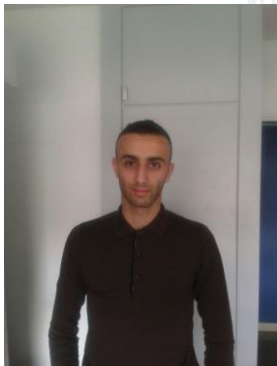


COMSOL Multiphysics® Based Identification of Thermal Properties for Mesoporous Silicon by Pulsed Photothermal Method

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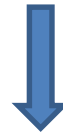


Outline

- 1) Motivation for thermal identification of TFM/CM
- 2) Pulsed Photo-Thermal technique (PPT)
- 3) Structural characterization
- 4) COMSOL Computation
- 5) Results & Conclusion

Motivation for mesoporous Si

- We are interested by MS Si for Luminescence, PV applications and microsystems like fuel cells, and for electronic (Front and Back-end). See references
- Thermal characterisation of MP Si is based on fast optical techniques like photothermal, and needs analytical models for 1 or 2D thermal problems.
- ~~• Analytical models + Complex surfaces (2D, thin films, mesoporous,...)~~



Numerical models are needed (Comsol®)!

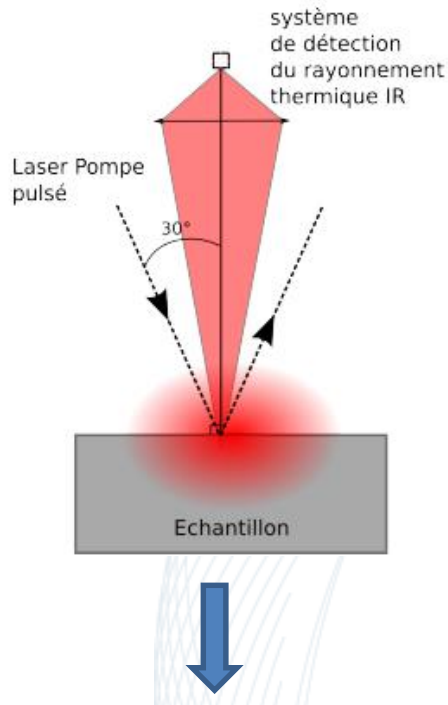
1) Experiments by PPT

2) Modelling of laser heating by COMSOL

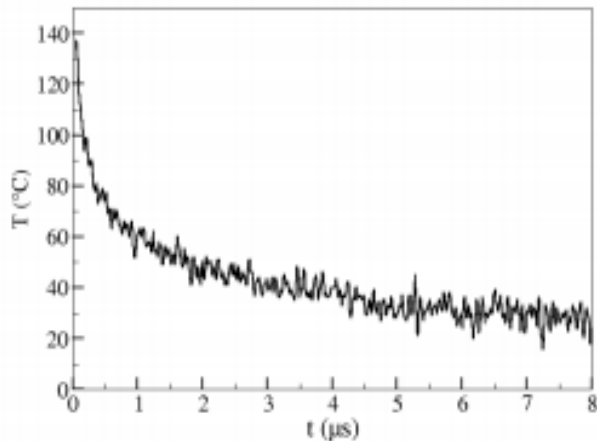


3) Identification of Thermal Properties (k, Rth, ...)

