Interest of the multi-scale characterization of a heterogeneous material for the prediction of its thermal radiative behaviour

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J.-F. Thovert

UPR 9028

(ex CRMHT) Conditions Extrêmes et Matériaux : Haute Température et Irradiation
1D, avenue de la Recherche Scientifique, 45071, Orléans, Cedex 02

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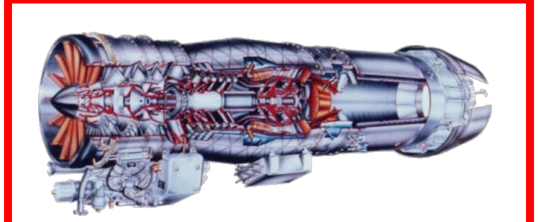
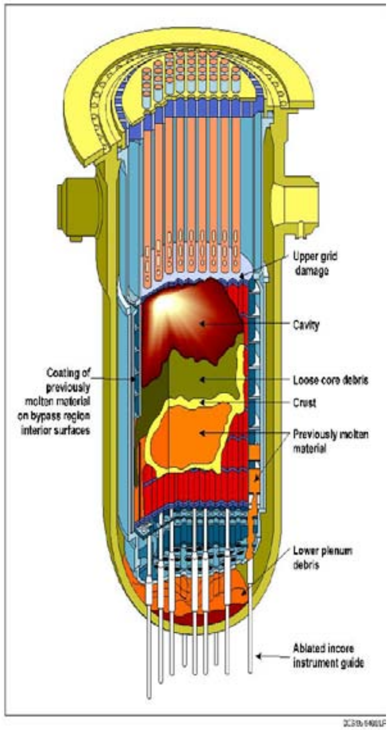
500 K 1000 K 1500 K 2000 K 2500 K

S. Gauthier, Ph. D, CETHIL, 2008



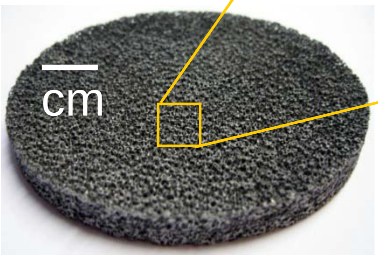


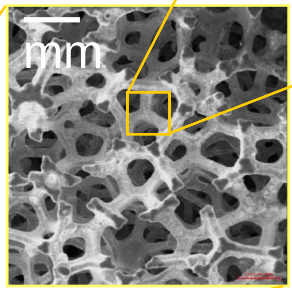
E. Chalopin, Ph. D, EM2C, 2008

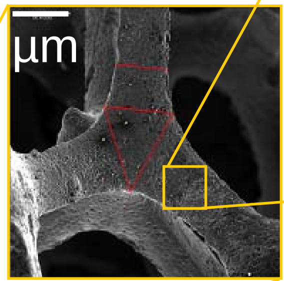
POROUS MEDIUM : RELEVANT LENGTH SCALE?

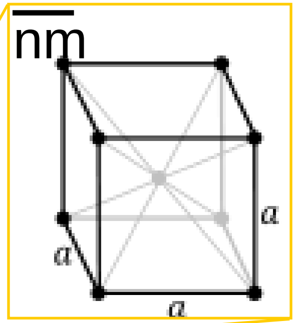
Heat Tranfer

Ex : Metallic Foam







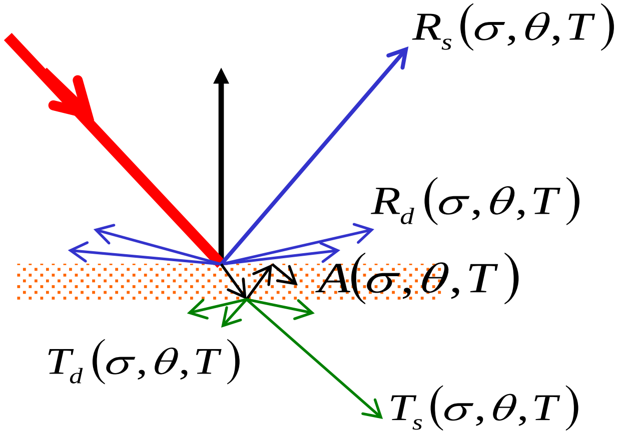


Thermal Radiative Properties

Microstructure + Chemistry

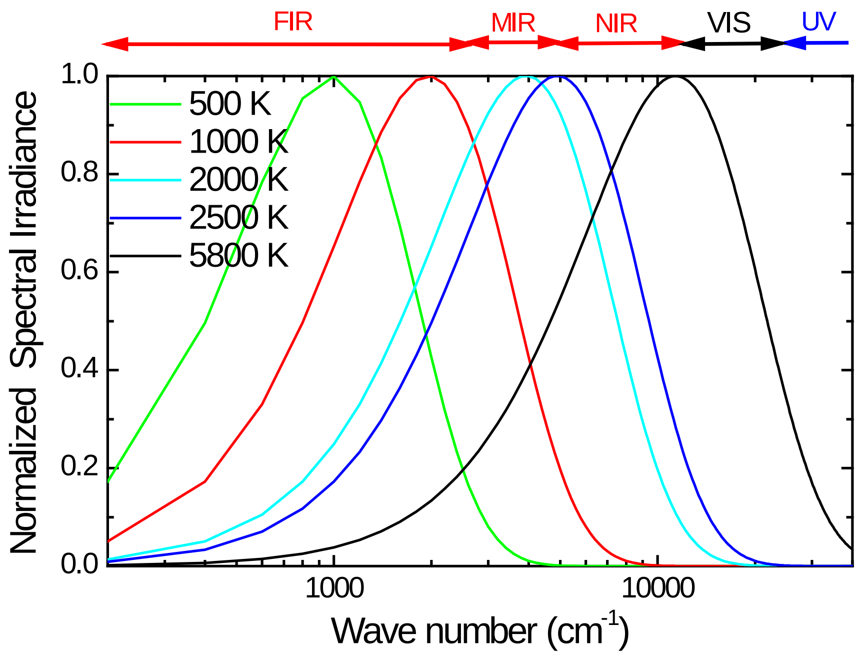
Material Characterization

DIRECT RADIATIVE PROPERTIES



$\hat{R} = R_s + R_d$

$\hat{T} = T_s + T_d$



Kirchhoff 's law:

Energy balance

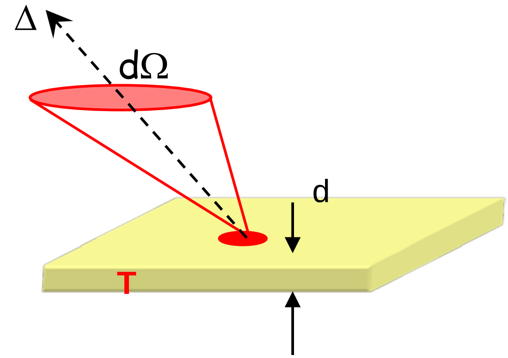
- $A(\sigma,\theta,T) = 1 - \hat{R}(\sigma,\theta,T) - \hat{T}(\sigma,\theta,T)$

