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

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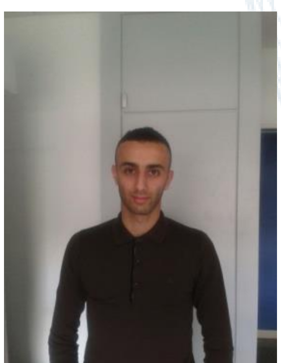


COMSOL CONFERENCE
2014 CAMBRIDGE

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 (3D, thin films, mesoporous,...)~~

↓

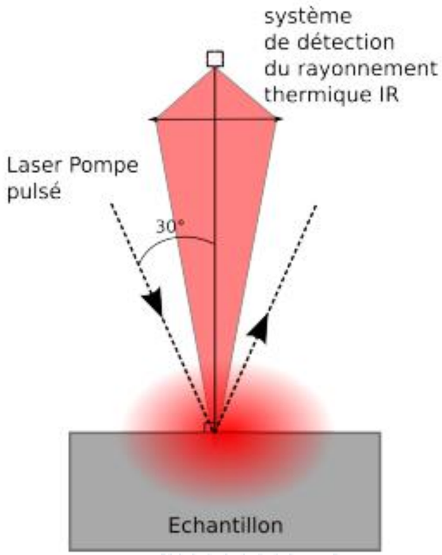
Numerical models are needed (Comsol®)!