PPT methods : Principles



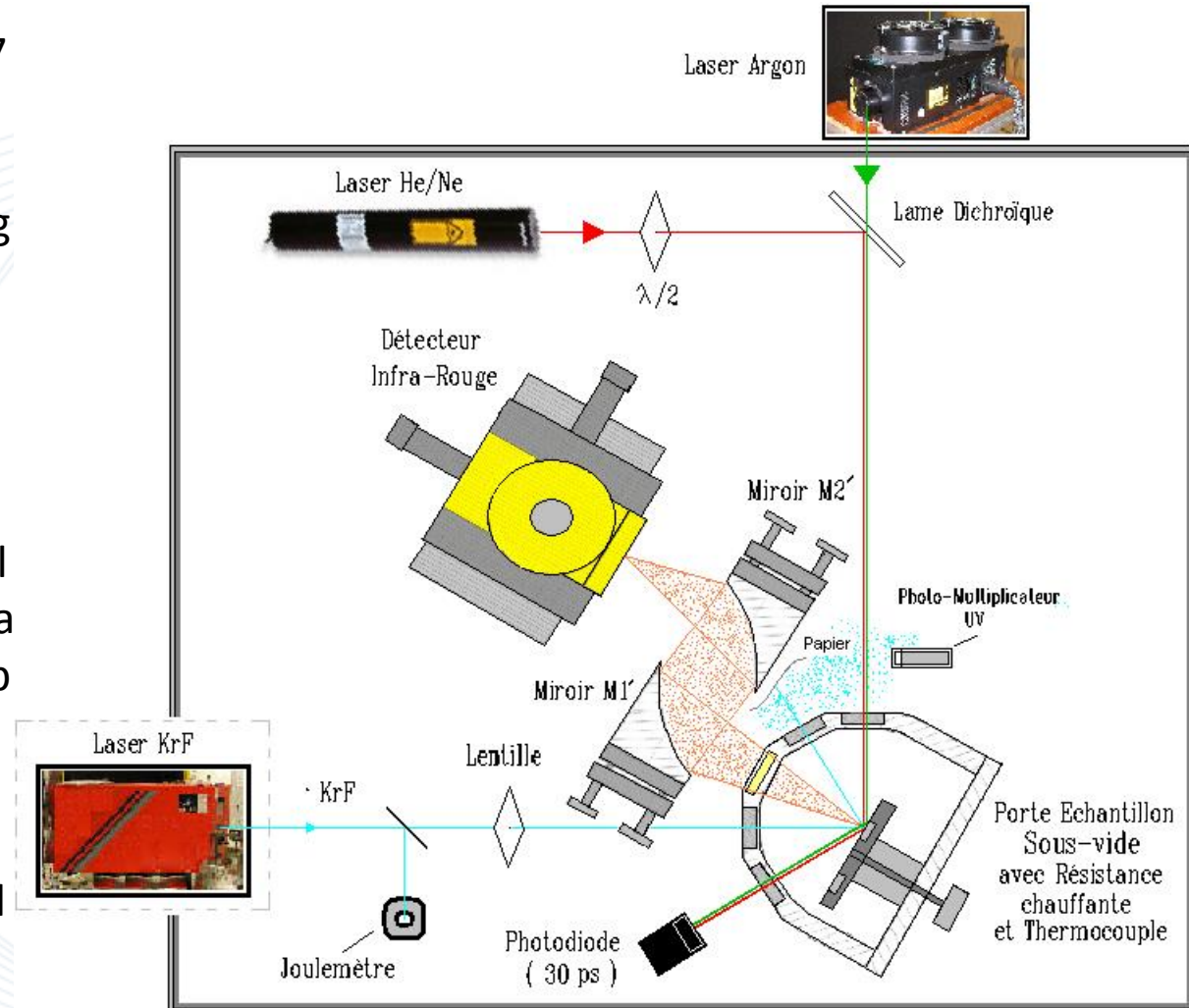
- 1) Near surface laser heating
- 2) IR detection (needs fast detectors!)
- 3) Recording of surface temperature versus time (in the nanosecond regime)
- 4) Optimisation of the computed thermal signal versus thermal parameters : Correlation between experiments and Comsol thermal curves.



k, ρ, C_p, \dots

Experimental device

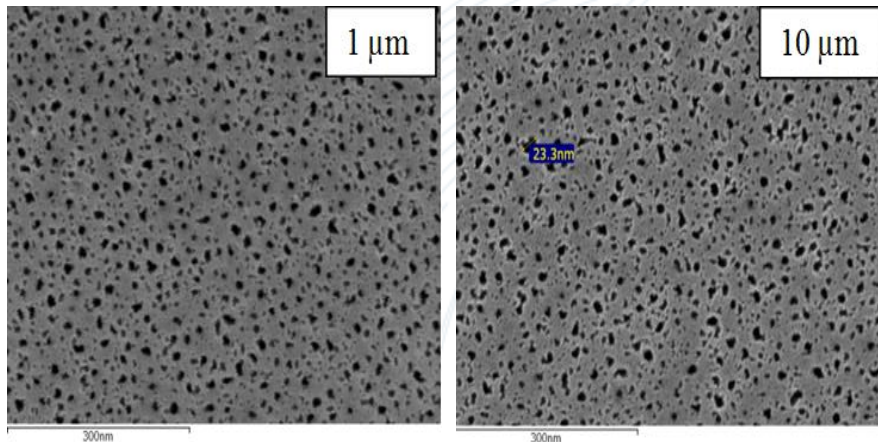
- 1) Pulsed laser heating of samples ($\lambda=248$ nm; $\tau = 27$ ns; $F= 100$ mJ/ cm²)
- 2) IR signals are focused using off-axis paraboloid mirrors (1 to 12 μ m) onto a fast HgCdTe detector, liquid nitrogen cooled.
- 3) The output electrical signal (voltage) is recorded onto a wide-band oscilloscope (up to 4 GHz).
- 4) Calibration procedure: conversion of the electrical signal into absolute temperature.



