'inclinaison	0.0253	°

Sensitive down to 1 layer (0.32 nm)

FLG thin films on Si

10 µm x 10 µm

Morphology / Roughness



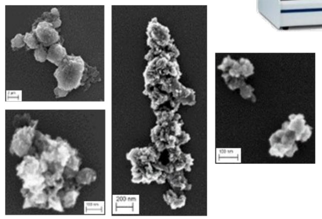
Thickness

Brunauer – Emmett – Teller (BET)

Graphene powders (GNP)

Specific Surface Area of 748.8 ± 4.3 m^2/g

Attempts to **correlate with morphology** of particles (thickness + agglomeration/aggregation)



* *Calibrated against metrological AFM through array transfer standard*

Characterization techniques: also used to measure transport properties (see part d)

Overview to be pursued and completed by most recent techniques or involving hybrid techniques

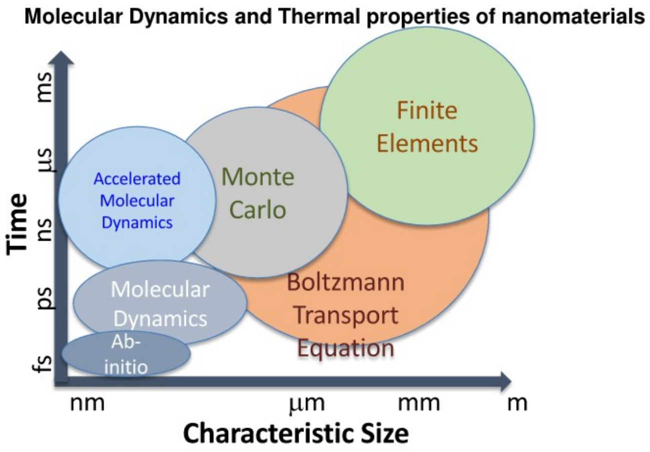
Need of other contributions!

c. Simulations of energy transport properties

Animator: Samy Merabia

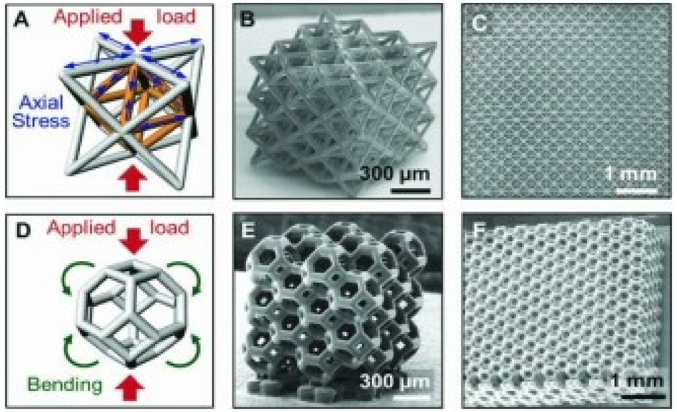
Starting an Overview on different simulations techniques

- ✓ Molecular dynamics
- ✓ Ab-initio NEGF calculations
- ✓ Anharmonic Lattice dynamics



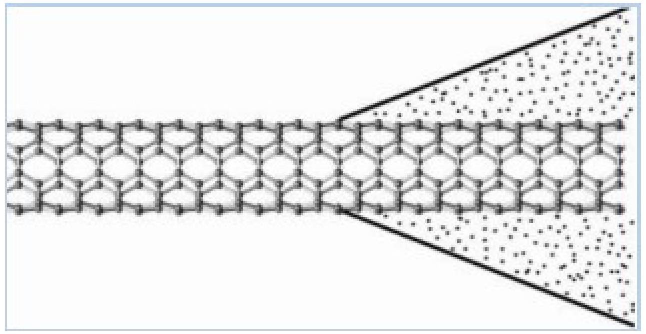
Modeling nanostructured materials: some recent trends

- ✓ Metamaterials
- ✓ Nanostructured interfaces (superlattices, atomic scale films, nanocomposites)
- ✓ Nanowires



Which property ?

- ✓ Thermal conductivity
- ✓ Nanoscale friction



Simulations of Lubrication at Nanoscale

c. Simulations of energy transport properties

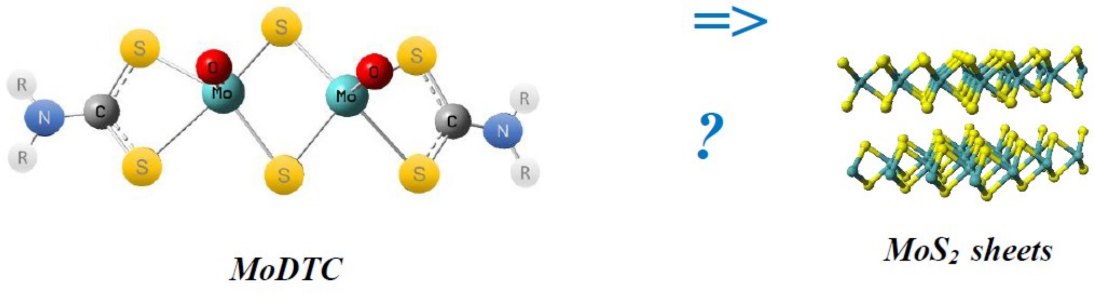
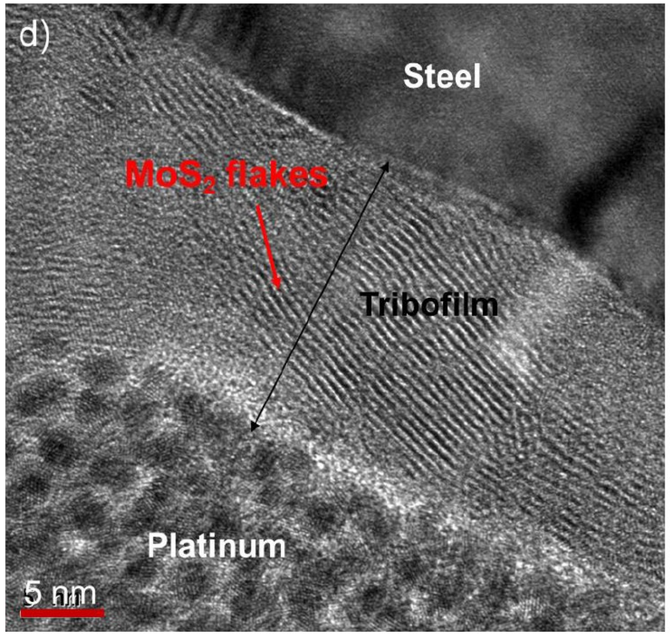
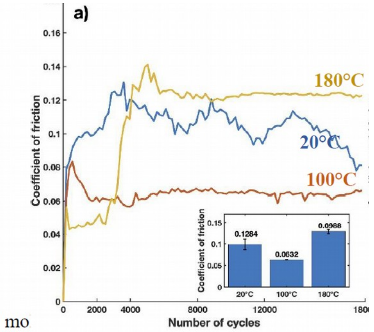
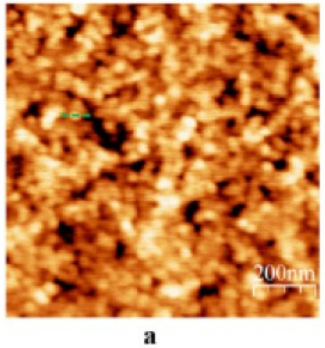


Figure 19: Schematic resuming the objective of the thesis: better understanding of MoS2 generation from MoDTC additives within boundary lubricated steel-steels contacts (Source figure MoS2 sheets Wikipedia).