1) Experiments by PPT

2) Modelling of laser heating by COMSOL

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

PPT methods : Principles

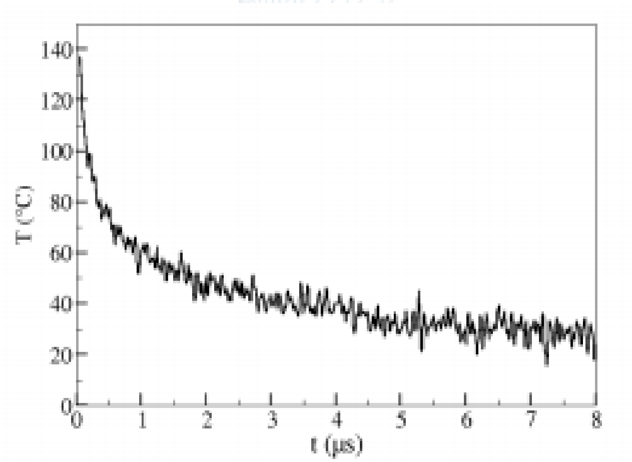


1) Near surface laser heating

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,Cp,…

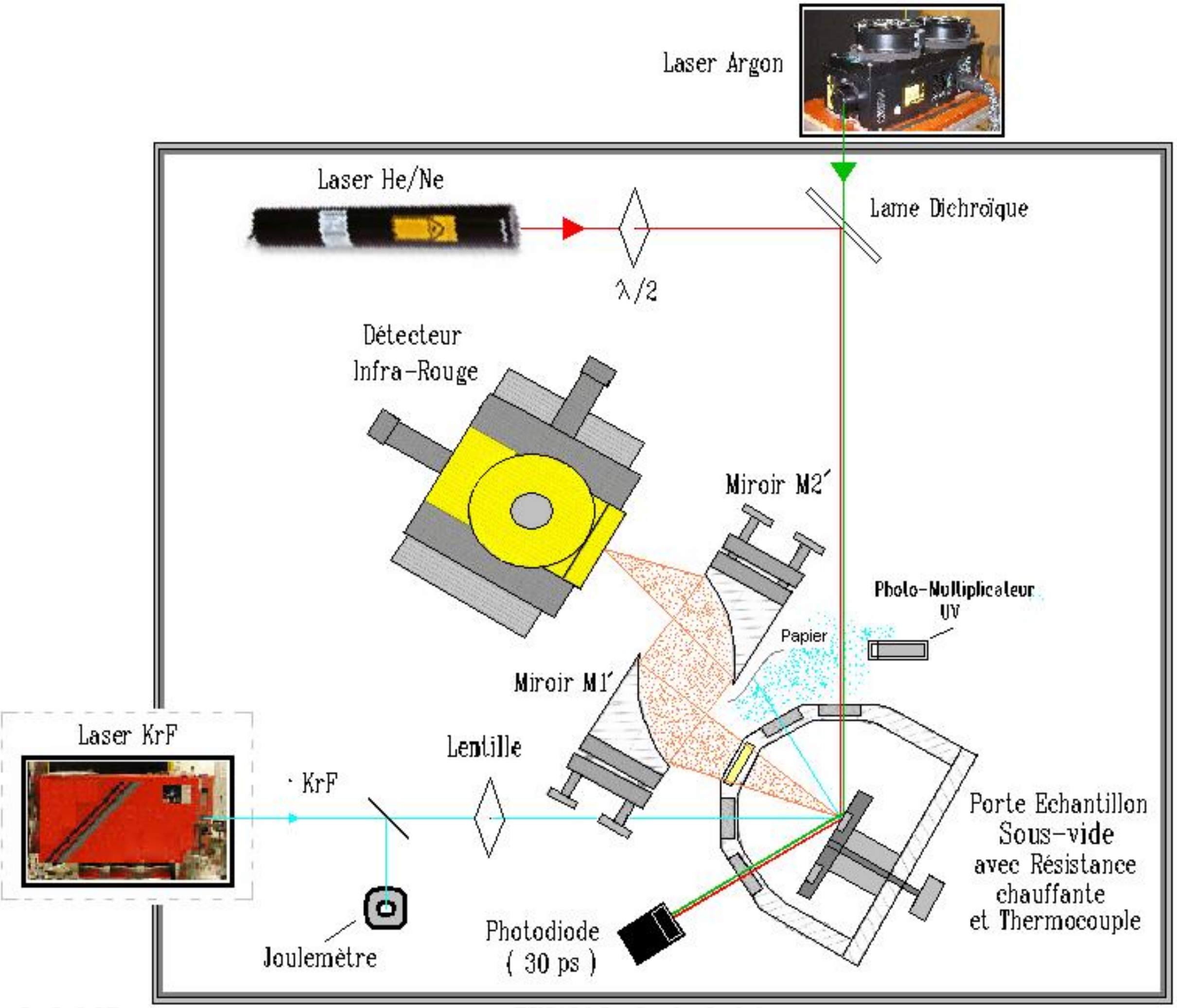
Experimental device