SEM and FTIR

for size and porosity implementation

- Electro-chemical etching for Mono-cristalline n type (100) fabrication at 0.2,1,10 & 50 μm depth.
- Sample sizes (10 X 10 X 0.5 mm)



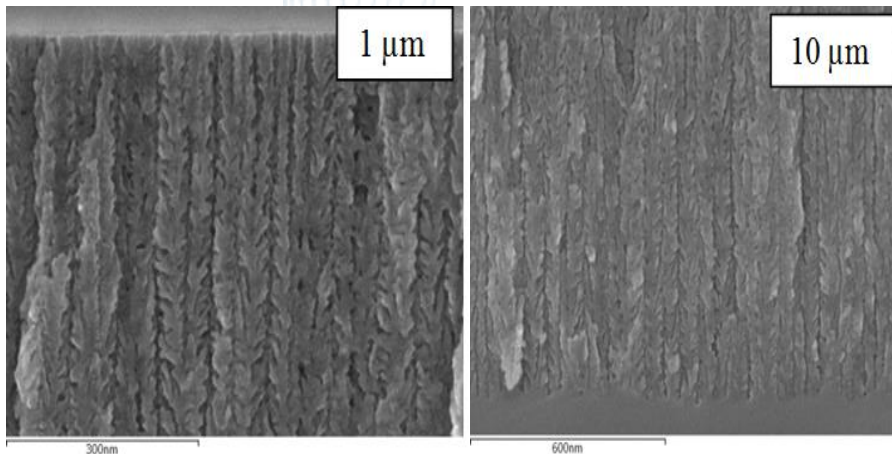
- Pore sizes are ranging from 5 to 25 nm
- Pore density is : $3.2\text{-}3.75 \times 10^3$ pores/ μm^2
- Coloumnar (fir-like) structures

SEM + FTIR



Etching depth Porosity

0.2 μm	34 %
1 μm	26 %
10 μm	33 %
50 μm	25 %

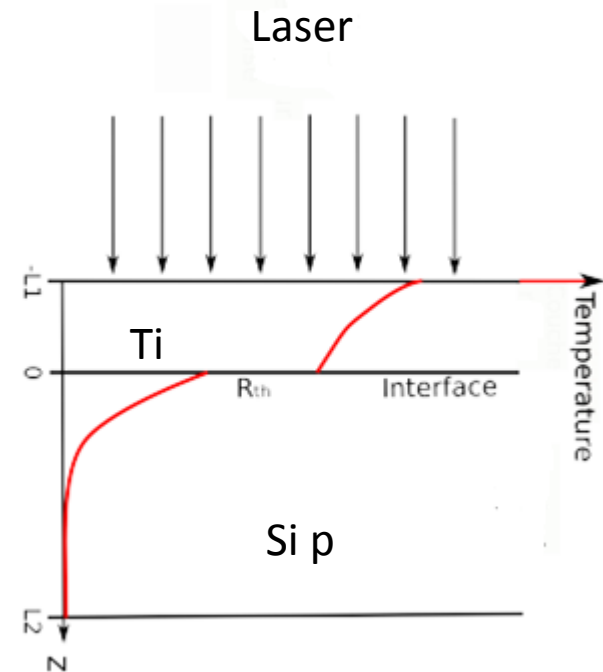
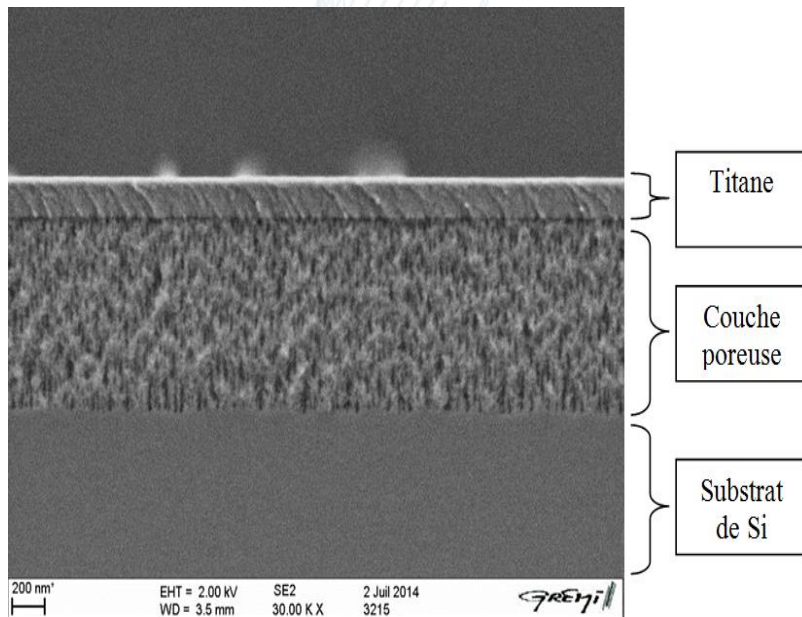