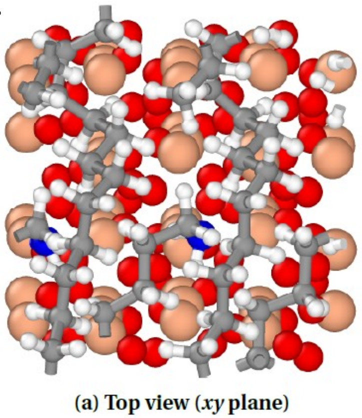




e

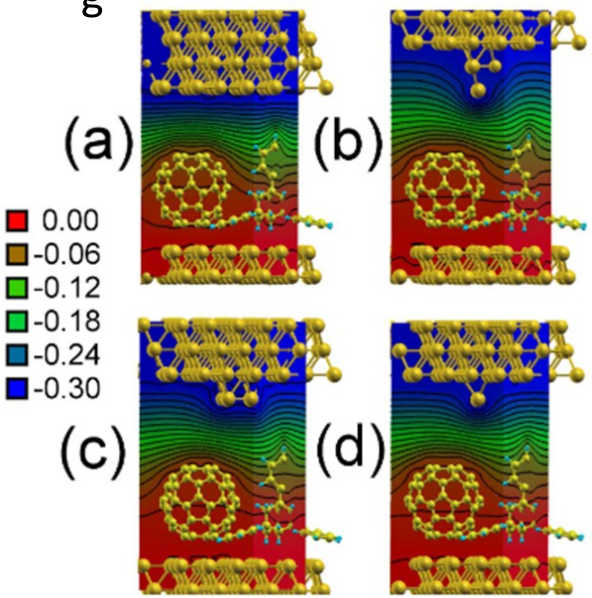


f



Molecular Dynamics Simulations
LAMMPS

g



DFT calculations
VASP
SIESTA

Electronic transport

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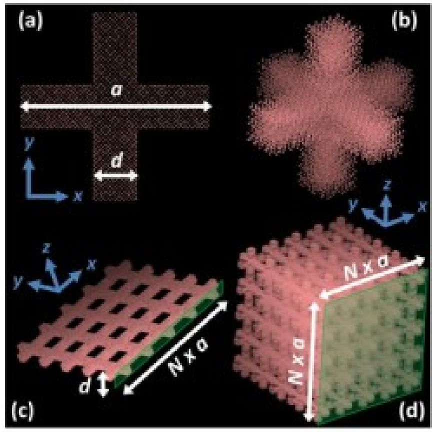
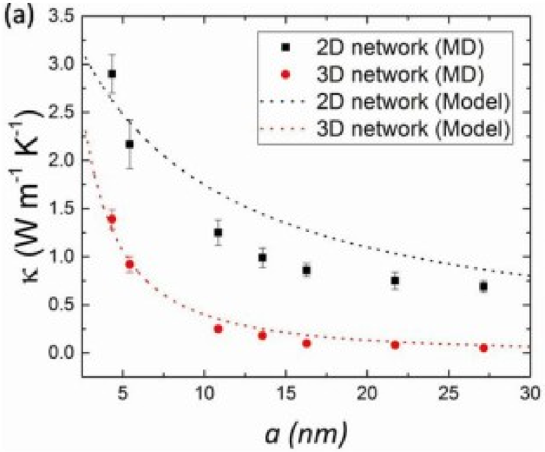
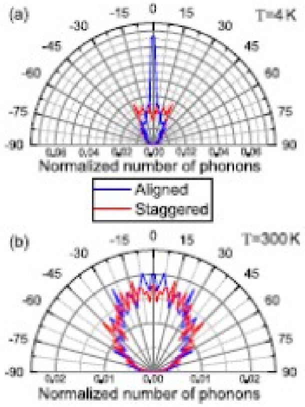
lemta Laboratoire Énergies & Mécanique Théorique et Appliquée

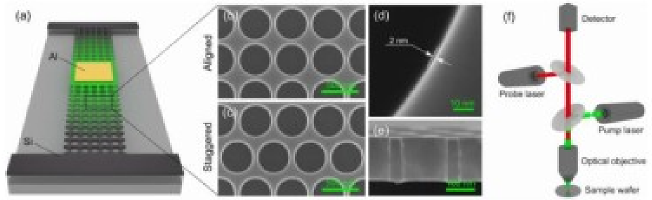
"Thermal Conductivity of 2D and 3D Nanowire Network", PHYSICAL REVIEW B **98**, 155434 (2018)



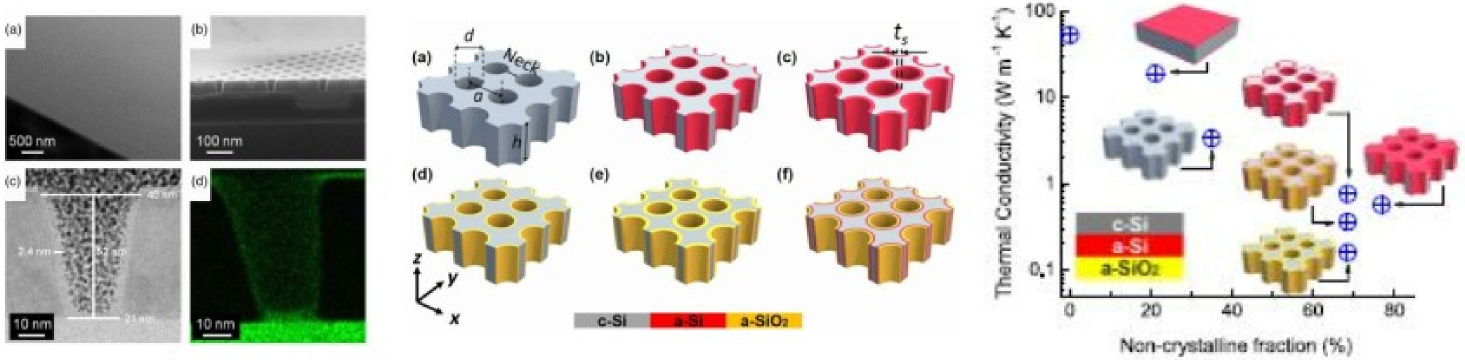


"Aligned/staggered holes of phononic crystals => focusing", PHYSICAL REVIEW B **95**, 205438 (2017)