1) Pulsed laser heating of samples (λ=248 nm; τ = 27 ns; F= 100 mJ/ cm²)

2) IR signals are focused using off-axis paraboloid mirrors (1 to 12 µm) 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).

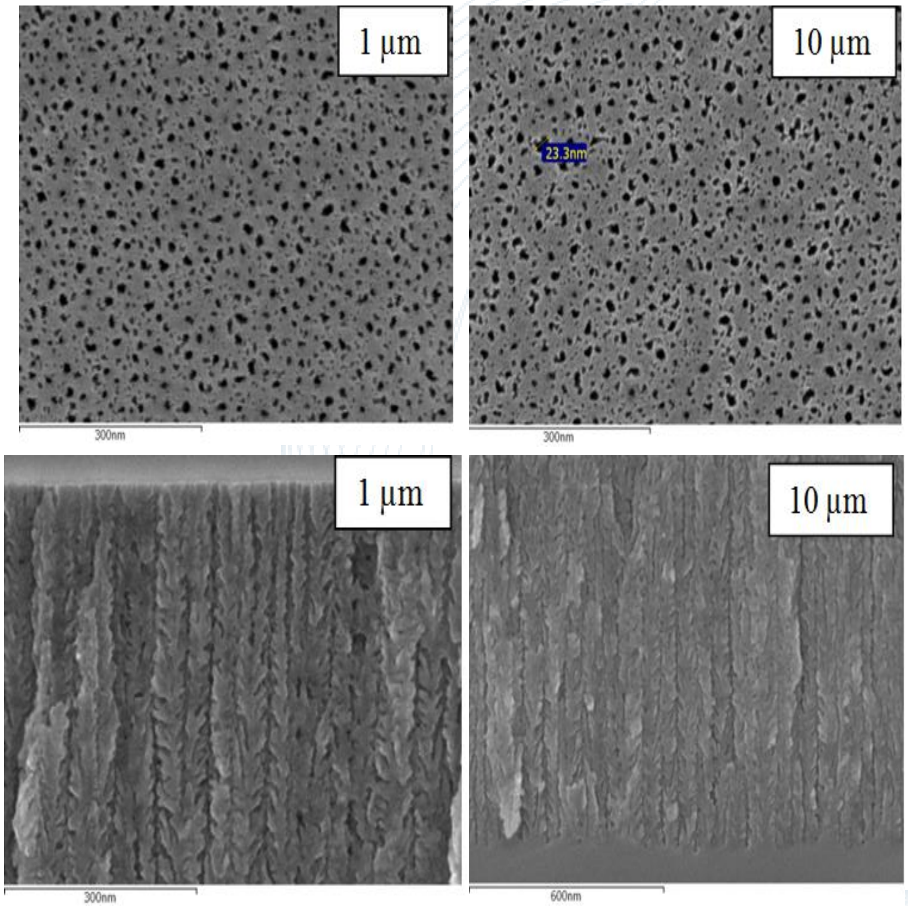
4) Calibration procedure: conversion of the electrical signal into absolute temperature.