Ti transducer by magnetron sputtering deposition

To ensure homogeneous absorption of the incident photons (UV) and a high and stable IR emission. Finally to create a surface (less than 200 nm) heat source

Thermal contact resistance (R_{th})

Induces by the Ti/MP Si interface. It's a very important parameter for thermal field and temperature response evaluation.



Comsol Multiphysics

The screenshot displays the COMSOL Multiphysics software interface. On the left is the **Model Builder** tree, showing a hierarchy from **Root (root)** down to **Geometry** (containing rectangles and points), **Materials**, **Heat Transfer in Solids (ht)**, **Mesh**, and **Study** (with a **Parametric Sweep** and **Step 1: Time Dependent**).

The central **Node Properties** pane shows details for a selected node:

- Name:** 1µm type n new last.mph
- Path:** E:\IBRAHIM\Si type N\New Folder\New Folder\1µm type n
- Program:** COMSOL 4.3b (Build: 189)
- Tag:** Model2
- Author:** (empty field)
- Date created:** (empty field)
- Date modified:** Jul 24, 2014 5:52:55 PM
- Modified by:** (empty field)
- License number:** 1037460
- Version:** (empty field)
- Comments:** Transient Axisymmetric Heat Transfer. This is a benchmark model for an axisymmetric transient thermal analysis. The temperature on the boundaries changes from 0 degrees C to 1000 degrees C at the start of the simulation. The temperature at 190 s from the analysis is compared with a NAFEMS benchmark solution.

The **Used Products** section lists COMSOL Multiphysics and Heat Transfer Module. The **Unit System** is set to SI, and the **Font** size is 9 pt.

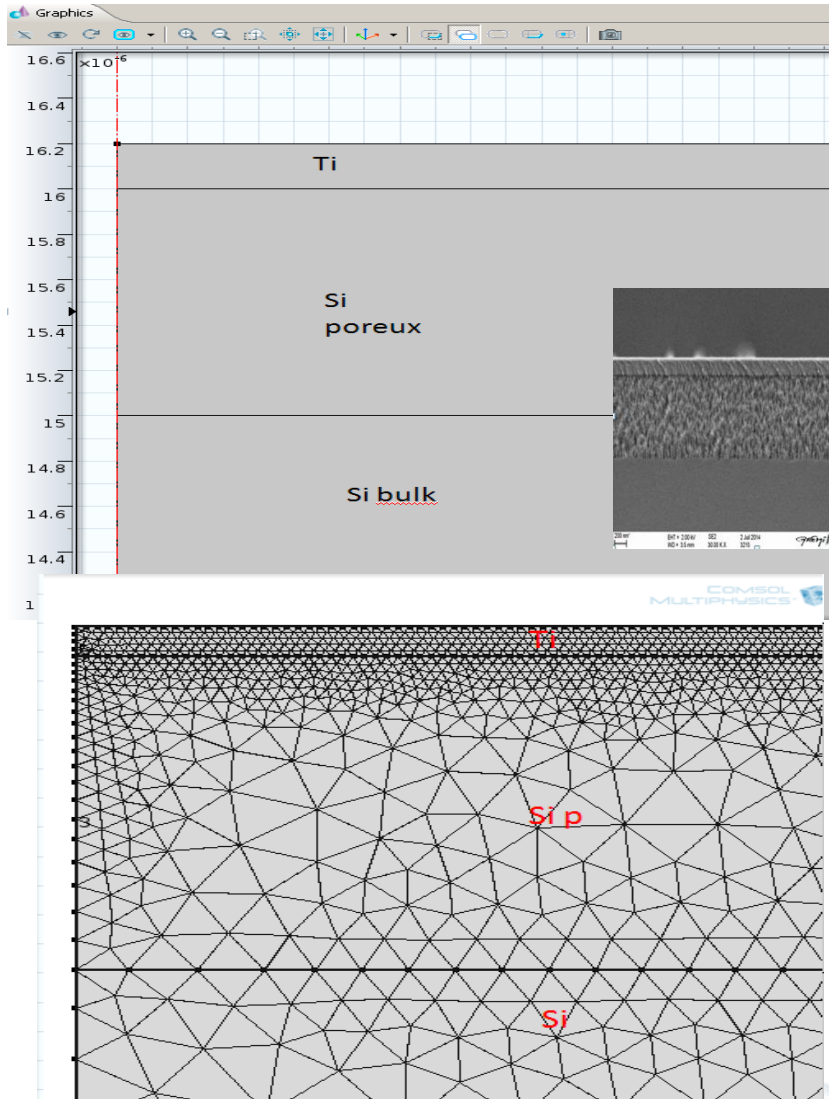
The **Graphics** window on the right shows a 3D visualization of a cylinder with a temperature distribution. The plot is titled "Time=0 Volume: Temperature (K)". A color scale on the right ranges from 293 K (blue) to 293 K (red), with intermediate values of 20 and 40. The cylinder is highlighted in green, and a coordinate system (x, y, z) is visible at the bottom left of the plot area.