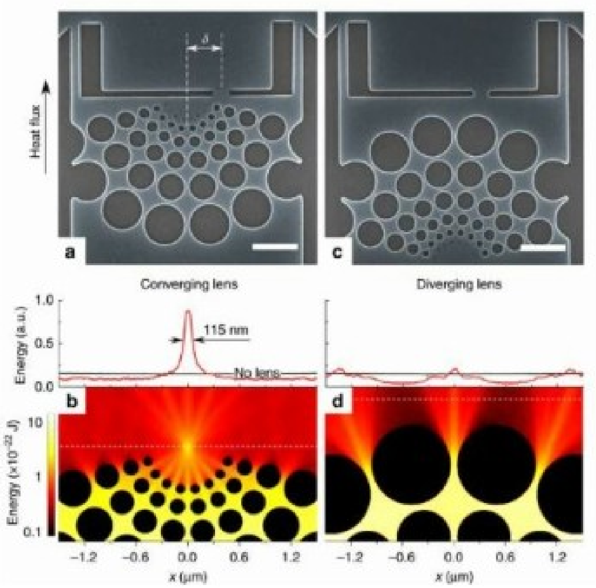




"Phononic Crystals and amorphisation", PHYSICAL REVIEW B **97**, 115435 (2018),

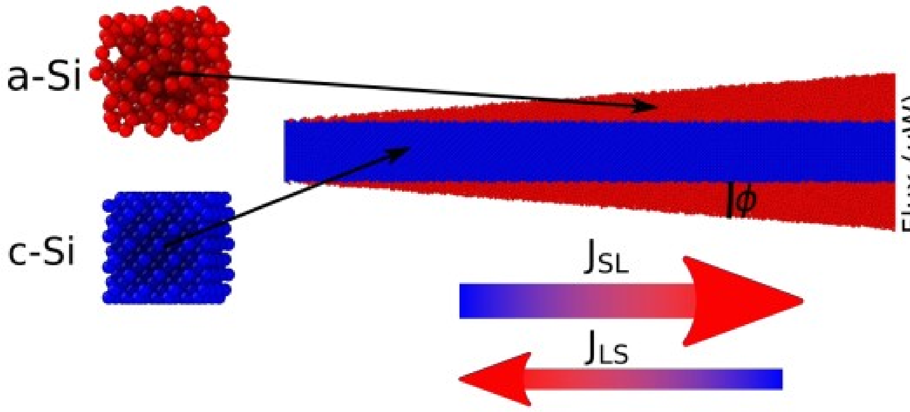


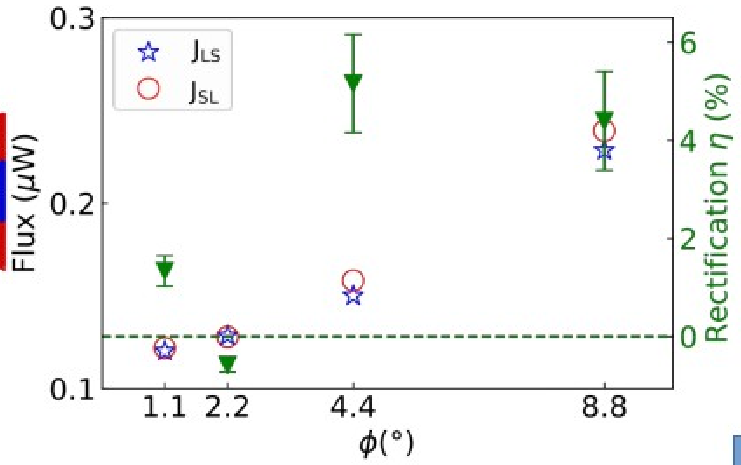
Heat guiding and focusing using ballistic phonon transport
Nature Communications volume 8, Article number: 15505 (2017)



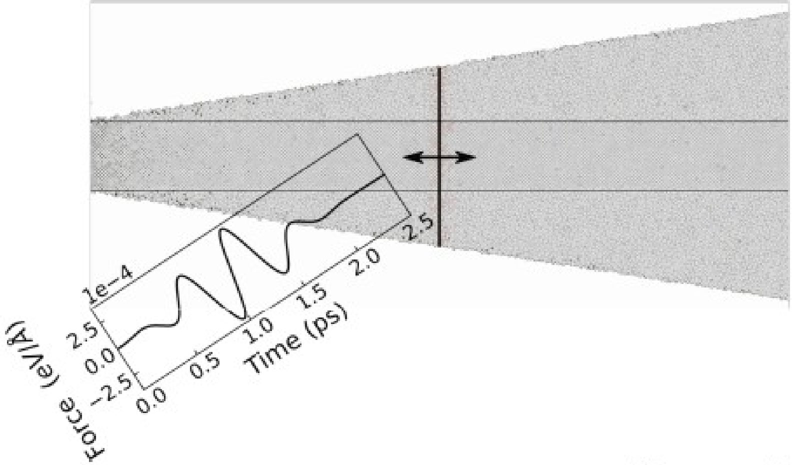
Asymmetrical Nanowires for Thermal Rectification

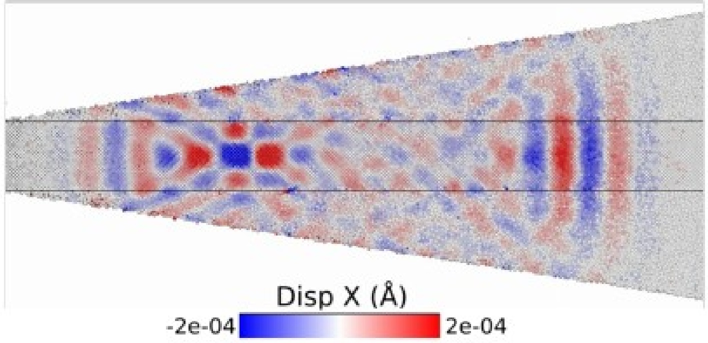
CETHIL UMR 5008 LaMCoS UMR 5259





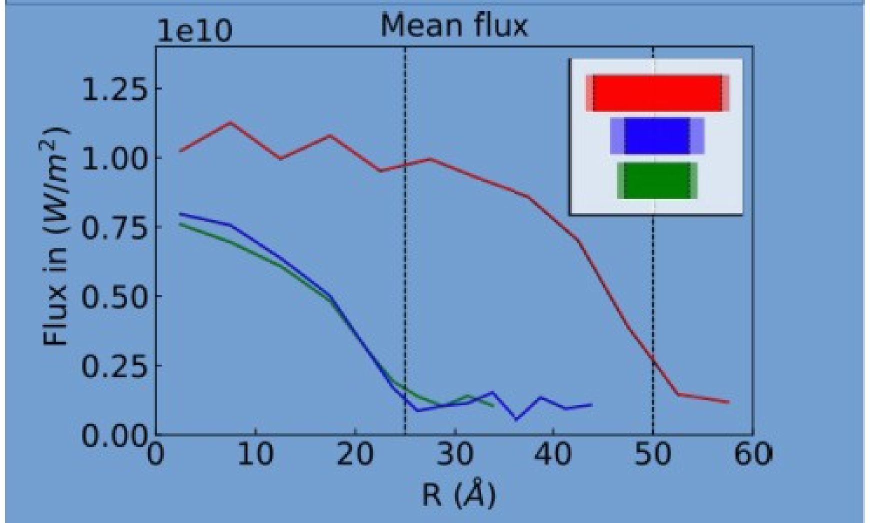
- Geometry
  - Variable thickness shell
- Effect of interface
  - Parallel to the flux
- Thermal properties
  - NEMD
- Vibrational properties
  - Wave Packet





[Desmarchelier, PRB, 2021]