SEM and FTIR

for size and porosity implementation

- Electro-chemical eching for Mono-cristallyne 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 : 3.2-3.75 x 10^3 pores/µm²

-Coloumnar (fir-like) structures

SEM + FTIR

⇩

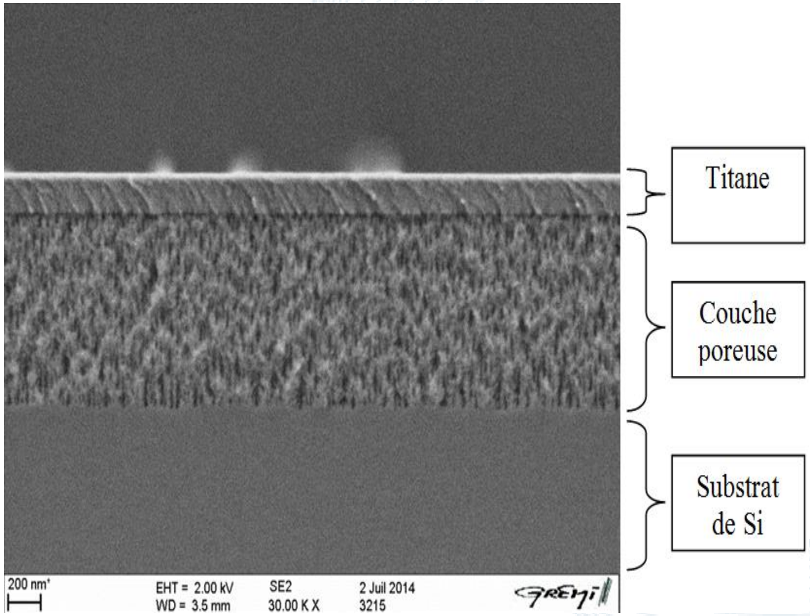
Etching depth	Porosity
0.2µm	34 %
1µm	26 %
10 µm	33 %
50 µm	25 %

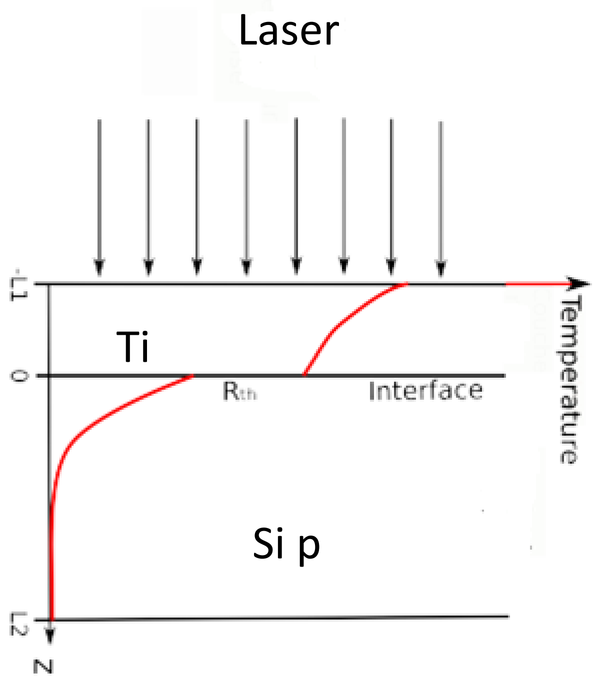
Ti transducer by magnetron sputtering deposition