At the bottom of the interface, there are tabs for **Messages**, **Progress**, **Log**, and **Table 5**. The version number **COMSOL 4.3.2.189** is displayed at the bottom left.

Geometry and meshes

- 3D model
- Multilayer model including interfaciale resistance and porous media

	Ti	Si bulk	Si poreux
Thickness	200 nm	50 μm	[0.2, 1, 10, 50] μm
k (W/m/K)	22	125	?
ρC_p (J.K-1.m-3) $\times 10^6$	2.5	1.5	?
Maillage	5 à 10 nm	Quelques μm	5 nm à quelques μm



Physics ?

➤ Heat Transfer in Solids module :

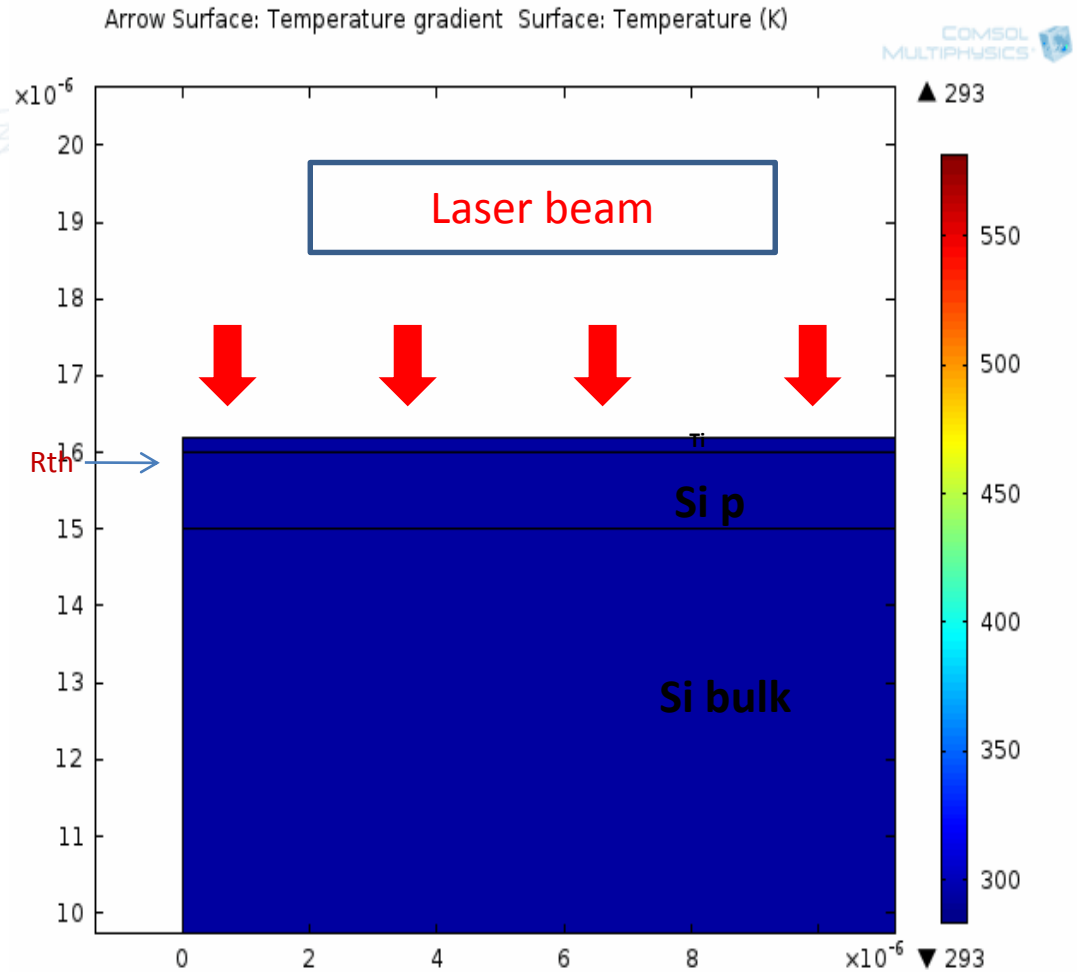
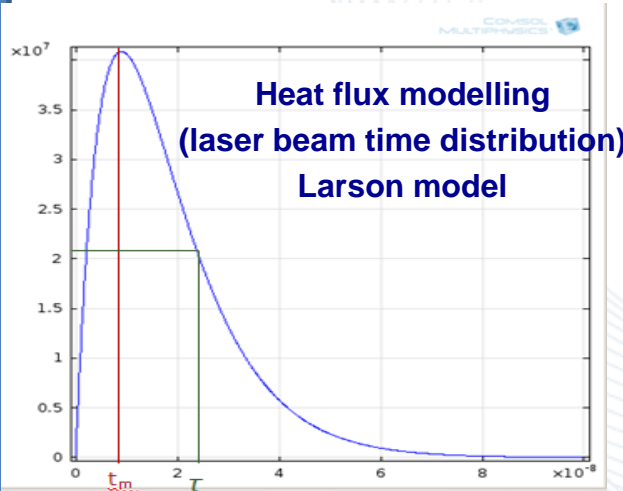
$$\rho \cdot C_p \frac{\partial T}{\partial t} = \nabla \cdot (k \nabla T)$$