Next Step



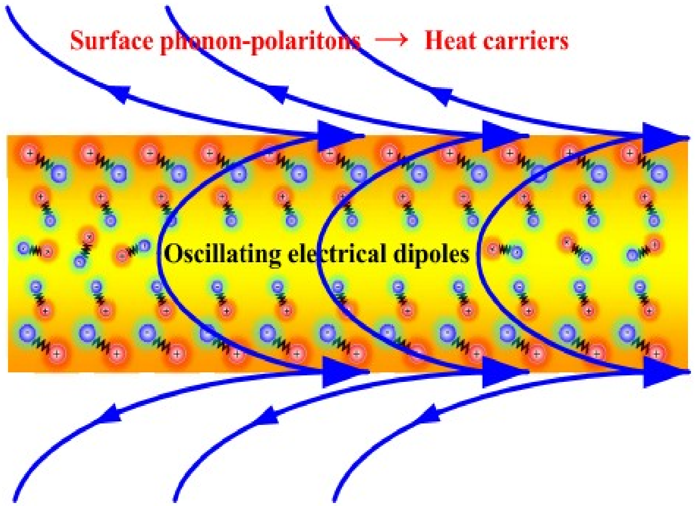
Surface Phonon-Polariton Heat Capacity of Polar Nanofilms

Subtopic: 2D heat transport by SPhPs

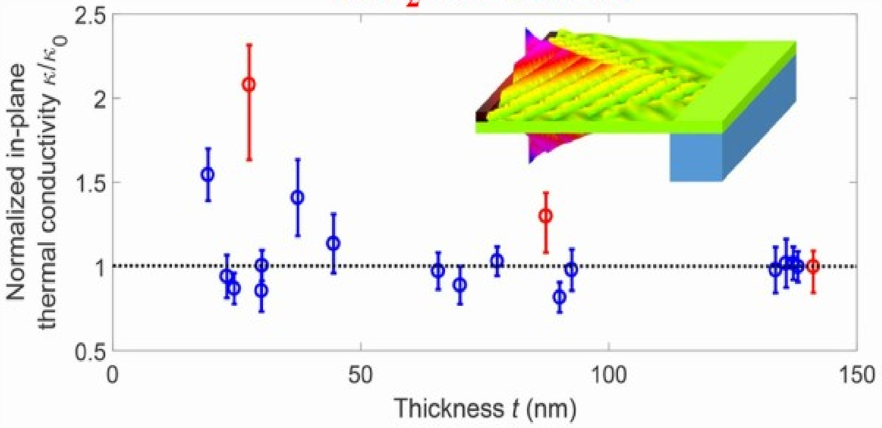
Jose Ordonez, LIMMS-CNRS.

LIMMS
Laboratory for Integrated Micro-Mechatronic Systems
LIMMS/CNRS-IIS UMI 2820

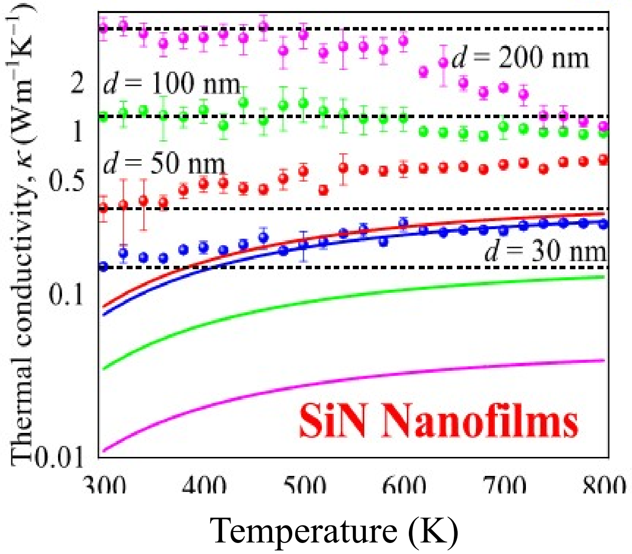
University of Tokyo



SiO_2 Nanofilms



L. Tranchant *et al.*, Nano Lett. 19, 6924 (2019).



Y. Wu *et al.*, Sci. Adv. 6, eabb4461 (2020).

Main Results & Perspectives

- Anharmonic phonon NEGF formalism

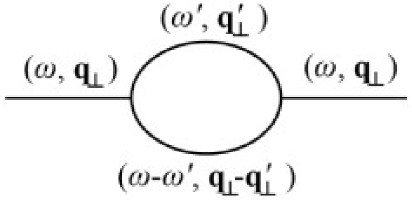
  - For heat conduction through 3D nanostructures (Thin film, SLs, multilayer, interface, *et al*.)

$$\mathbf{G}^{\mathrm{R}}(\omega;\mathbf{q}_\perp)=[\omega^2\mathbf{I}-\tilde{\mathbf{\Phi}}(\mathbf{q}_\perp)-\mathbf{\Sigma}^{\mathrm{R}}(\omega;\mathbf{q}_\perp)]^{-1},$$

$$\mathbf{G}^{>,<}(\omega;\mathbf{q}_\perp)=\mathbf{G}^{\mathrm{R}}(\omega;\mathbf{q}_\perp)\mathbf{\Sigma}^{>,<}(\omega;\mathbf{q}_\perp)\mathbf{G}^{\mathrm{A}}(\omega;\mathbf{q}_\perp),$$

$$\mathbf{\Sigma}_{\mathrm{s}}^{\mathrm{R}}(\omega;\mathbf{q}_\perp)=\frac{1}{2}[\mathbf{\Sigma}_{\mathrm{s}}^{>}(\omega;\mathbf{q}_\perp)-\mathbf{\Sigma}_{\mathrm{s}}^{<}(\omega;\mathbf{q}_\perp)]+iP\int_{-\infty}^{\infty}\frac{d\omega'}{2\pi}\frac{\mathbf{\Sigma}_{\mathrm{s}}^{>}(\omega';\ \mathbf{q}_\perp)-\mathbf{\Sigma}_{\mathrm{s}}^{<}(\omega';\ \mathbf{q}_\perp)}{\omega-\omega'},$$

$$\Sigma_{\mathrm{s},\,l_x l'_x}^{<,>ij}(\omega;\mathbf{q}_\perp)=\frac{1}{2}i\hbar\sum_{l_{1x}l_{2x}l_{3x}l_{4x}}\sum_{j_1j_2j_3j_4}\frac{1}{N}\sum_{\mathbf{q}'_\perp}\tilde{\Phi}_{l_x l_{1x} l_{2x}}^{ij_1j_2}(\mathbf{q}'_\perp,\mathbf{q}_\perp-\mathbf{q}'_\perp)\tilde{\Phi}_{l'_x l_{3x} l_{4x}}^{jj_3j_4}(\mathbf{q}'_\perp-\mathbf{q}_\perp,-\mathbf{q}'_\perp)$$
$$\times\int_{-\infty}^{\infty}\frac{d\omega'}{2\pi}G_{l_{1x}l_{4x}}^{<,>j_1j_4}(\omega';\mathbf{q}'_\perp)G_{l_{2x}l_{3x}}^{<,>j_2j_3}(\omega-\omega';\mathbf{q}_\perp-\mathbf{q}'_\perp).$$



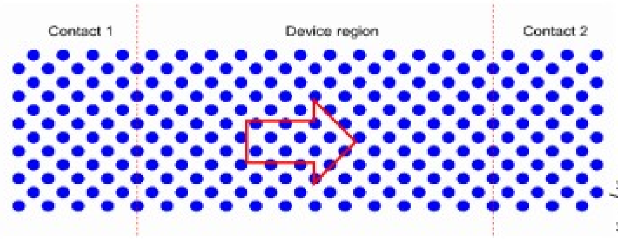
- Numerical implementation
  - Recursive algorithm
  - MPI parallelization
  - DFT input

"Large-scale quantum heat transport simulation"