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

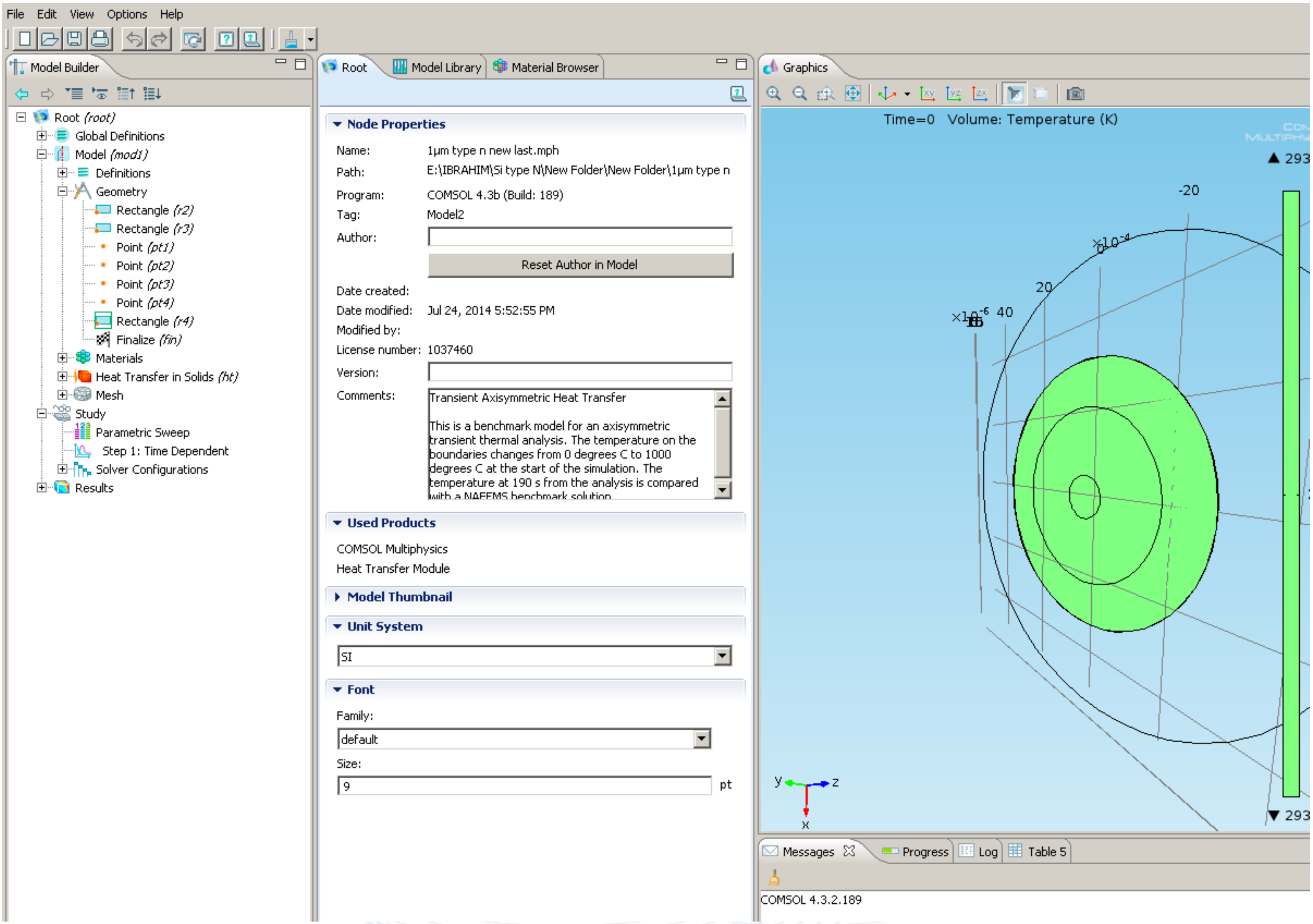
Thermal contact resistance (R_{th})

