Optimization of Thermal Properties Identification of Complex Thin films Using MATLAB® and COMSOL Multiphysics®

Birane Wane, Nadjib Semmar
GREMI-UMR 7344,
CNRS- University of Orleans, FRANCE

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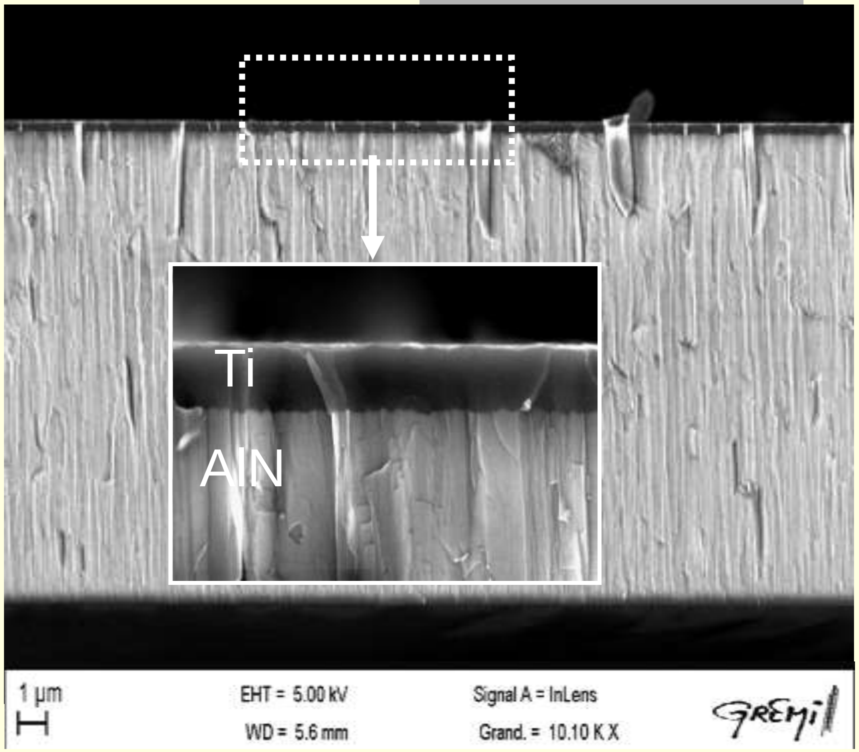
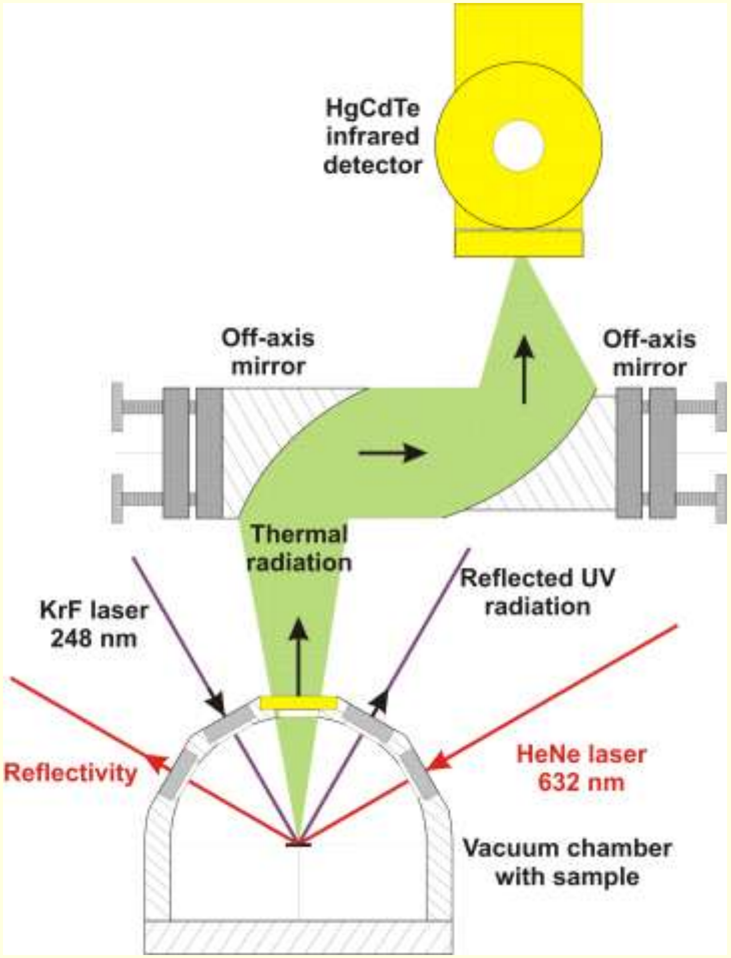
Motivations

- *Study of thermal properties for thin films :*
  - AlN (Highly conductive)
  - YSZ (ceramics thin film)
  - Metals
  - Dielectric films…
- Their applications in next generation microelectronic devices :
  - QCL, HEMT, Thin film fuel cells
- Fundamental knowledge of condensed matter thin film state : mesoporous Si, CNTs…
  - *J.Phys.D 2011, J.A.P. 2012, …*