➤ Heat Transfert in Porous Media :

✓ $\rho C_p \mathbf{u} \cdot \nabla T = \nabla \cdot (k_{eq} \nabla T)$

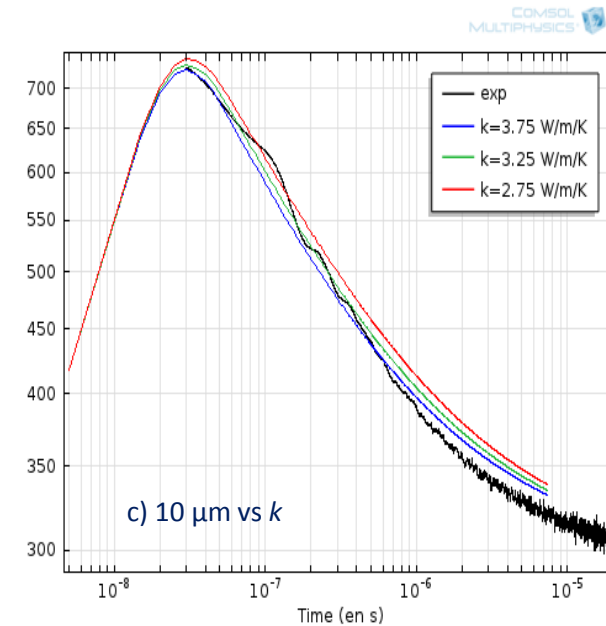
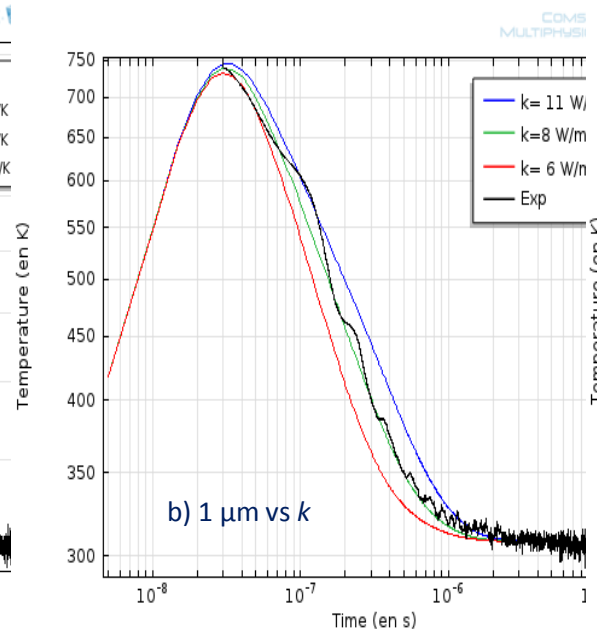
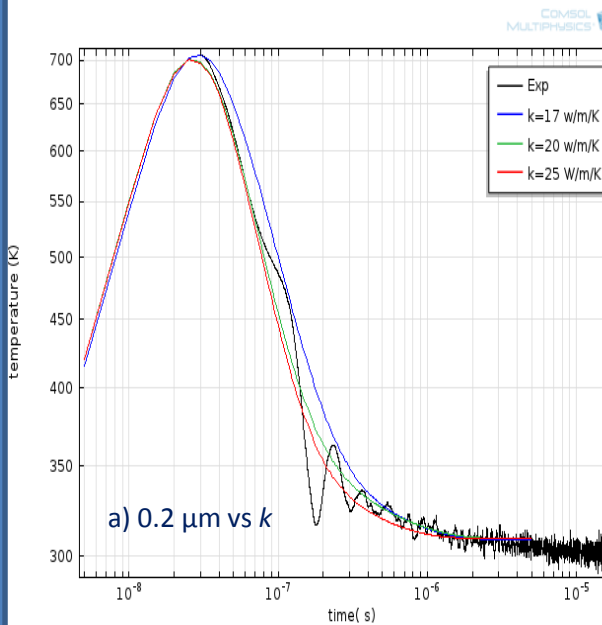
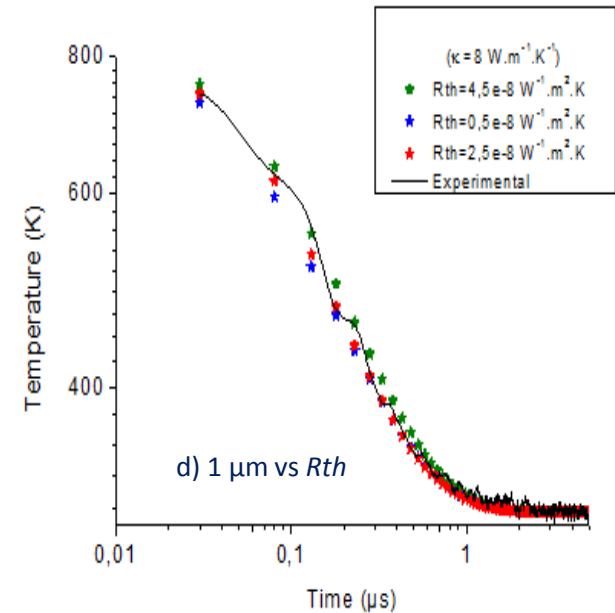
✗ $k_{eq} = \theta_p k_p + (1 - \theta_p) k$