Local Thermodynamic Equilibrium

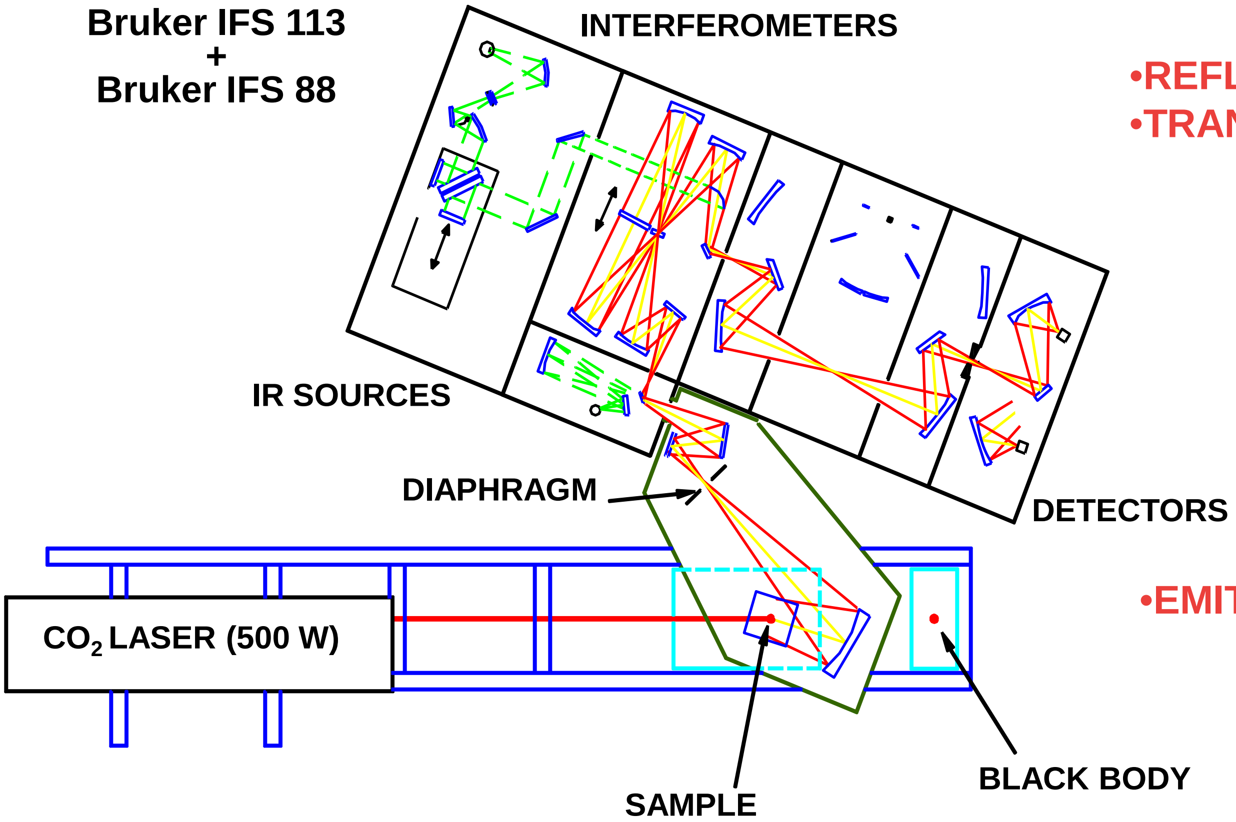
- $E(\sigma,\theta,T) = A(\sigma,\theta,T)$

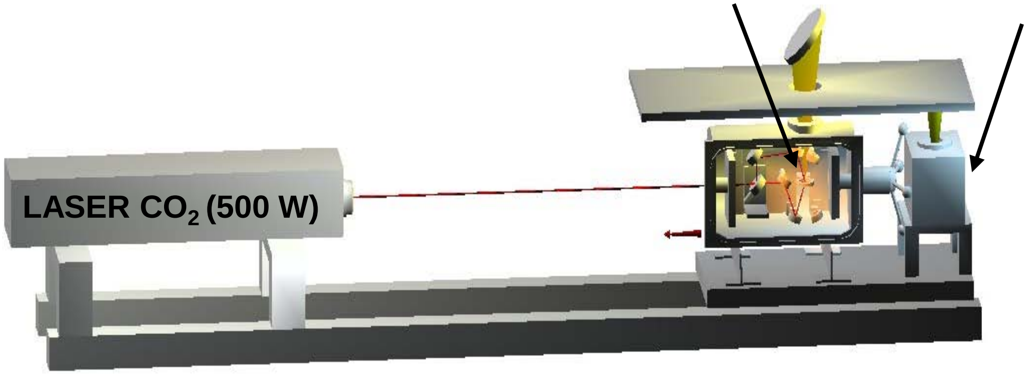
$$E(\sigma,\theta,T) = \frac{L(\sigma,\theta,T)}{L^0(\sigma,T)}$$

- $L^0(\sigma,T) = \dfrac{C_1\sigma^3}{e^{\frac{C_2\sigma}{T}} - 1}$ Planck's law
- $L(\sigma,\theta,T)$



EXPERIMENTAL SET UP





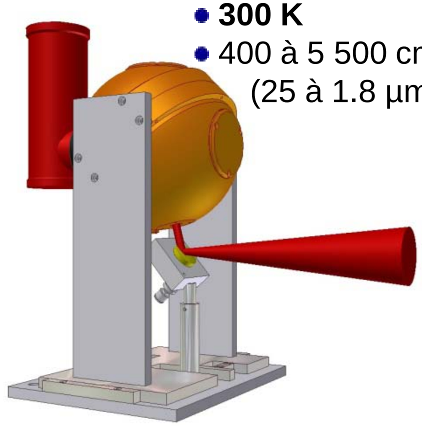
•REFLECTANCE
•TRANSMITTANCE

- **4 - 1200 K**
- 10 - 40 000 cm^{-1} (1 000 - 0.25 µm)