JPCS 2012

Principle of PhotoThermal method

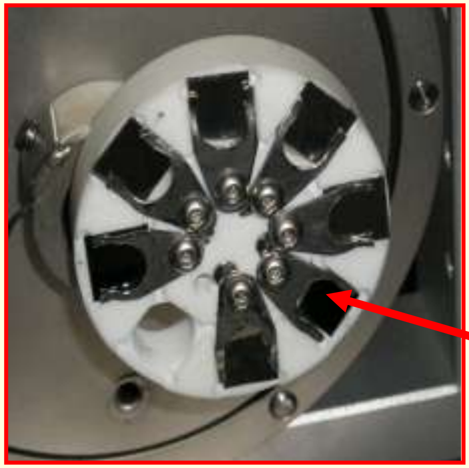


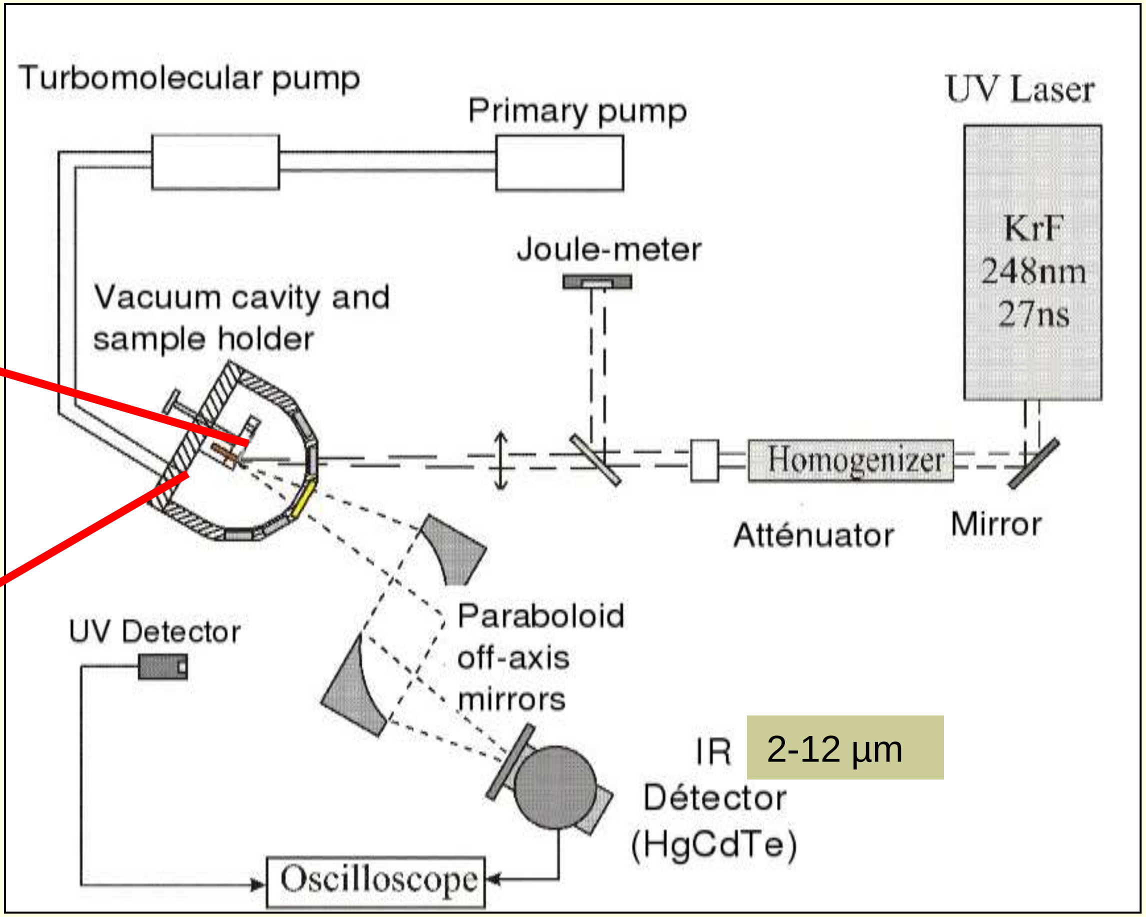
- Absorption of laser pulse energy ⇨ rapid increase of temperature and then relatively slow temperature decrease
- Detector calibration curve $U(T)$ – heating support
- Experiment evaluation:
  U(t) ⇨ T(t)