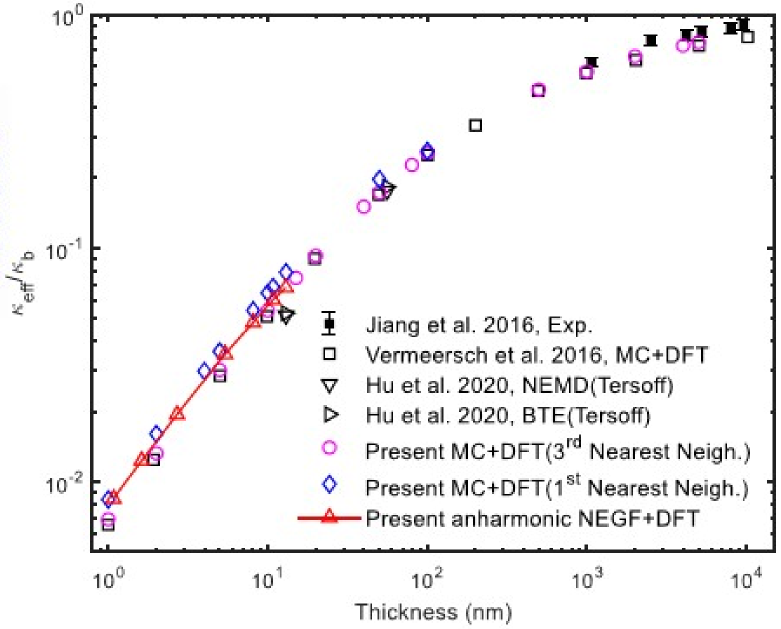
Y. Guo, M. Bescond, Z. Zhang, *et al*. PRB **102**, 195412(2020)

- Benchmark

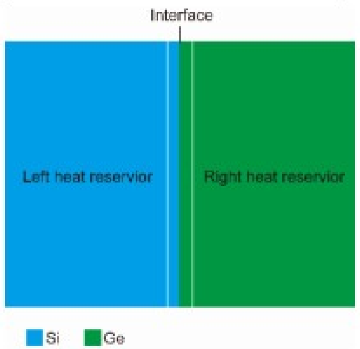
c. Simulations of energy transport properties



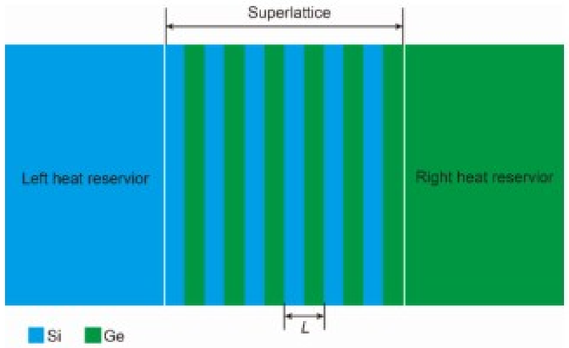
Heat conduction across a Si thin film at 300K



- Application & Perspective



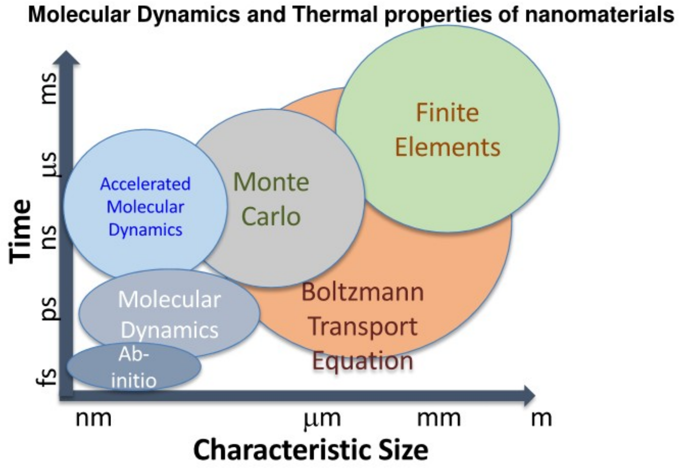
Si/Ge interface



Si/Ge SLs

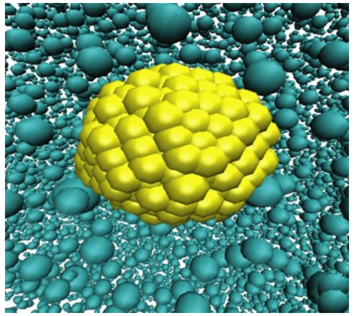
Starting an Overview on different simulations techniques

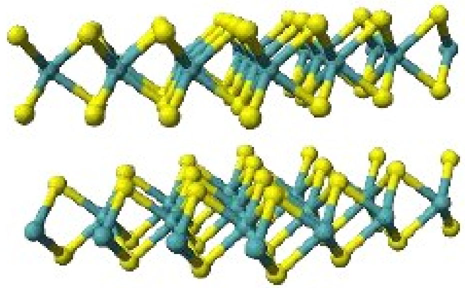
- ✓ Boltzmann Transport Equation (Monte-Carlo,..)
- ✓ Anharmonic Lattice dynamics
- ✓ Approximate ab initio methods



Modeling nanostructured materials: some recent trends

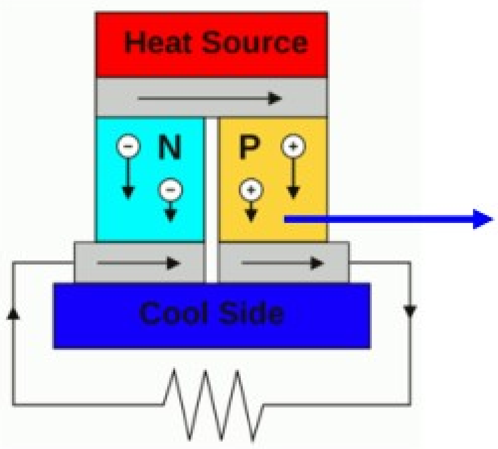
- ✓ Nanoparticles
- ✓ 2D materials

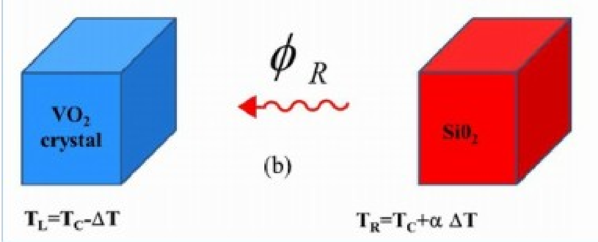




Which property ?

- ✓ Electronic conductivity
- ✓ Seebeck coefficients
- ✓ Radiative heat transfer





[Ben-Abdallah, APL, 2013]

d. Measurements techniques of energy transport and conversion properties

Animator: Séverine Gomès

Energy transport and conversion properties

From axis 3, analyzed energy conversion

- Conversion « Thermal 🔔 Electrical »
- Conversion « Optical 🔔 Electrical »
- Conversion « Mechanical 🔔 Electrical »
- Conversion « Chemical 🔔 Electrical »
- Hybrids / Cogeneration

Properties and parameters to be measured:

- **Thermal** conductivity, diffusivity, flux, resistance, heat capacity, temperature,…
- **Electric** electrical resistivity, I V curve, permittivity …
- **Thermoelectric** Seebeck effect, electrical resistivity, thermal conductivity, Peltier coefficient
- **Optical** emissivity, reflectivity, properties of absorption and fluorescence
- **Mechanical** displacement, deformation, flexibility, stiffness, friction…
- **Chemical** electrochemical properties, ionic retention, catalyze kinetic
- …

How to measure them for nanomaterials?