➤ Boundary conditions



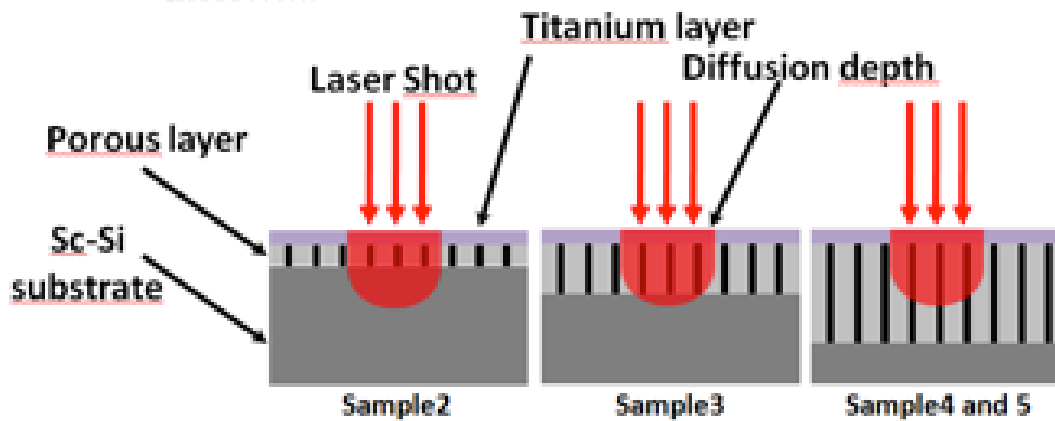
Results, Experiments Vs Modelling

- Parametric Sweep is employed to optimise the identification of each parameter.
- Here examples for k identification 0.2, 1, and 10 μm , and R_{th} for 1 μm .