Experimental Setup

Photo-thermal nano-second

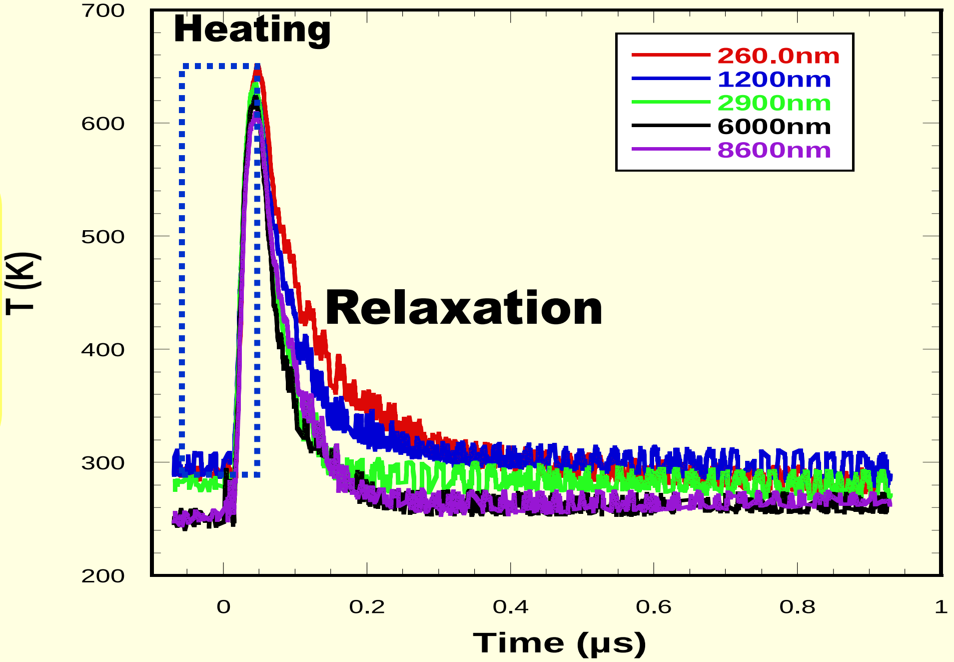
Sample holder





What is thermal identification?

Temperature of the IR detector from Ti/AlN sample surface after laser beam fluence of 4,8 mJ/cm^2



Built a realistic model to fit well the experimental curves based on the multilayer system physical parameters

1- 1D analytical model for multilayer thin films (Balageas) :

Matlab Experiments gives 3 group of parameters

$$V_D(t) = \frac{\theta_D(t)}{\theta_\infty} = 1 + 2\frac{\sum_{i=1}^{2} x_i\omega_i}{\sum_{i=1}^{2} x_i} \sum_{K=1}^{\infty} \frac{\sum_{i=1}^{2} x_i \cos(\omega_i\gamma_K) + (-1)^i \mathcal{R}\gamma_K \sin(\omega_i\gamma_K)}{\sum_{i=1}^{2} x_i\omega_i \cos(\omega_i\gamma_K) - (-1)^i \mathcal{R} \cos(\omega_i\gamma_K) + (-1)^i \mathcal{R}\gamma_K\omega_i \sin(\omega_i\gamma_K)} \exp\left(-\frac{\gamma_K^2 t}{\eta_2^2}\right)$$

Eingenvalues problem

2- Comparison with the 3D model namely for low conductive and complex thin films :

Creation of full model under Comsol :

Thin films/participating media (Heat Transfer Module)

3D Model in COMSOL – heat source

- Laser penetration into depth of sample is ruled by Beer-Lambert law

$$I(z) = I_0 \cdot e^{-az}$$

Material	n_1	n_2	a (m^{-1})	δa (nm)
Al	0.19	2.94	$0.1490 \cdot 10^{-9}$	13.4253
Cu	1.12	1.88	$0.0953 \cdot 10^{-9}$	20.9949
W	3.4	0.14	$0.1444 \cdot 10^{-9}$	13.8493

- Optical properties:

complex refractive index

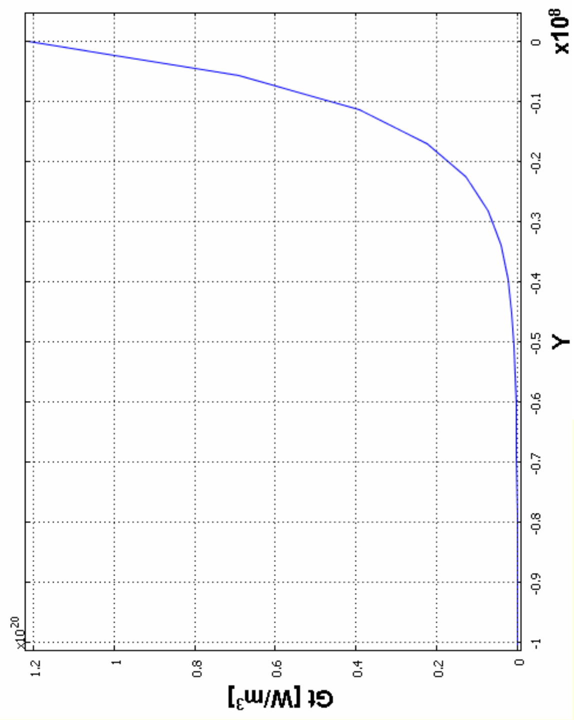
$$n = n_1 + in_2$$

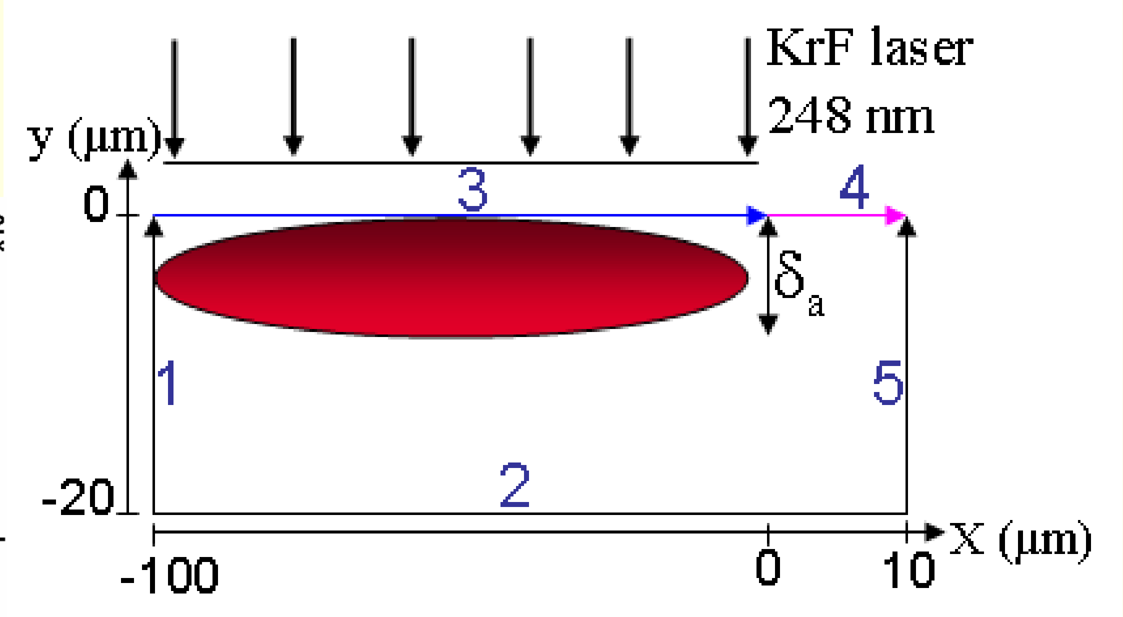
absorption coefficient

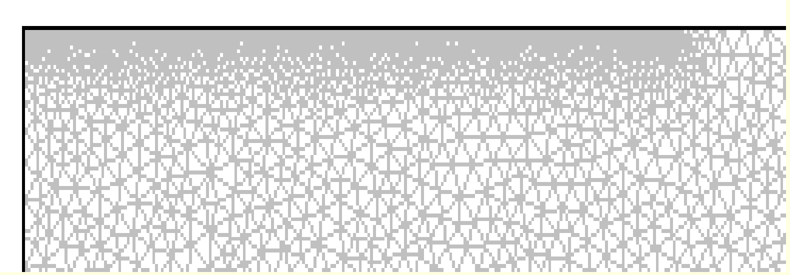
$$a = \frac{2\omega n_2}{c} = \frac{4\pi n_2}{\lambda} = \frac{2}{\delta a}$$