Thermal properties and parameters (1)

Generalities

Thermal conductivity, thermal diffusivity, effusivity, thermal barrier resistance, surface phonon-polaritons heat transfer

The methods currently employed and developed invariably associate

Thermal stimulation of the sample under test

+

Measurement of sample temperature response **associated to** Direct or inverse modeling

Information on the thermal properties of the sample.

Depending on the excitation and measurement method, several broad categories can be identified.

Thermal properties and parameters (2)

Photothermal methods

Thermal conductivity, thermal diffusivity, effusivity,
thermal barrier resistance, surface phonon-polaritons heat transfer

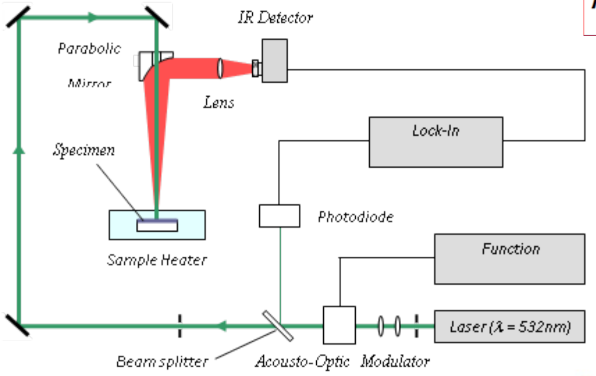
Frequency domain photothermal radiometry (PTR)

Thin films (materials and nanocomposites)

0.1 Hz — 100 Hz — 100 KHz — 10 MHz — f

0.1 Hz – 100 Hz	100 Hz – 100 KHz	100 KHz – 10 MHz
Thermal diffusivity, effusivity, heat capacity	**Thermal diffusivity and effusivity**	**Thermal diffusivity and effusivity and Thermal Boundary Resistance**
Thickness 500 µm – 2 mm Back and front detection	Thickness of 1-50 µm	Thickness < 500 nm
• Nanocomposites • Metal sheet • Anisotropic material	• Organic thin films • Metal alloys • Irradiated materials	• Phase changing materials • Metal/semiconductor • Interfaces

$$\mu = \sqrt{\frac{a}{\pi f}}$$



Spatial resolution limited to diffraction (≈500 nm)

Minimum studied thin film thickness depends on thermal properties of materials (few tens of nm): Fourier's law

Excited layer opaque to the laser wavelength otherwise coating needed

Other techniques to be presented

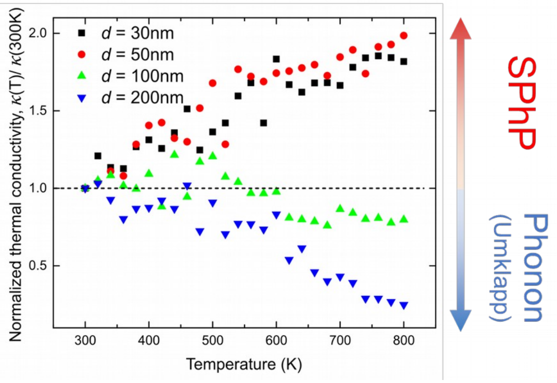
Frequency domain thermoreflectance

Raman spectroscopy

Time domain thermoreflectance

……

SiN nano-membranes



Laboratory for Integrated Micro-Mechatronic Systems LIMMS/CNRS-IIS UMI 2820

Y. Wu et al., Science Advances ***6****, eabb4461 (2020).*

Thermal properties and parameters (3)

Temperature, Thermal conductivity, heat flux, or specific heat

Electrothermal methods

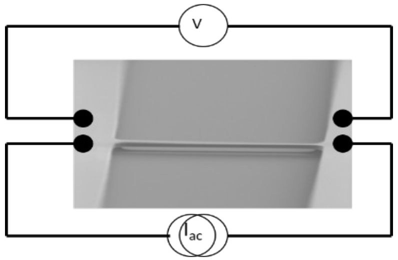
NÉEL institut

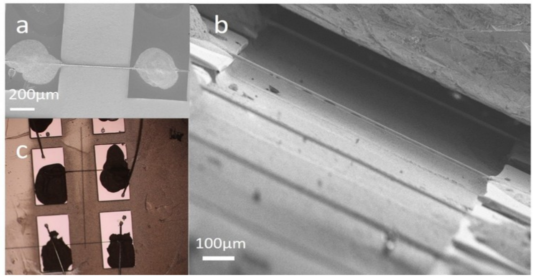
3 omega in various geometries

1D individual nanowires (0K-400K)

Longitudinal technique for nanowires to microbundles or fibers

Phonon regime: Ziman to diffusive



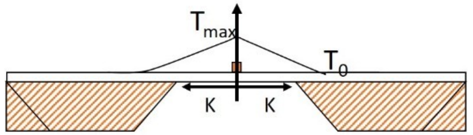


JAP 2007, NanoLetter 2009, PRB 2015, PRB 2017

NbN

2D membranes and thin films (4K-400K)

Phonon regime: Bound. Scatt to diffusive



RSI 2013 2015, PRB 2015

NbN

3D thin films and bulk substrates (4K-400K)

- For thin films (e>100nm): from 0.01 W/mK to 30 W/mK
- For forest of nanowires
- For bulk 3D: 0.01 to 400W/mK

Phonon regime: Bound. Scatt to diffusive

Nanofluids (RT→ 450K)

iTheMM

- *k* and *a* simultaneously,
- Absolute or comparative measurements,
- TBR estimation between particles and fluid

Differential platform (0K-400K)

Temperature range : 0.03K ->400K

Monolithic nanostructures

Suspended 2D materials

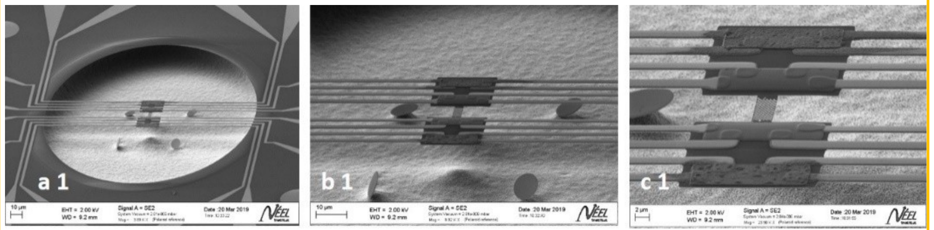
(graphene, HBN, WSe_2, MoS_2, etc…)

Individual nanowires or nanobundles

(but contact thermal resistance!)

Phonon regime:

quantum/ballistic to diffusive



Thermal properties and parameters (4)

Temperature, thermal conductivity/conductance, heat flux

AFM - electrothermal methods

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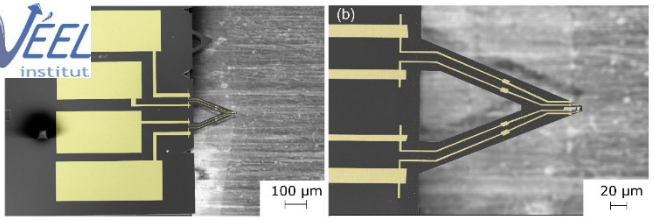
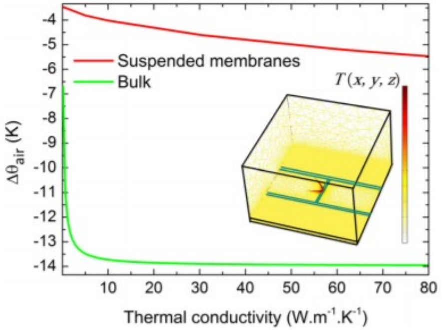
Scanning Thermal Microscopy (SThM)

Widely used over the 



New probe 4 wires, NbN thermometers (5-10 times more sensitive).