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

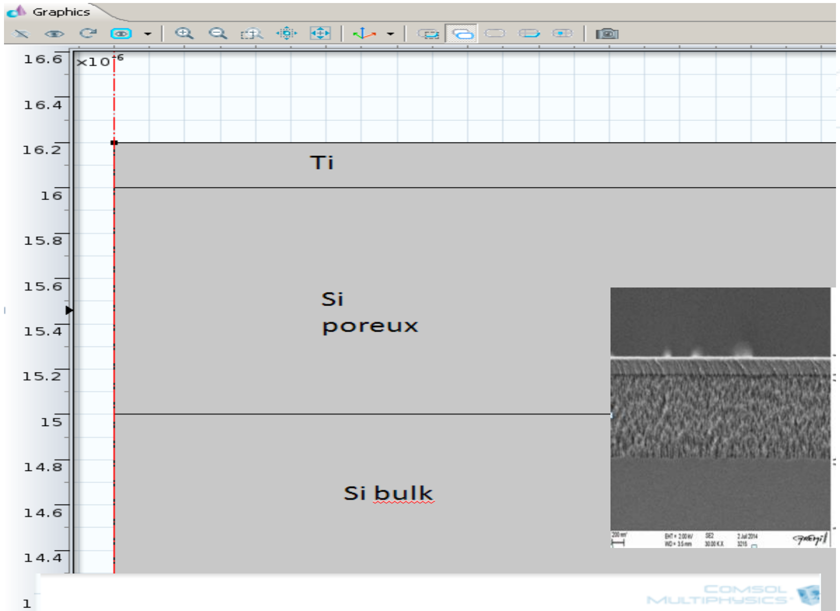


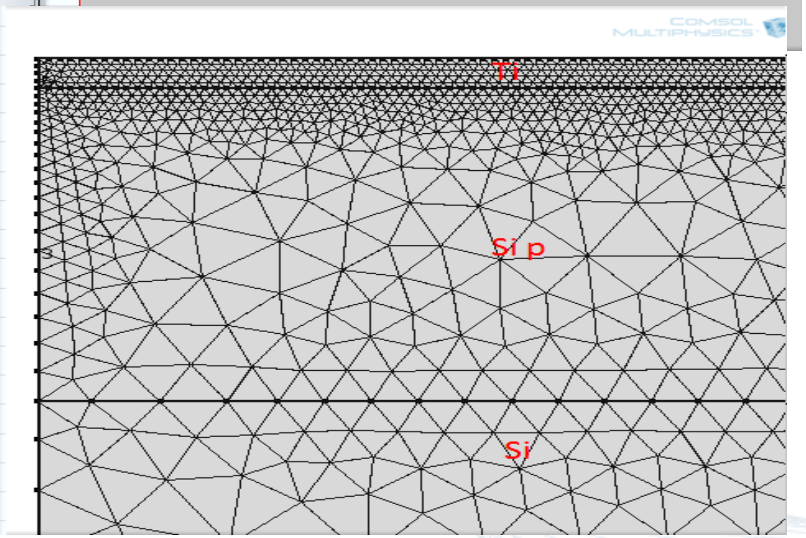


Comsol Multiphysics



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	?
ρCp (J.K-1.m-3) x 10^6	2.5	1.5	?
Maillage	5 à10 nm	Quelques µm	5 nm à quelques µm

Physics ?

- Heat Transfer in Solids module :

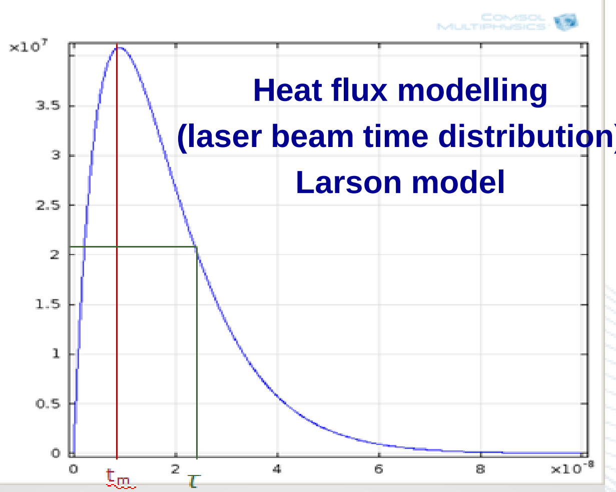
$$\rho \cdot C_p \frac{\partial T}{\partial t} = \nabla \cdot (k \nabla T)$$

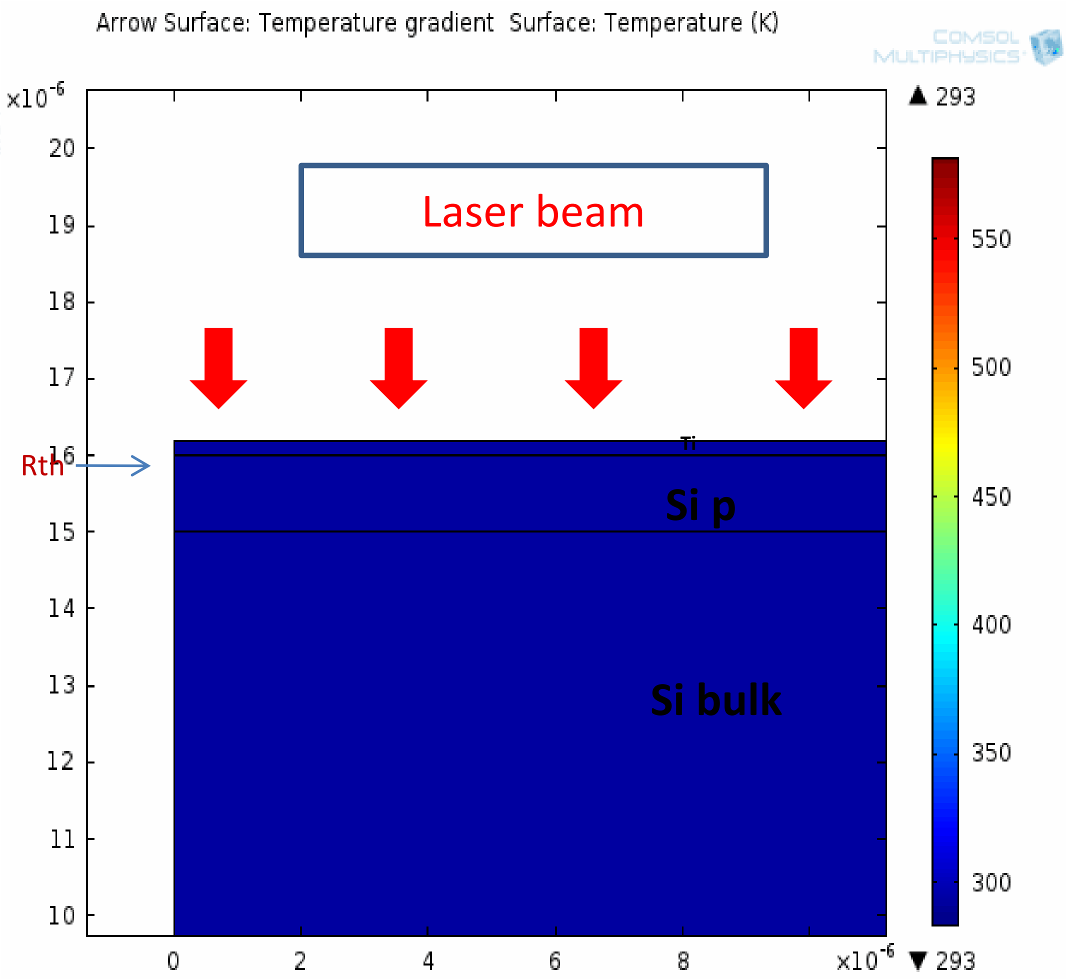
- Heat Transfert in Porous Media :