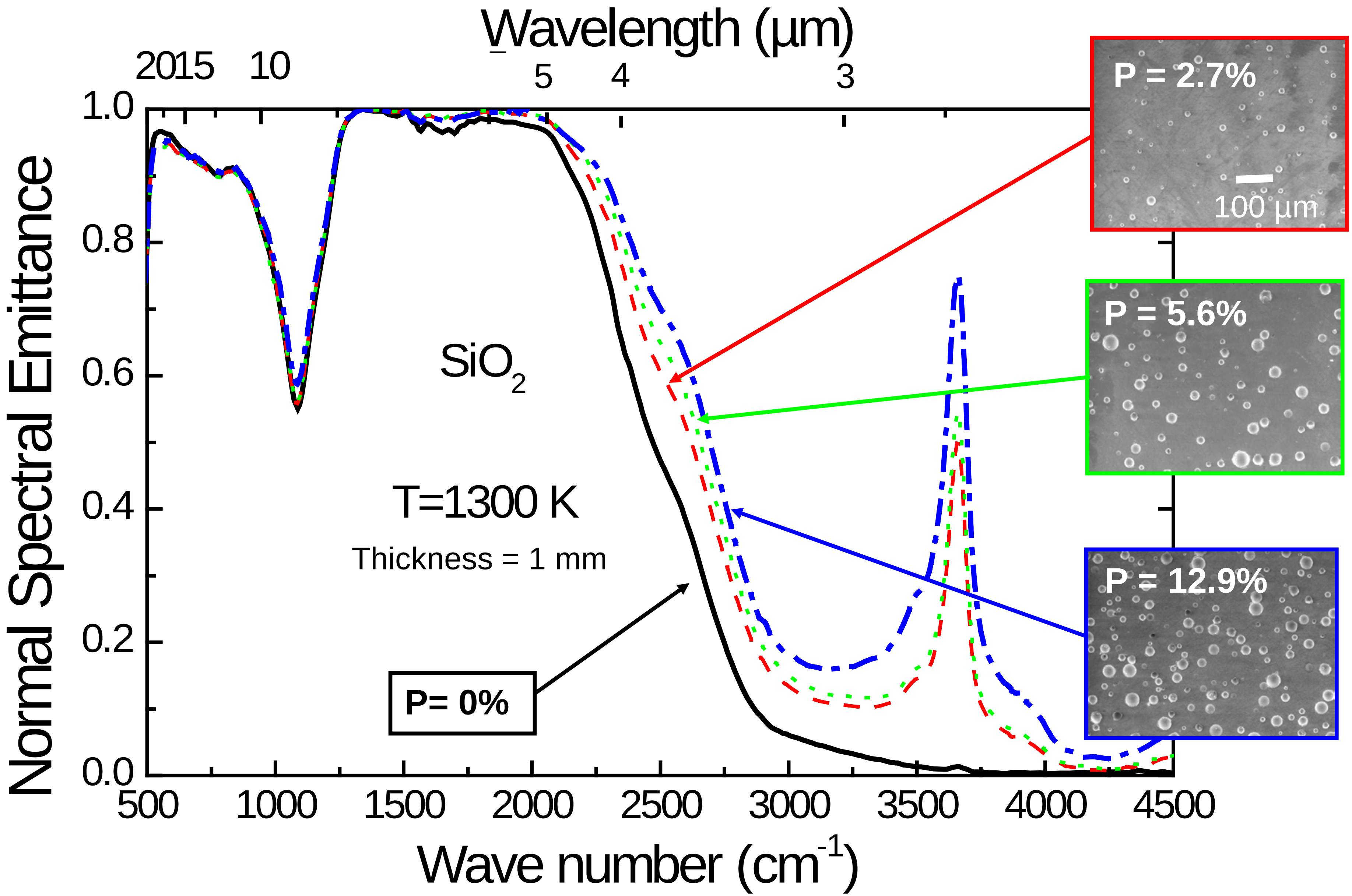
•EMITTANCE

- **500 - 2 500 K**
- 10 - 14 500 cm^{-1} (1 000 - 0.7 µm)

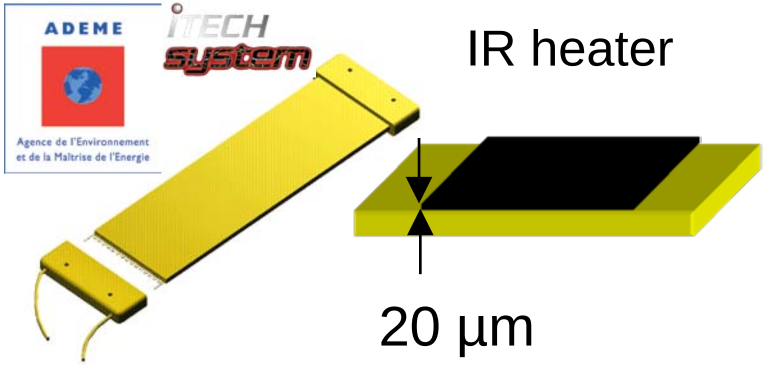
- **300 K**
- 400 à 5 500 cm^{-1} (25 à 1.8 µm)



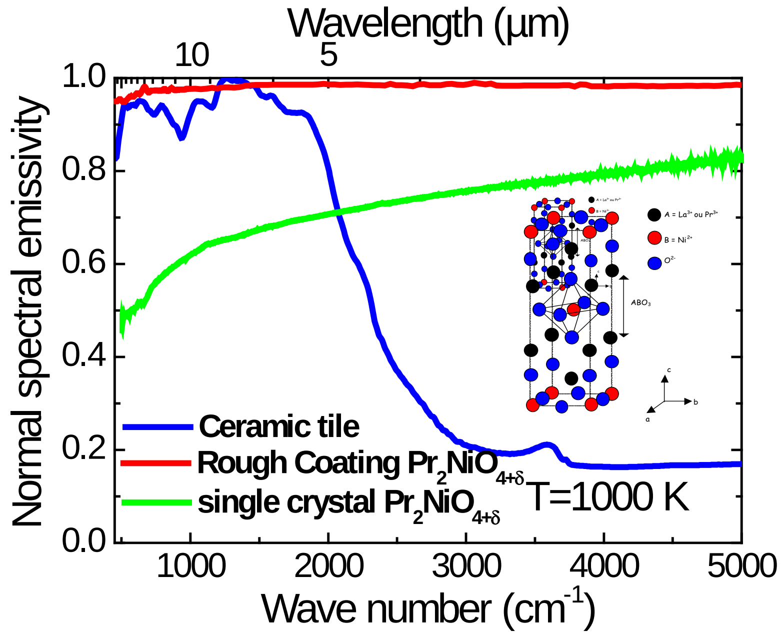
MODEL POROUS MEDIUM : SILICA GLASS WITH BUBBLES

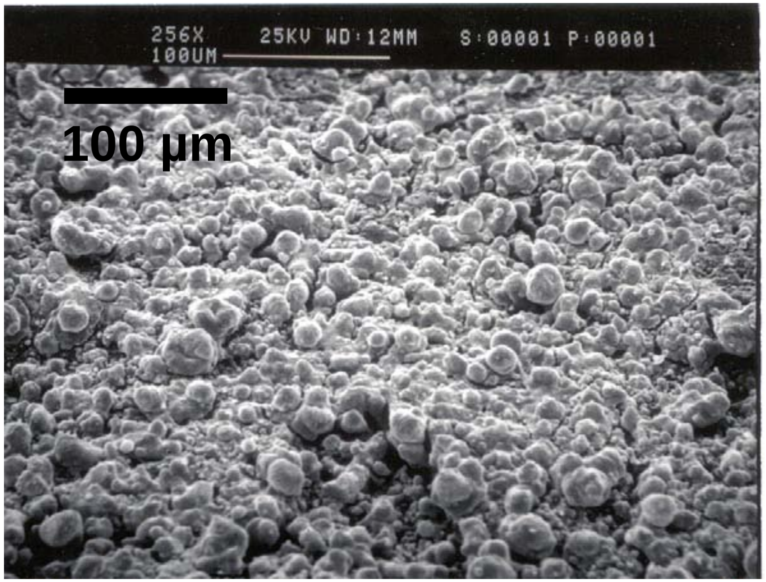


BLACK BODY COATING



Rousseau et al., *Appl. Phys. Lett.*, 79 (2001), 3633.