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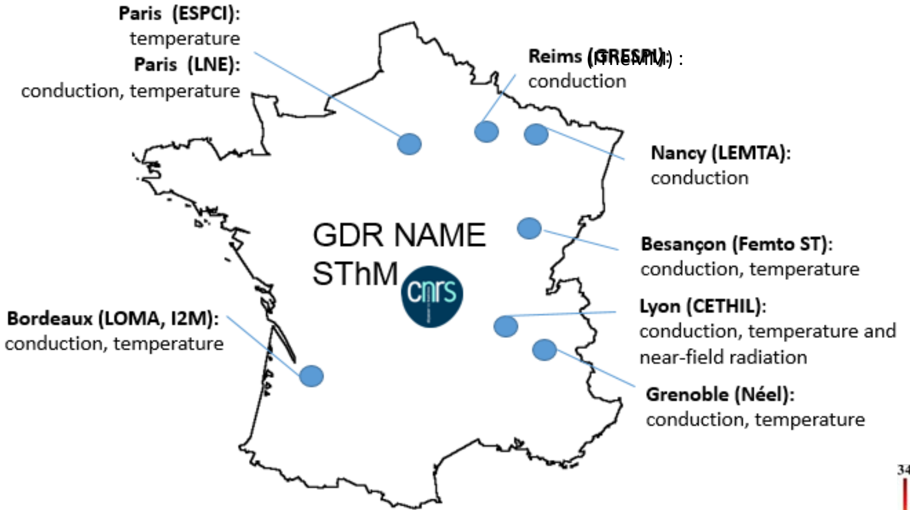
Massoud et al., APL 2017



Application

- Bulk materials
- Thin films on substrate
- Suspended membranes
- Nanowires (in matrix or suspended)
- 2D materials (on substrate or suspended)
- Imaging of local Joule and Peltier effects of a self-heated nw

Depending on probe

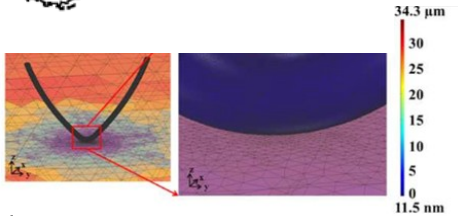
(conventional mode)

Lateral spatial resolution: 10 nm (UHV)

TC-sensitivity range:

- < 10 $W.m^{-1}.K^{-1}$ for bulk samples
- larger for samples reshaped for reducing their thermal conductance (suspended membrane, nw)

Last trends



- Low temperature measurements
- Numerical electro-thermal modelling of probe-sample system
- New probes with better sensitivity
- Combined instruments & SPM modes

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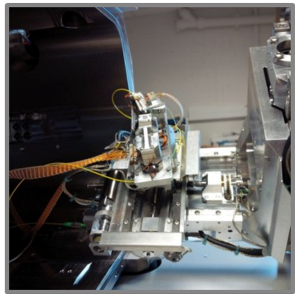
Integration in the SEM



Electric properties and parameters (1)

AFM – various electrical modes

Electric current, voltage, surface potentiel,
Work function, barrier height , electric resistance, capacitance

Scanning Capacitance Microscopy (SCM)

Scanning Spreading Resistance Microscopy (SSRM)

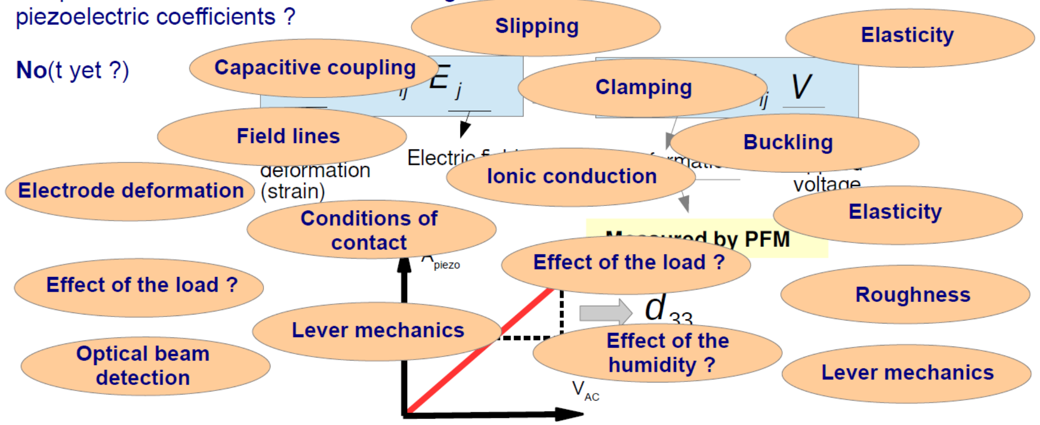
Spatial resolution < 10 nm
Mesurable sample parameters:

- Active dopants and dopant (p ou n)
- Global electrical resistance of nano-contact (probe and sample, (SSRM)

Piezoresponse Force Microscopy

Is it possible to use cantilever motion to gain access to nanoscale measurement of piezoelectric coefficients ?

No(t yet ?)



Kelvin probe force microscopy (KPFM)

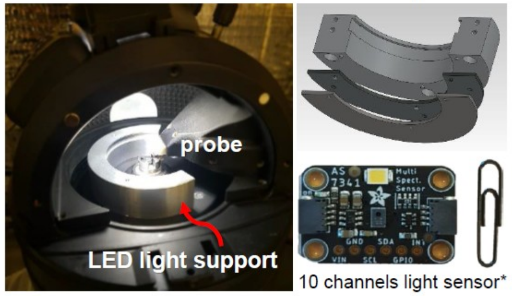
UHV

Conductive AFM (C-AFM)

Metrology of surface potentials and currents

Goal: Estimate uncertainty on the photovoltaic performance of Nanowire arrays

Instrumentation needs and developments



LED based solution for a fiber-coupled sun simulator source**

Illumination & Dark measurements

KPFM

- High-resolution
- E_F local variations
- Capacitance gradients in Z (correlation with SMM)

C-AFM

- I-V spectroscopy
- Current maps vs Voltage
- Extraction of photovoltaic performance: V_{oc}; I_{sc}; η

Challenges:

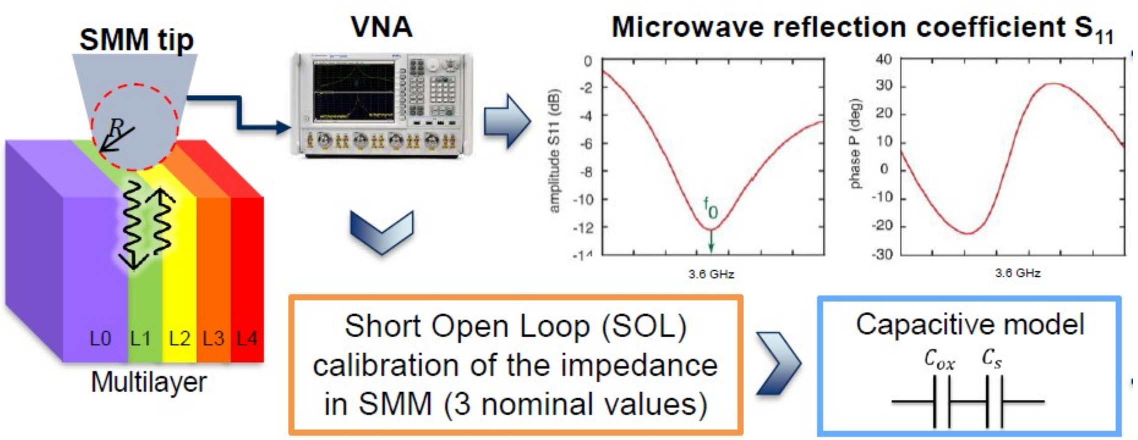
- Force constant of the cantilever: effect of force on currents.
- Positioning of tip on NWs: spectroscopy vs stack imaging.
- Reproducibility and repeatability.
- Environment and surface quality.
- Illumination conditions: intensity, spectrum range, angle.

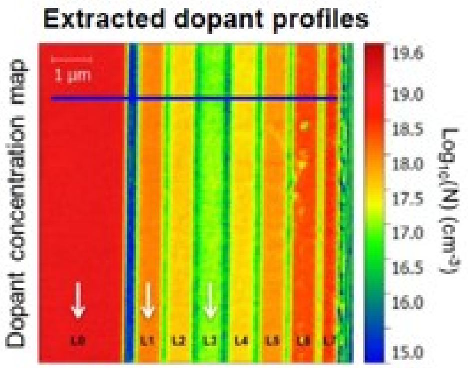
Electric properties and parameters (2)

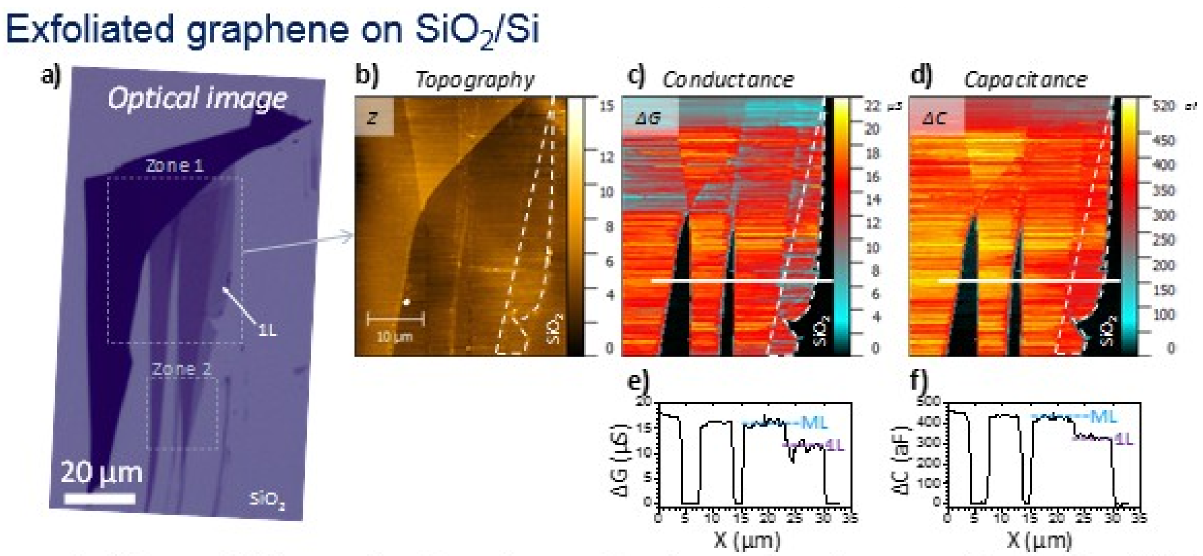
AFM - various electrical modes

Dopant concentration, electric conductance and capacitance

Scanning microwave Microscopy (SMM)







Calibrated (through plane) **conductance** and **capacitance** (~GHz)
+ sensitive to **number of layers**

State of art:
- Comprehensive traceability of capacitance metrology in SMM – 3% relative uncertainty budget on micro MOS structures [2].

Challenges:
- Reduce uncertainty (10%) on the measured values of concentrations.
- Is it ever possible to identify « *real* » dopant concentrations? *(see perspectives)*

Conclusion

Properties and parameters to be measured:

From axis 3, analyzed energy conversion

- Conversion « Thermal 🔔 Electrical »
- Conversion « Optical 🔔 Electrical »
- Conversion « Mechanical 🔔 Electrical »
- Conversion « Chemical 🔔 Electrical »
- Hybrids / Cogeneration

Properties and parameters to be measured:

- **Thermal** conductivity, diffusivity, flux, resistance, heat capacity, temperature,…
- **Electric** electrical resistivity, I V curve, permittivity …

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- **Thermoelectric** Seebeck effect, electrical resistivity, thermal conductivity, Peltier coefficient
- **Optical** emissivity, reflectivity, properties of absorption and fluorescence
- **Mechanical** displacement, deformation, flexibility, stiffness, friction…
- **Chemical** electrochemical properties, ionic retention, catalyze kinetic
- …

Associations with CnM

Club nanoMétrologie

for the both kind of SPM – techniques

Still defined at nanoscales?

Limitation of modeling for the analysis of raw data ?

Need of other contributions for completing the list of properties and of measurements techniques

CONCLUSION
PERSPECTIVES

Main conclusions

- A very broad variety of compounds and nanomaterials available
- Requirements in terms of thermal characterization

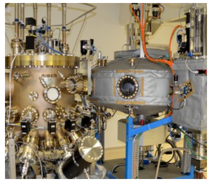
- Overviews started on:
  - synthesis methods
  - recent techniques or hybrid techniques for microstructural and chemical characterization
  - simulations techniques
  - measurement techniques

Need of other contributions!

- Which physical properties and parameters ?

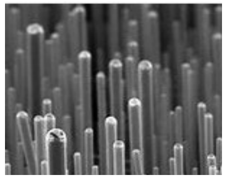
- Necessity to be in relation and connected with others workshops.

Four scientific topics



a. Elaboration-Synthesis

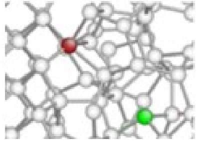
- ➢ Real nanomaterials and synthesis processes



b. Measurements techniques for microstructural definition

- ➢ Characterized nanomaterials and processes

Nanomaterials for Energy applications



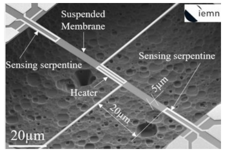
- ➢ Design laws at the nanoscales

c. Simulations of energy transport and conversion properties

- Based on modeling tools and theories available

- ➢ Physical property understanding and prediction

Comparison validation



d. Measurements techniques of Energy transport and conversion properties

- ➢ Physical property understanding and measurement

Expected input from Axis 2 due to modelling and theory limitations from other Axes nanomaterial property specification

Expected input from other axes nanomaterial property specification

Thanks to the participants in workshops

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Thanks a lot for your attention

Some questions?