Modeling of UV laser beam absorption

Heat source distribution





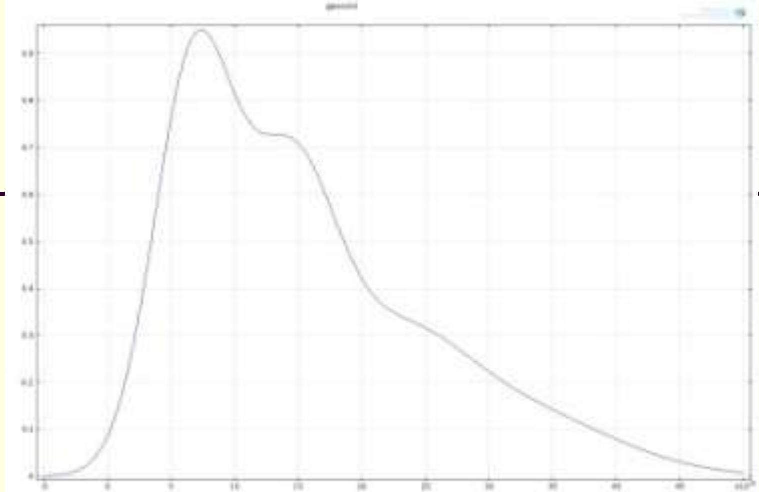


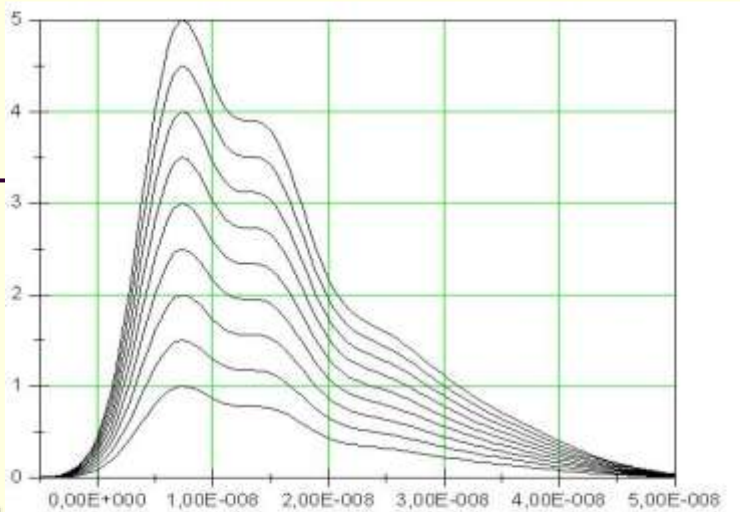
1 to 3 nm

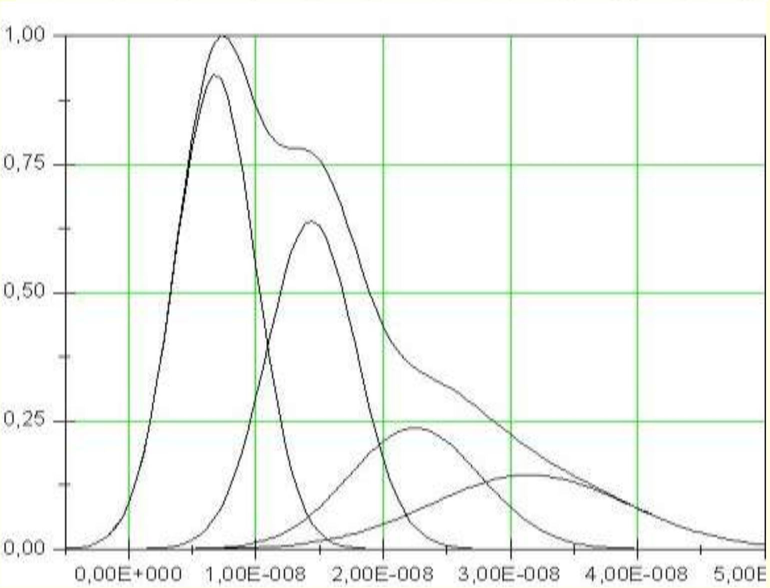
100 nm

But also the real time distribution ….

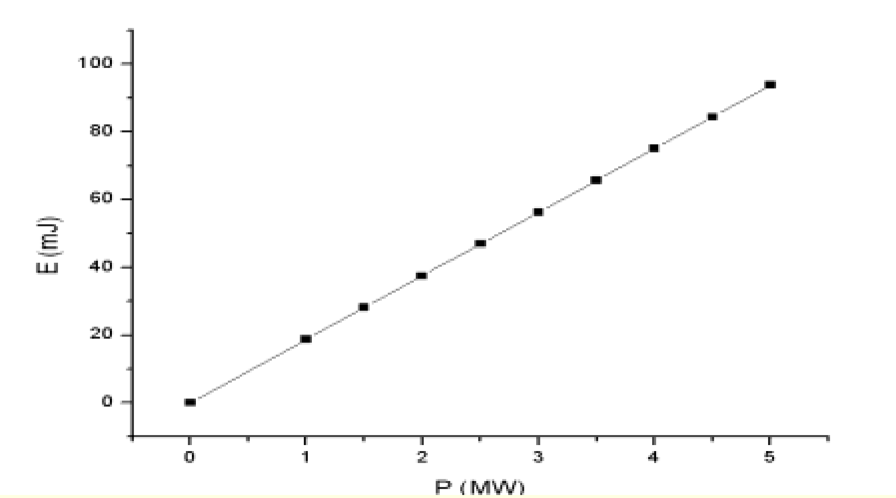
Function of laser energy







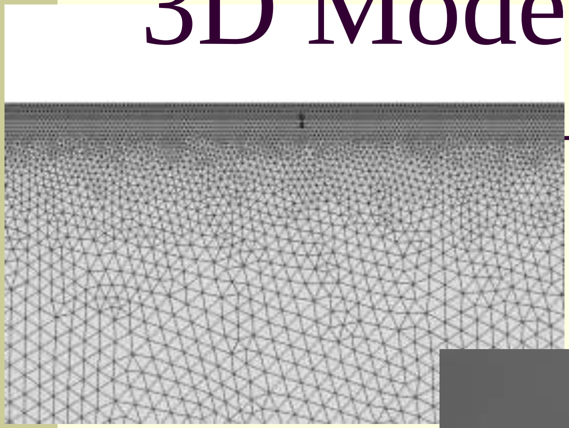
New



deconvolution ….

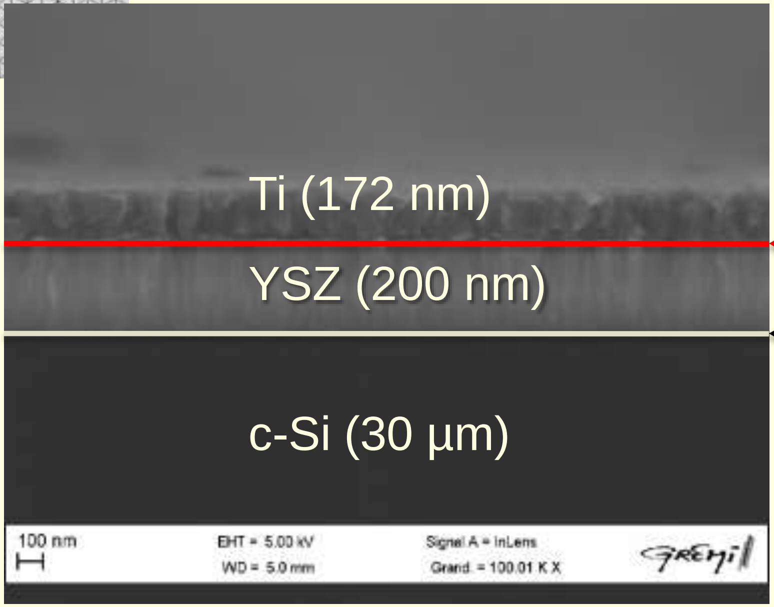
and linear variation of pics

3D Model in COMSOL : Si/YSZ/Ti



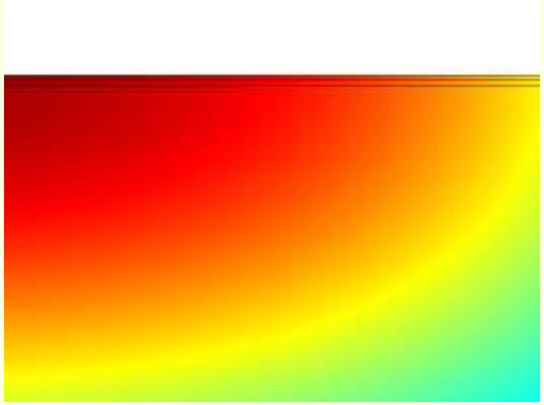
Ti : ρ1, c1, k1

YSZ : ρ2, c2, k2 ?