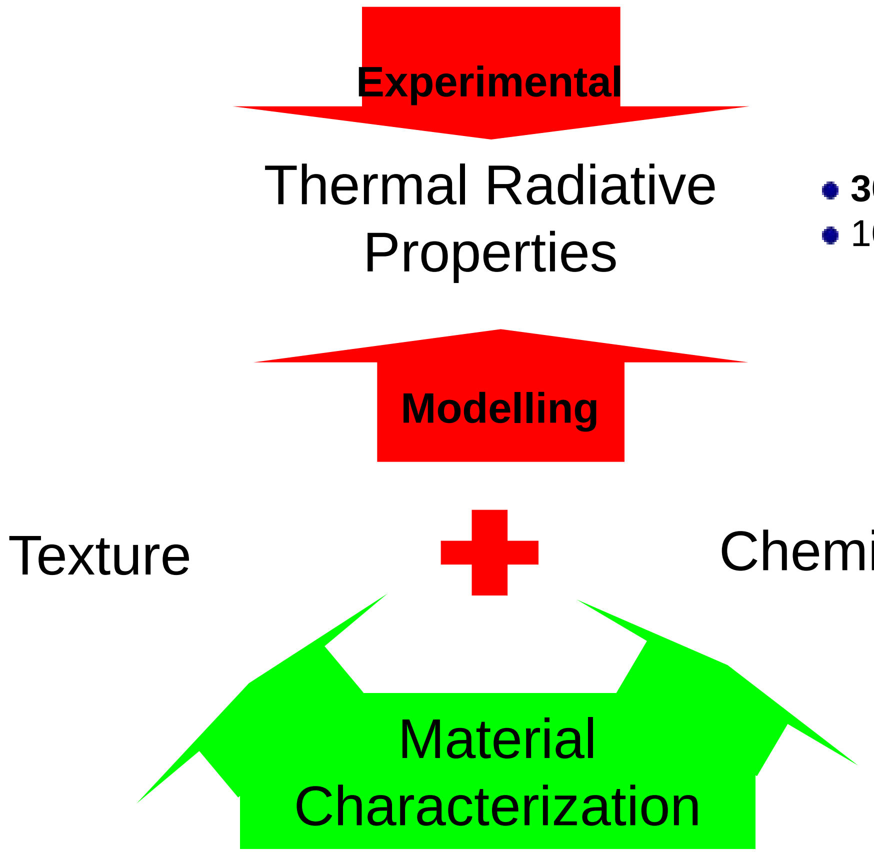


IR heaters

- Ceramic tile
- Praseodymium nickelate ($Pr_2NiO_{4+\delta}$)

- roughness
- nearly black body behavior

Infared emission spectroscopy



- **300 - 2500 K**
- 10 - 40 000 cm^{-1}
  (1 000 - 0.25 µm)

A SEMI TRANSPARENT COMPOUND :

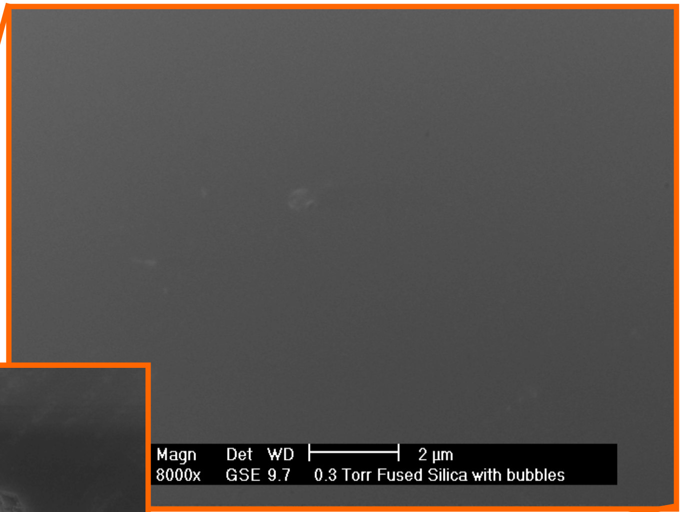
SILICA GLASS WITH BUBBLES

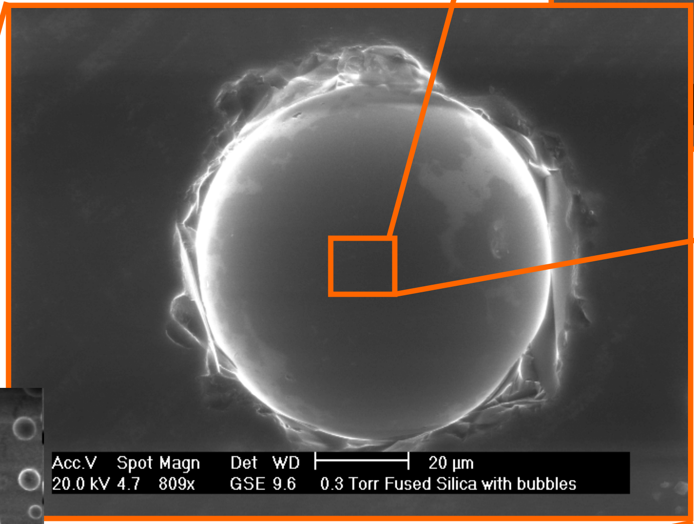
CLASSICAL CHARACTERIZATION OF THE GLASS

Chemical Analysis

-fused silica based on grain quartz grains of high purity (99.99 %)
-amount of metallic impurities ~ 100 ppm

Textural Analysis





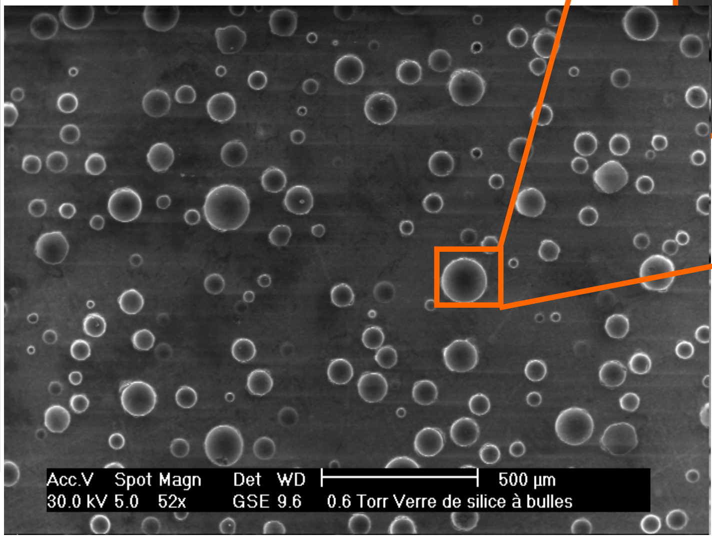
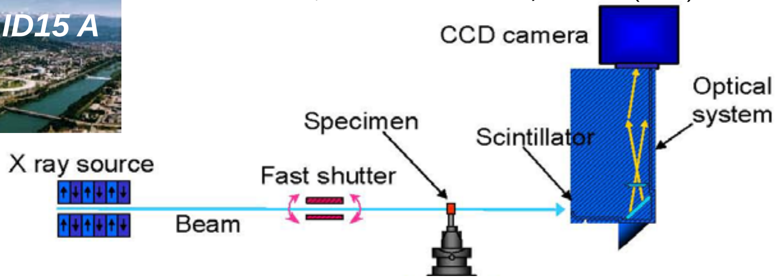


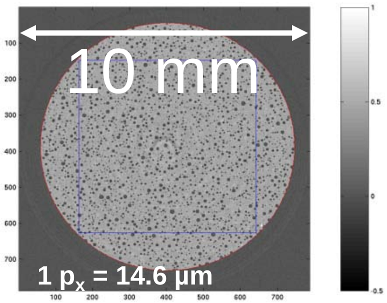
IMAGE ANALYSING OF 3D DATA (P = 12.9 %)