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

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

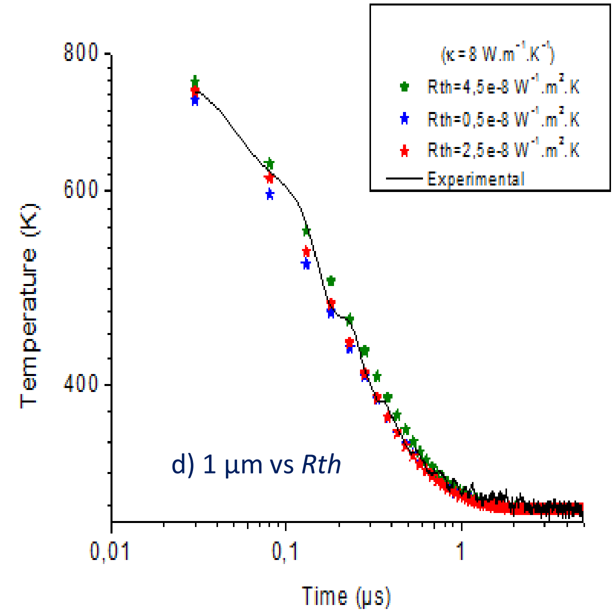
- Boundary conditions

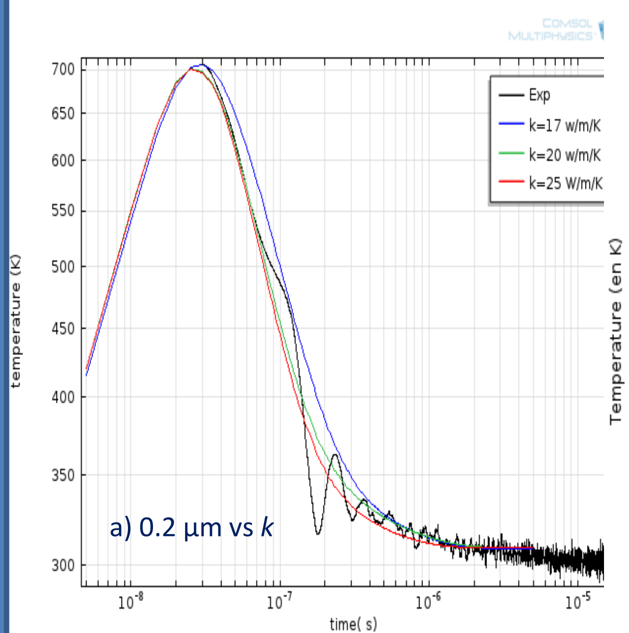


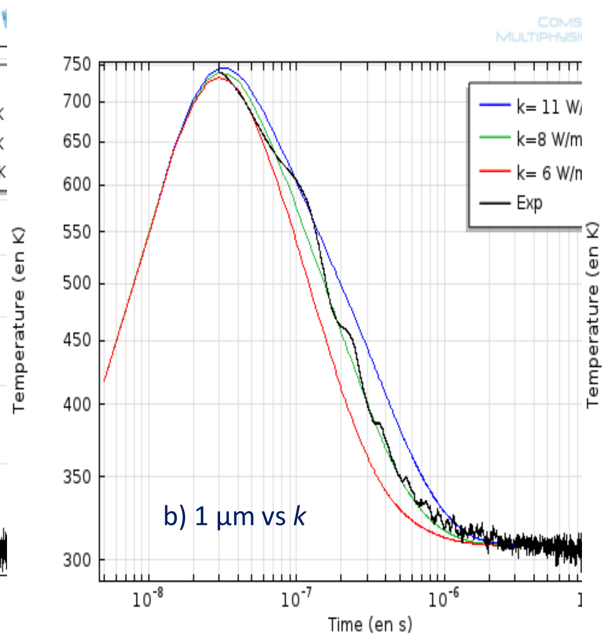


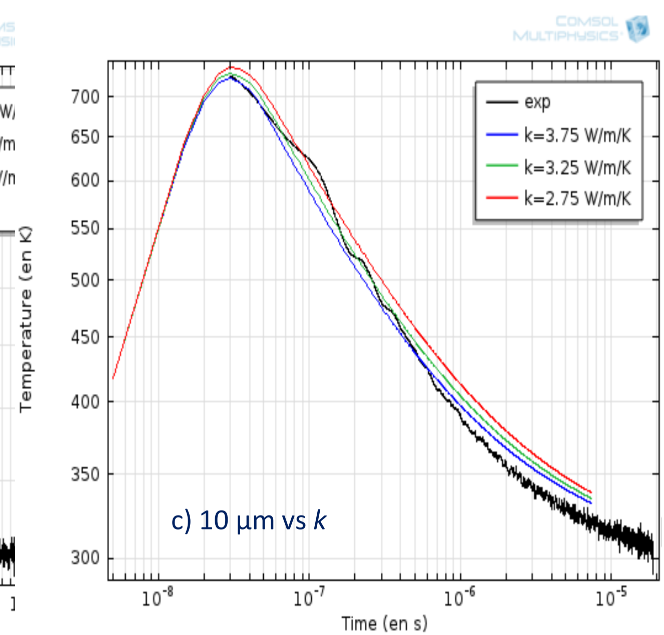
Results, Experiments Vs Modelling

➢Parametric Sweep is employed to optimise the identification of each parameter.
➢Here examples for k identification 0.2, 1, and 10 µm, and Rth for 1 µm.



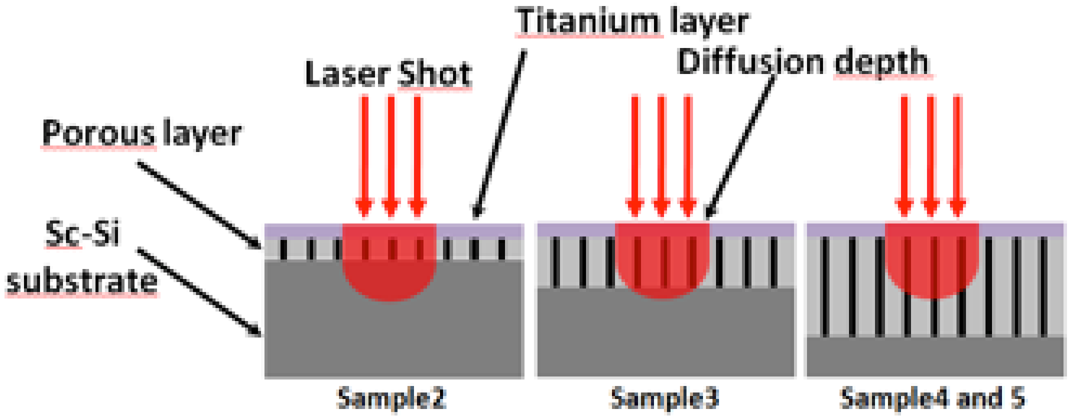






Results summarizing

	Ti	Bulk	0.2µm	1µm	10µm	50µm
k_p(W/m/K)	22	125 ± 17	20 ± 4	8 ± 2	3± 0.5	2±0.5
ρCp(J.K^{-1} .m^{-3})(x 10^{6})	2.5± 0.05	1.5 ± 0.05	1.25 ± 0.05	1.15 ± 0.05	1.22 ±0.05	1.25±0.05
R th(m².K/W)	-	2 x10^{-8}± 2	1x10^{-8} ± 2	2.5x10^{-8}±2	20x10^{-8}±2	80x10^{-8}±2
T max(K)	-	590	700	727	740	752
Tps relax(µs)	-	1.1	1.2	2.0	5	5