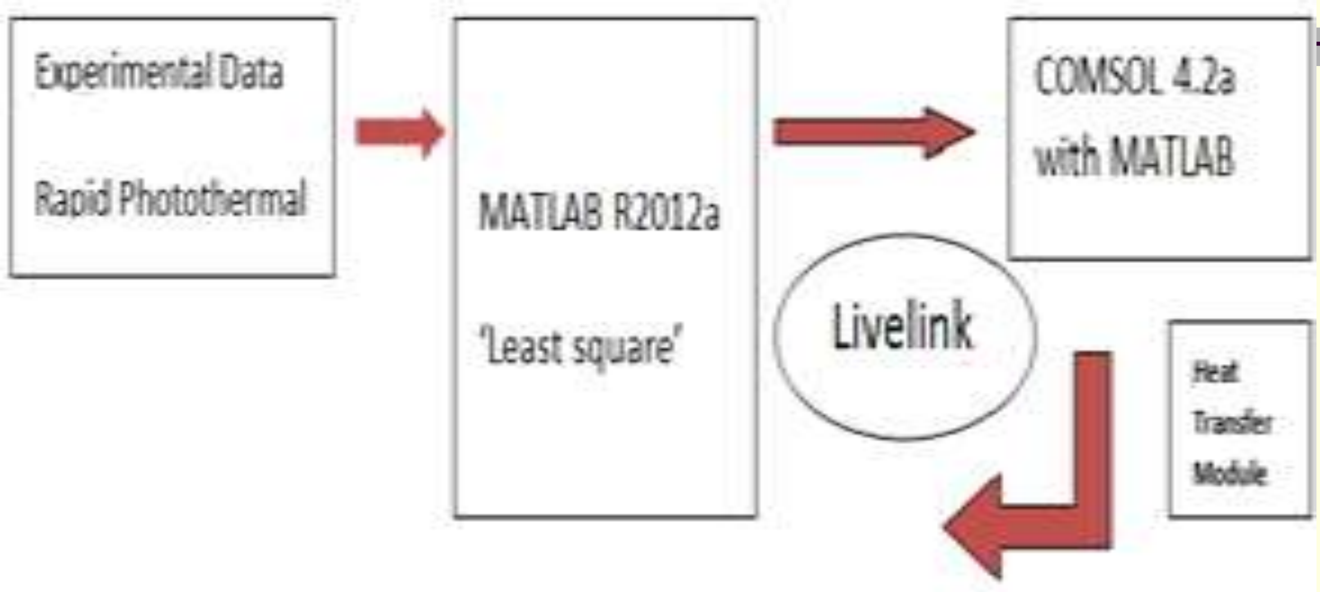
Rth1

Rth2



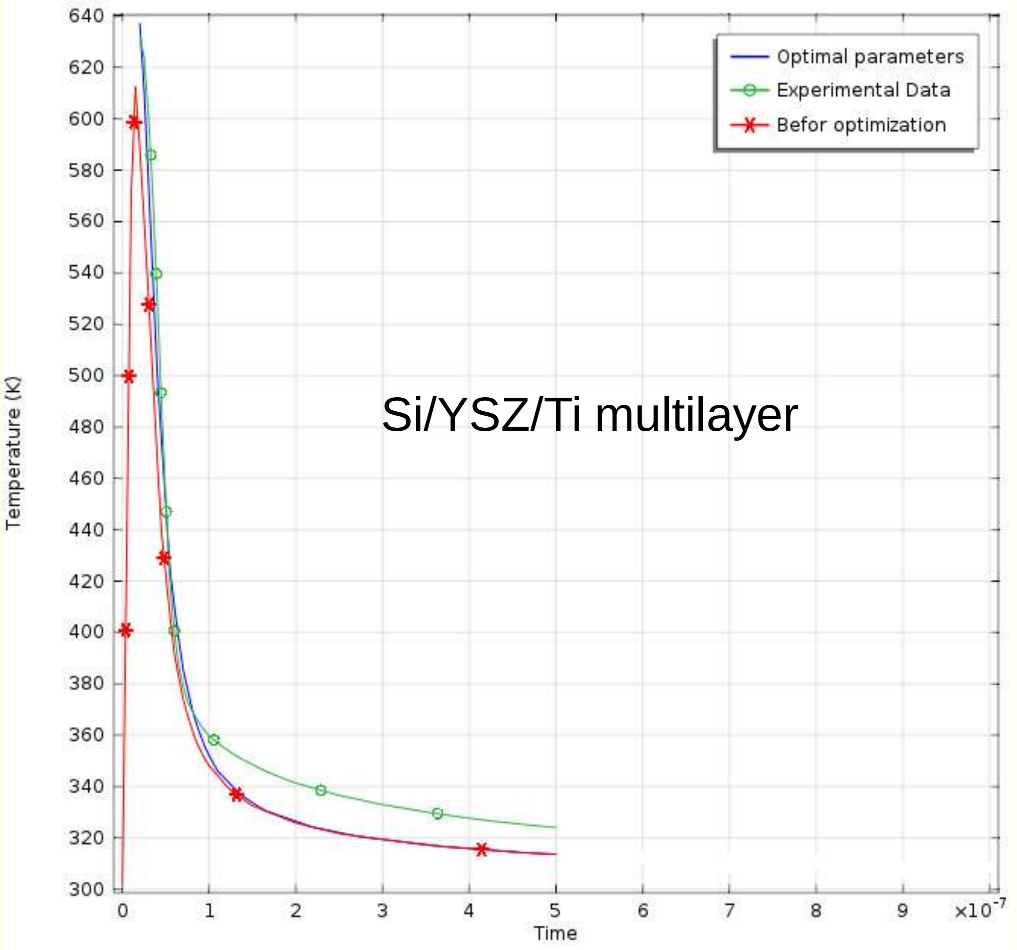
Bulk silicon : well known properties

Livelink loop



Our new strategy :
1 - Starting 1D with Matlab (Balageas model)
2 - Then Livelink to Run Comsol.
Runing this loop until convergence of thermal fields :