M. Di Michiel, Rev. Sci. Instrum. **76,** 0432702 (2005)

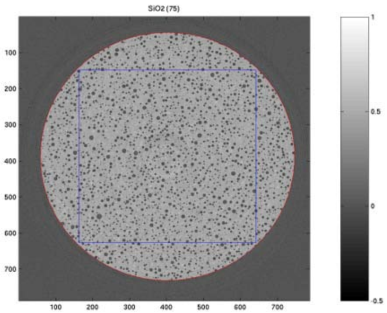


150 slides

SiO2_plane_**01**.jpg



SiO2_plane_**075**.jpg



SiO2_plane_**150**.jpg

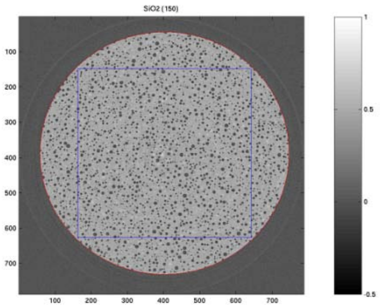
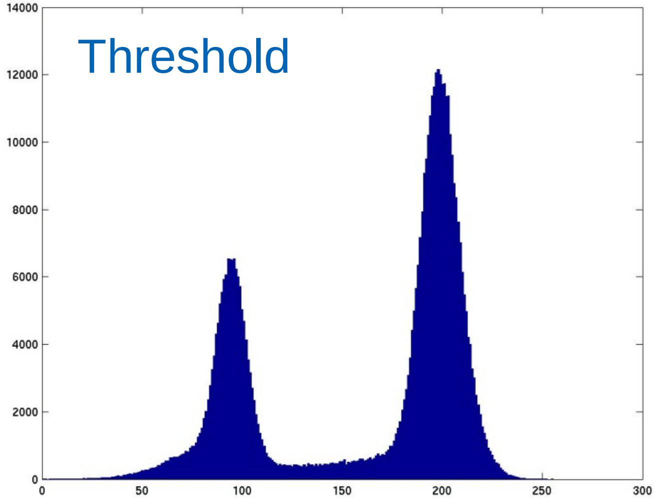
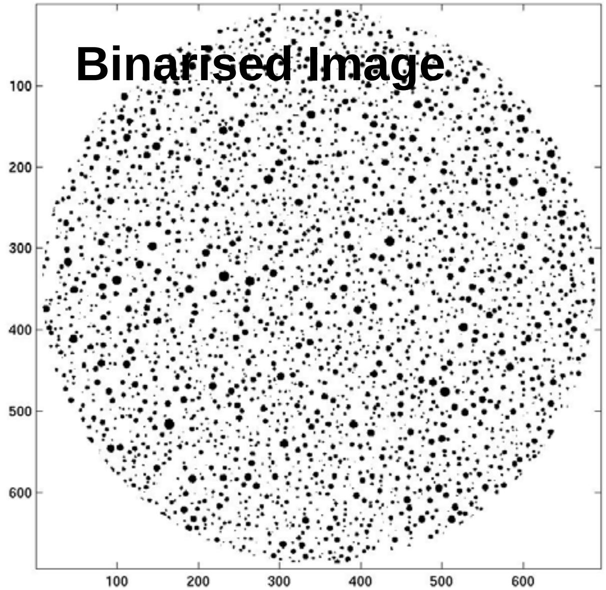


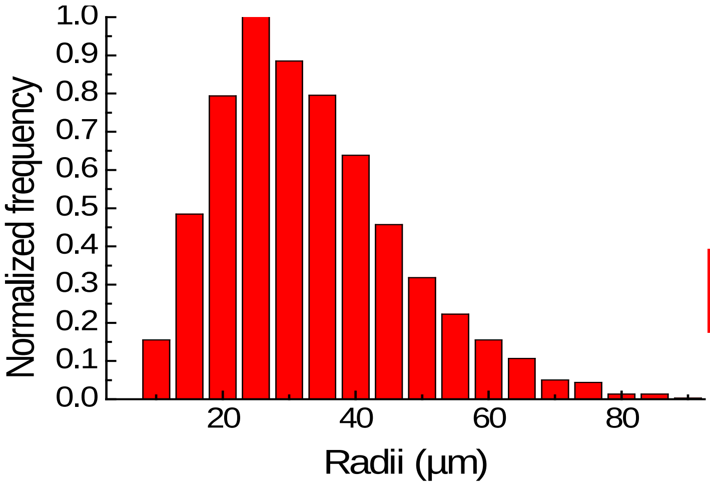
Image analyzing

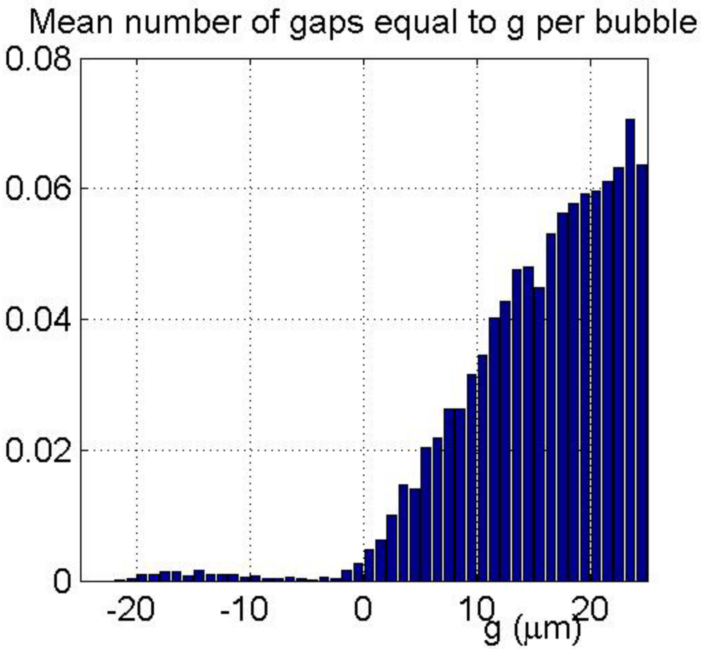




Coll. J.-F. Thovert LCD Poitiers

"MATERIAL PARAMETERS"→ RAY TRACING?



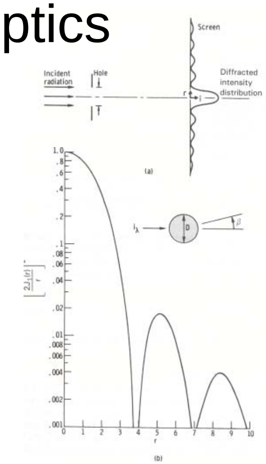


25 < λ < 2 µm (400 < σ < 5000 cm[-1])