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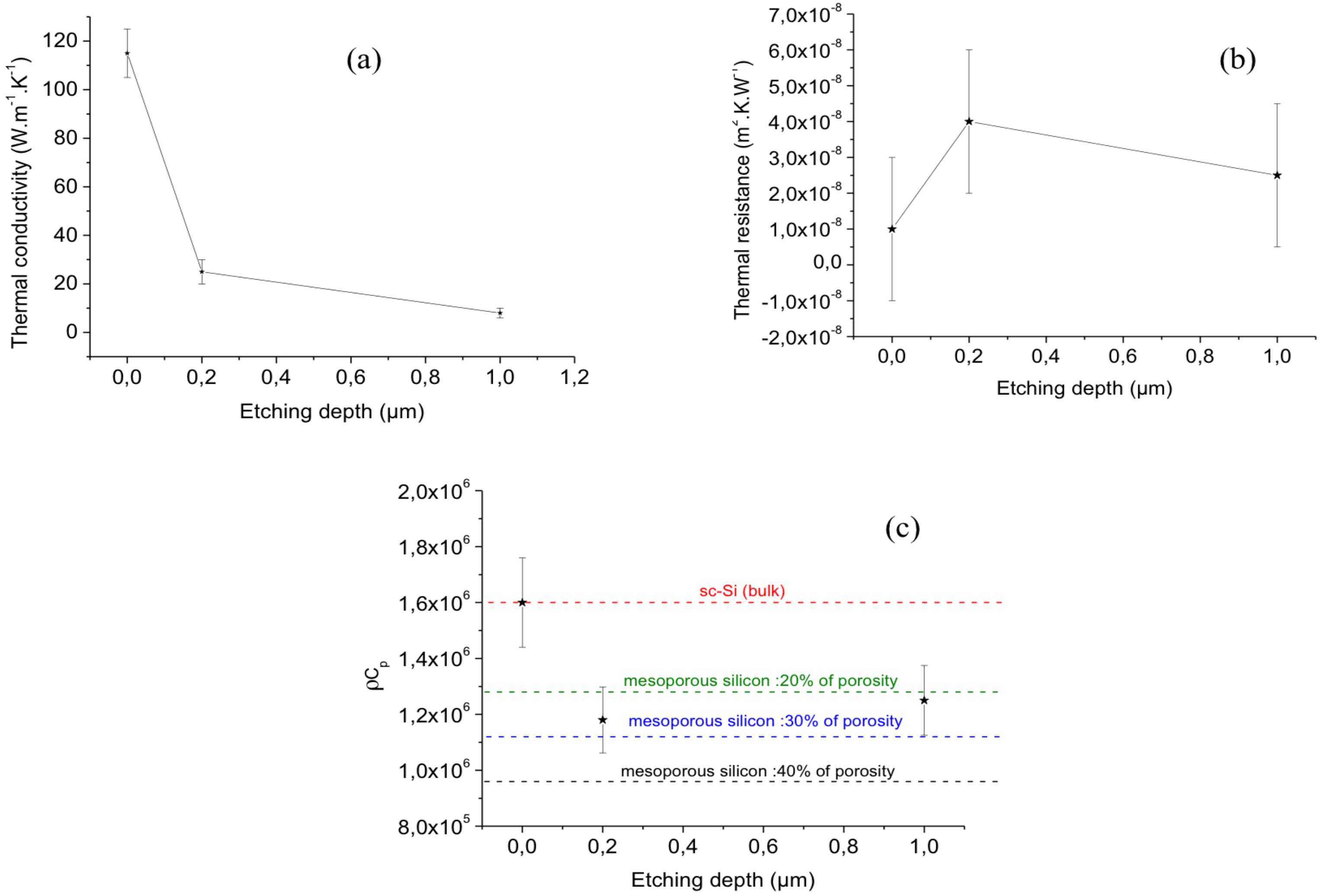
Thermal properties vs etching depth

(Submitted to J. Phys.D)



Conclusion

- New results are evidenced in this work for the <100> 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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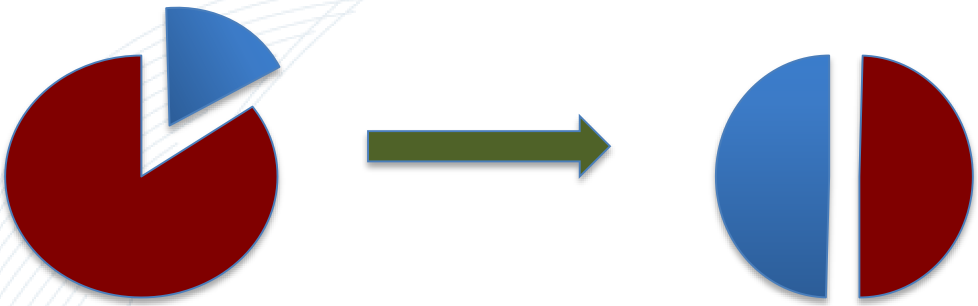
1 + 4 days to 1 + 1 days



Thanks

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