3 - **Outpout data :** density, thermal conductivity, heat capacity

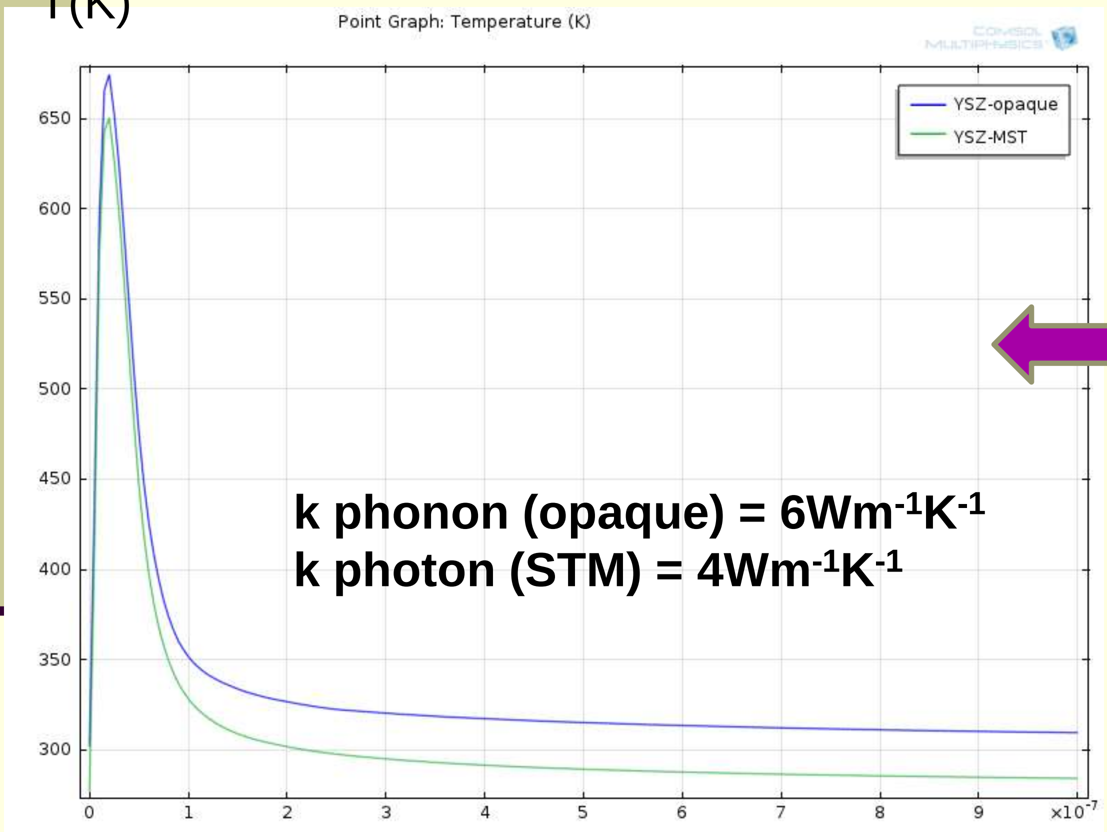
Output data: best results!



ρ = 3600 kg.m^{-3}
c = 550 J.K^{-1}.kg^{-1}
k = 7 W.m^{-1}.K^{-1}

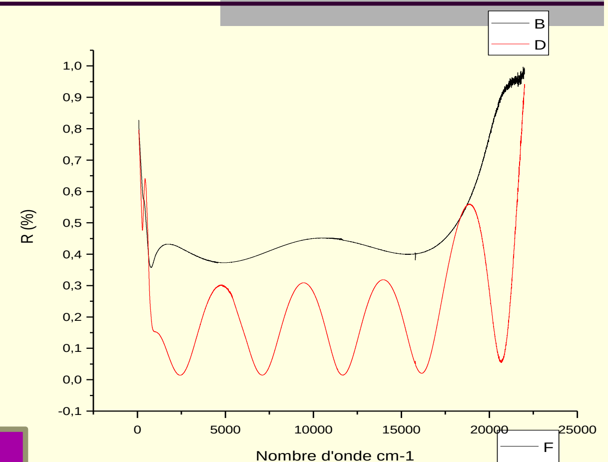
Yttria-Stabilised-Zirconia (YSZ)