$$x = \frac{2\pi \langle r \rangle}{\lambda} > 1$$

❖Geometrical optics

❖No diffraction



Siegel & Howell, 1992

$$g/\lambda > 1/2$$

$$\langle r \rangle \approx g$$

❖No interferences

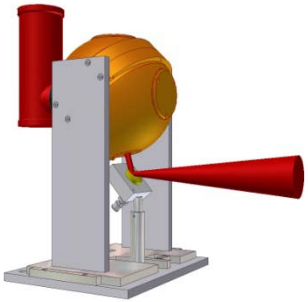
❖Multiple scattering

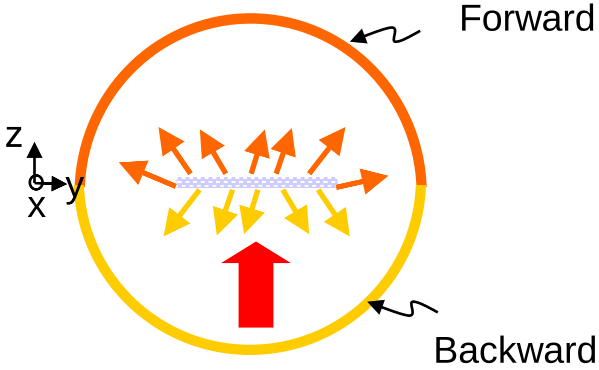
Multiple reflection

B. Rousseau et al., Applied Optics (2007)

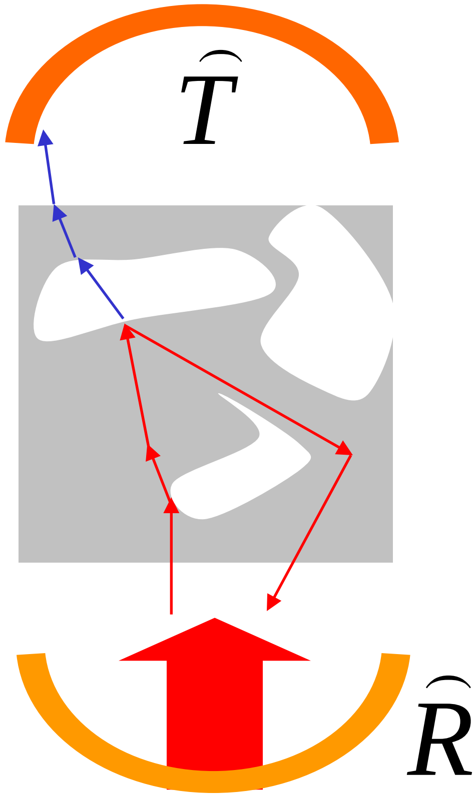
NUMERICAL EXPERIMENT

$$E(\sigma,\theta,T)=1-\widehat{R}(\sigma,\theta,T)-\widehat{T}(\sigma,\theta,T)$$



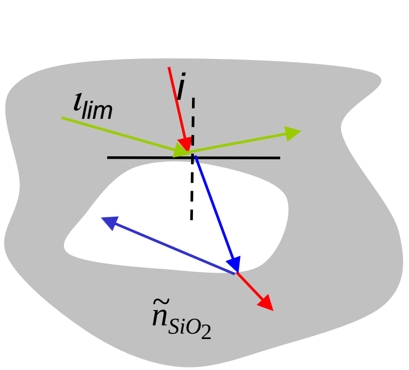


- ***Large number of rays : 10^5-10^6***
- ***Simulation in a realistic reconstructed volume***
- ***Large spectral domain [1-25 µm]***
- ***Large set of statistic data***
  - *path length in the solid phase (transparent, semitransparent, opaque)*
  - *path length in the void phase*
  - *number of intercepted interfaces*
  - *position and incident angle of a photon (at the beginning of its travel)*
  - *position and exhaust angle of a photon (at the end of its travel)*



ABSORPTION/SCATTERING PROCESS

❖Refraction index gradient : **scattering**



MCRT procedure (0< ξ <1)

ξ<ρ : reflexion
ξ>ρ : refraction

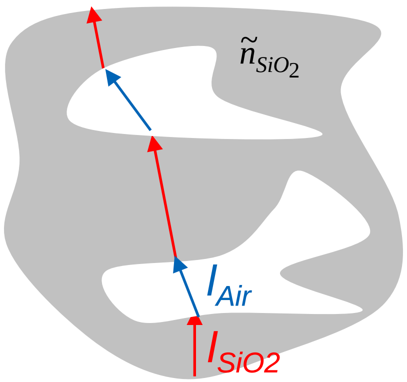
Fresnel's law

$$\rho(\sigma,T)=\frac{1}{2}\left[\left|\frac{\dfrac{\cos i}{\cos\tilde{r}(\sigma,T)}-\dfrac{\tilde{n}_1(\sigma,T)}{\tilde{n}_2(\sigma,T)}}{\dfrac{\cos i}{\cos\tilde{r}(\sigma,T)}+\dfrac{\tilde{n}_1(\sigma,T)}{\tilde{n}_2(\sigma,T)}}\right|^2+\left|\frac{\dfrac{\cos\tilde{r}(\sigma,T)}{\cos i}-\dfrac{\tilde{n}_1(\sigma,T)}{\tilde{n}_2(\sigma,T)}}{\dfrac{\cos\tilde{r}(\sigma,T)}{\cos i}+\dfrac{\tilde{n}_1(\sigma,T)}{\tilde{n}_2(\sigma,T)}}\right|^2\right]$$

Snell-Descartes 's law

$$\tilde{n}_{SiO_2}\sin i=\sin\tilde{r}$$

❖Chemin optique : **absorption**



MCRT procedure $\sum_i I_i < 0.01$

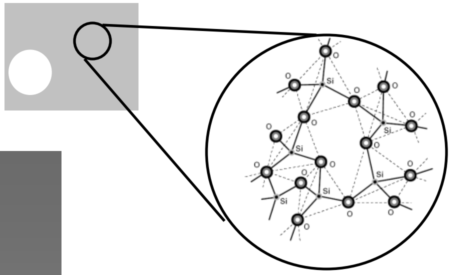
Beer-Lambert 's law

$$I_i = I_0 e^{-l_i K_i}$$

Key role :

Optical function (n, k , K)

OPTICAL FUNCTIONS OF SiO_2

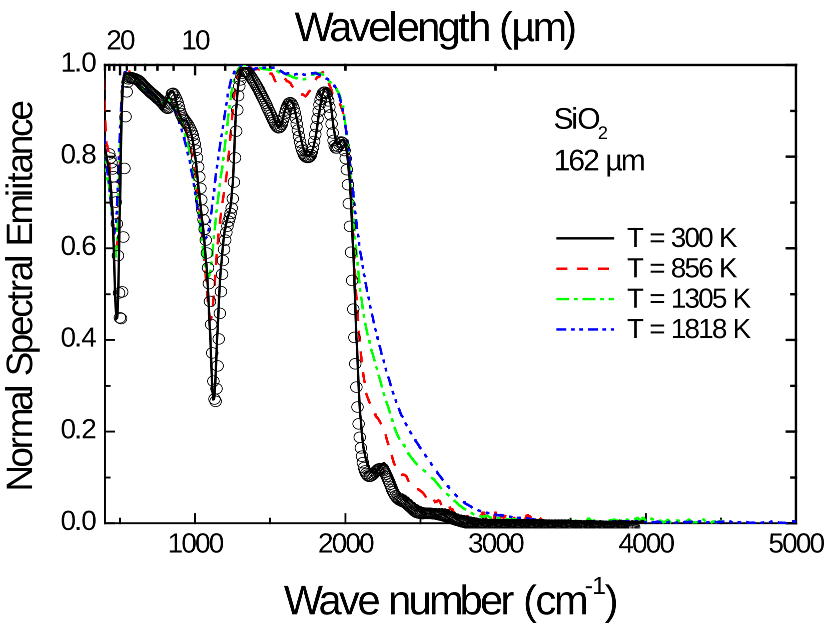


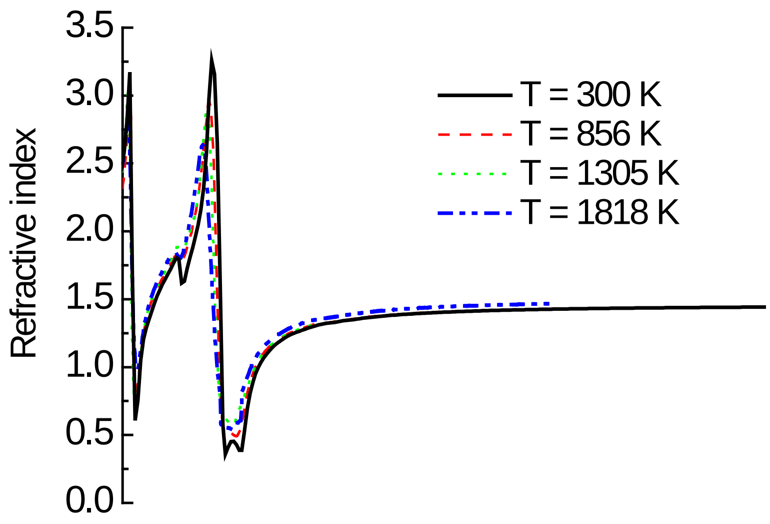
$$\begin{cases}\tilde{n} = \sqrt{\tilde{\varepsilon}} \\ \tilde{n}(\sigma,T) = n(\sigma,T) + ik(\sigma,T) \\ K(\sigma,T) = 4\pi\sigma k(\sigma,T)\end{cases}$$