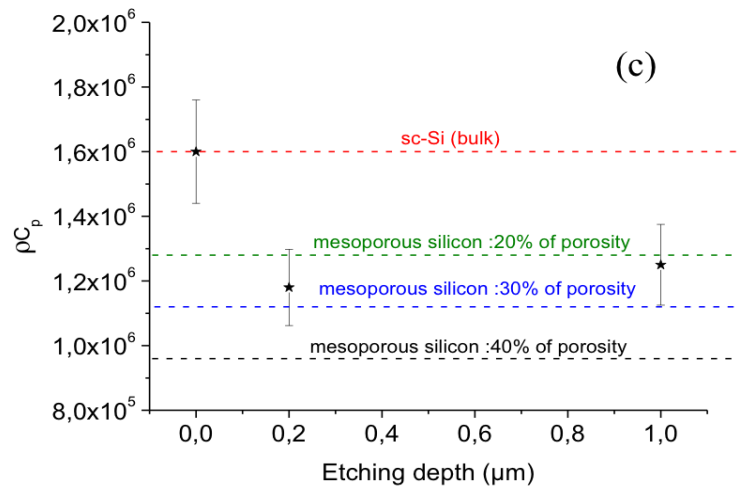
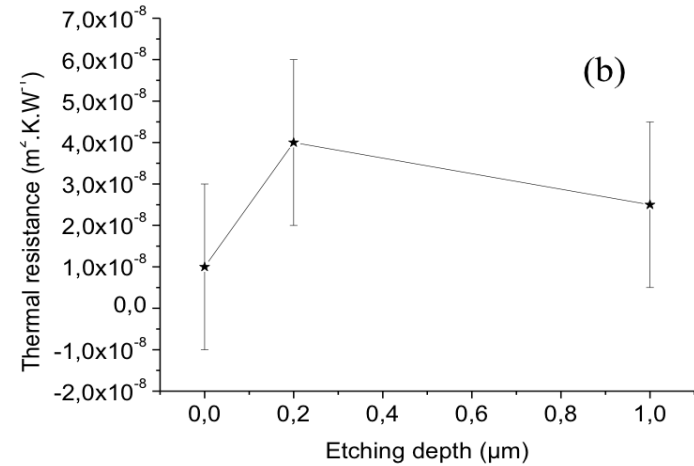
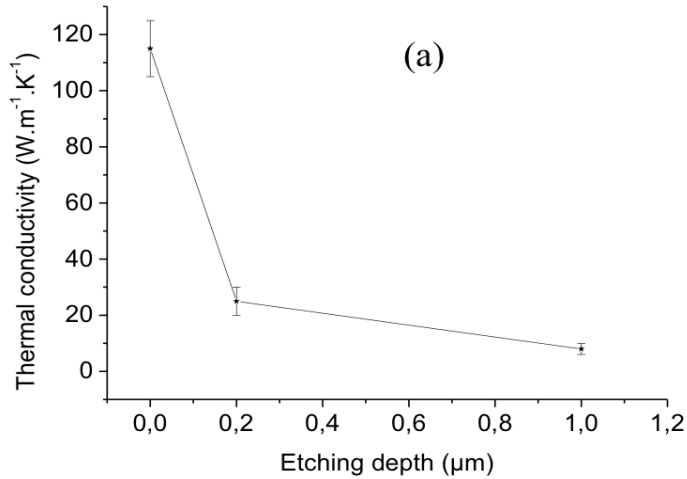
Results summarizing

	Ti	Bulk	0.2 μ m	1 μ m	10 μ m	50 μ m
k_p (W/m/K)	22	125 \pm 17	20 \pm 4	8 \pm 2	3 \pm 0.5	2 \pm 0.5
ρC_p (J.K ⁻¹ .m ⁻³)(x 10 ⁶)	2.5 \pm 0.05	1.5 \pm 0.05	1.25 \pm 0.05	1.15 \pm 0.05	1.22 \pm 0.05	1.25 \pm 0.05
R th (m ² .K/W)	-	2 x 10 ⁻⁸ \pm 2	1x10 ⁻⁸ \pm 2	2.5x10 ⁻⁸ \pm 2	20x10 ⁻⁸ \pm 2	80x10 ⁻⁸ \pm 2
T max(K)	-	590	700	727	740	752
Tps relax(μ s)	-	1.1	1.2	2.0	5	5



Thermal properties vs etching depth

(Submitted to J. Phys.D)



Conclusion

- New results are evidenced in this work for the $\langle 100 \rangle$ n-type porous Si based on Comsol[®] builder with more adapted physics.
- Comsol[®] program is able now to take into account the porosity (global one).
- Future effort will be done on the junction between local and global porosity.
- Also, the anisotropic thermal parameters are already in progress using a combination of PPT and TRR methods.

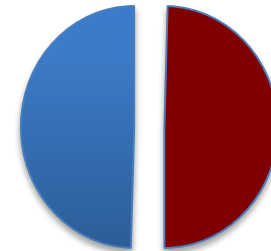
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to

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