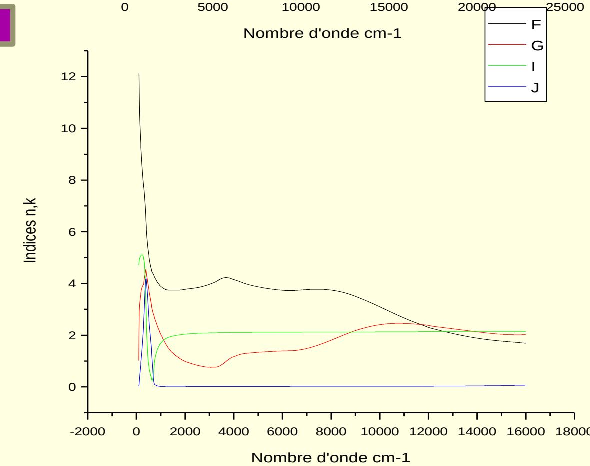
T(K)



k phonon (opaque) = 6$Wm^{-1}K^{-1}$
k photon (STM) = 4$Wm^{-1}K^{-1}$

t(s)





Optical parameters :
R, n1, n2

Conclusions

- New way for the optimization of thermal properties identification.

- But high number of loops, and long computation time.

- *Is the 'Optimization Module' able to do faster computations using more adapted models?*

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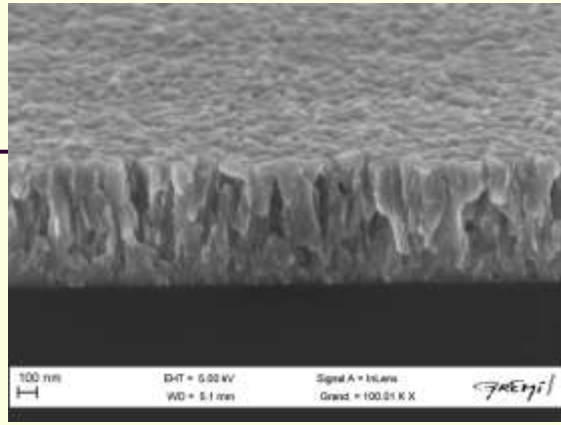

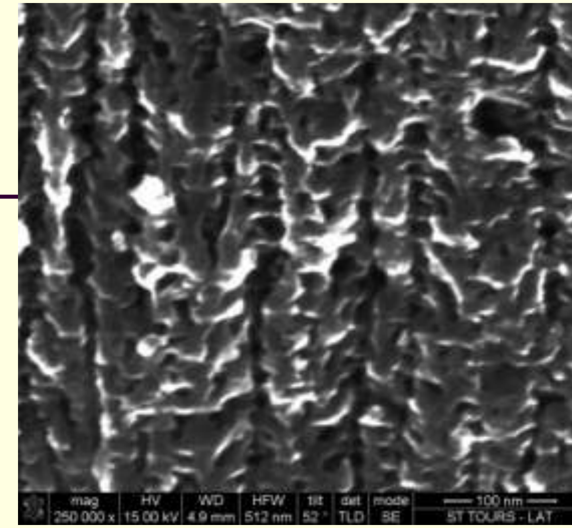

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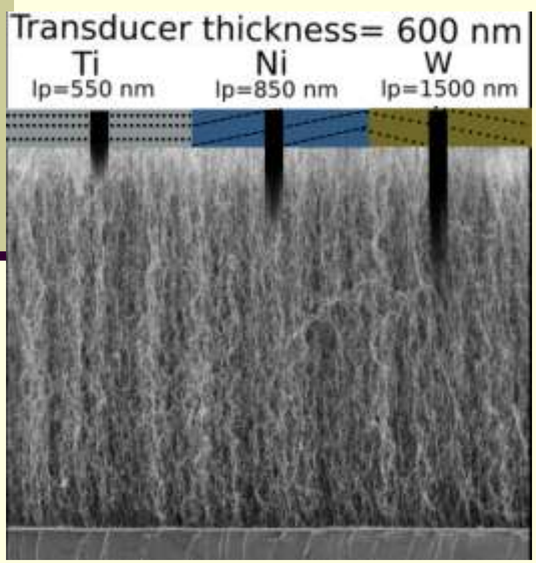

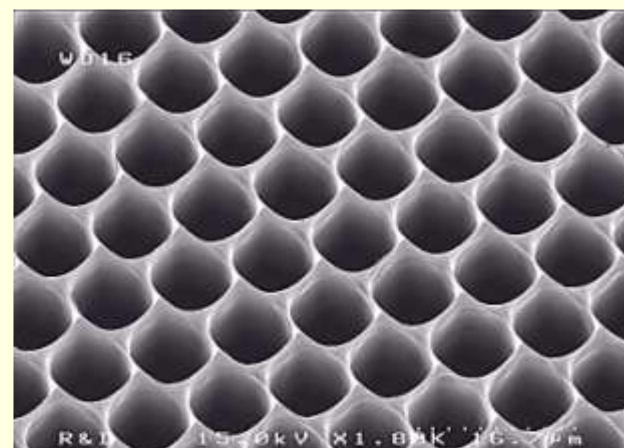

Experimental system - schematic view