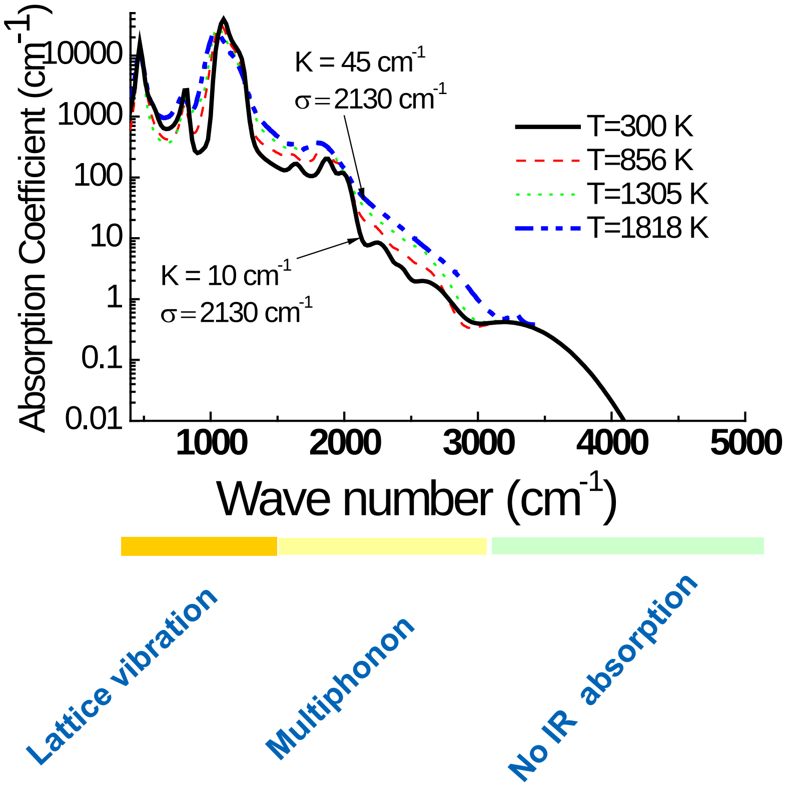
$$\tilde{\varepsilon}(\omega,T) = \varepsilon_\infty + \sum_j C_{V_j}(\omega; \omega_{0j}, \gamma_{Gj}, \gamma_{Lj})$$

De Sousa Meneses et *al.*, *JNCS*, **351**, (2005)

$$E(\omega,T) = \frac{(1-\rho(\omega,T))(1-e^{-K(\omega,T)d})}{1-\rho(\omega,T)e^{-K(\omega,T)d}}$$

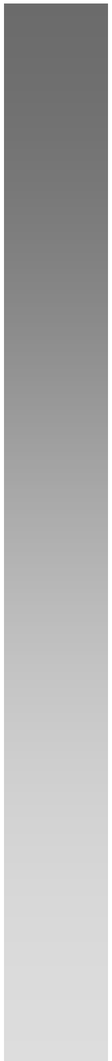


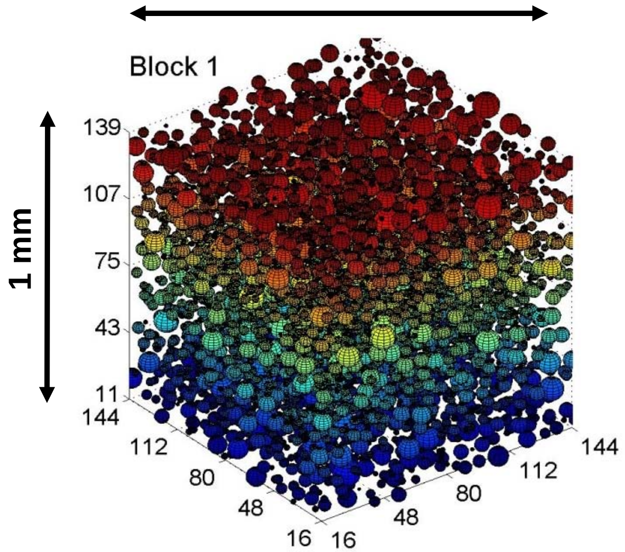




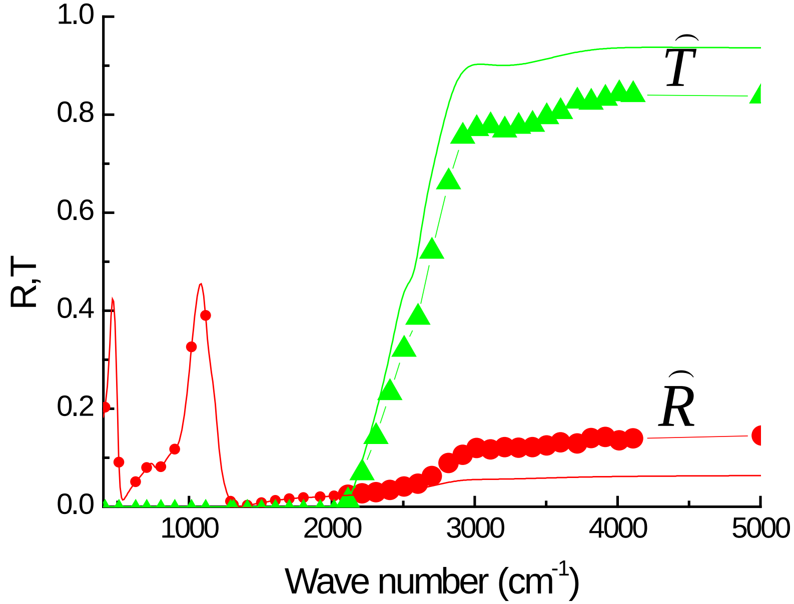
CHEMISTRY+MICROSTUCTURE ?

10 mm (× 10)

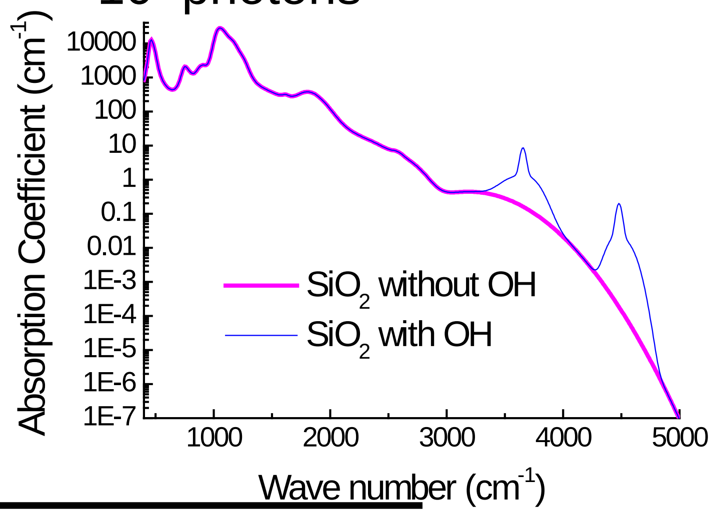


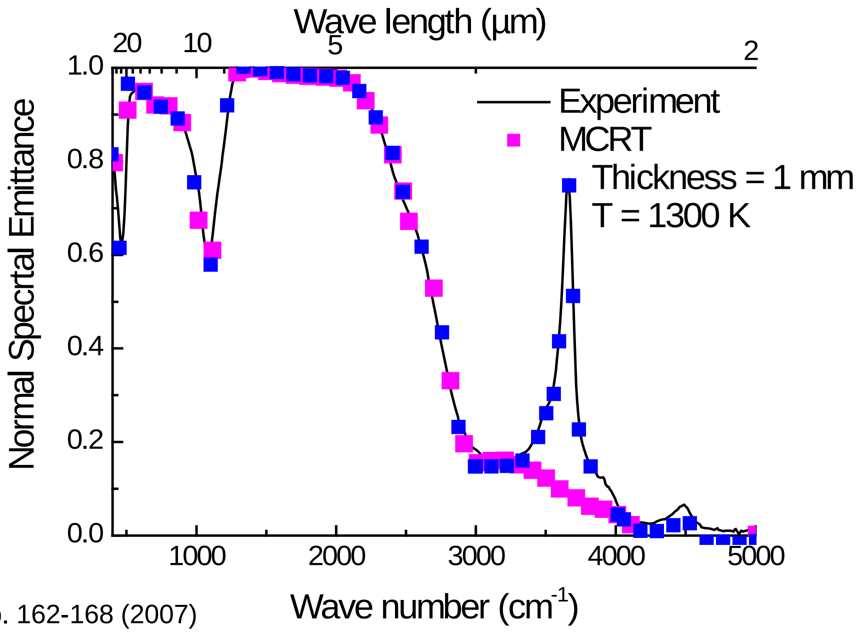


$$E = 1 - \hat{R} - \hat{T}$$



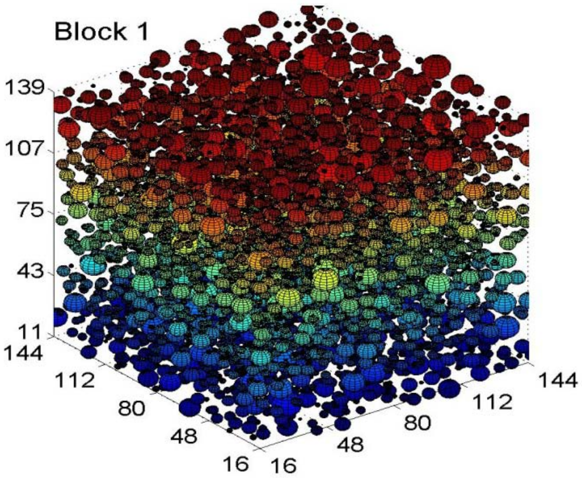
10^6 photons



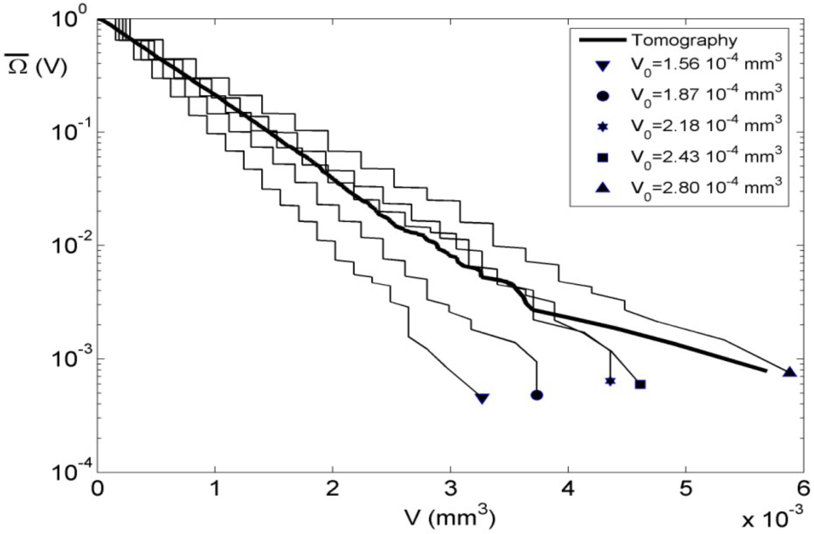


B. Rousseau et al. COLSUA, 300, pp. 162-168 (2007)

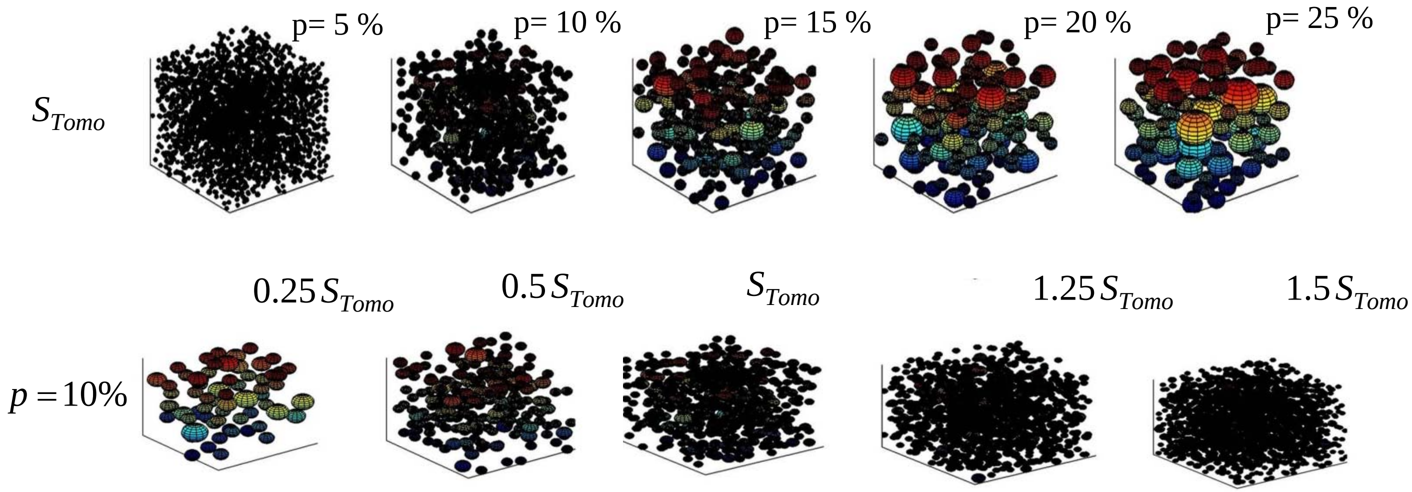
DESIGN OF POROUS GLASSES



S_{Tomo} = 89 cm^{-1}



COALESNCE MODEL

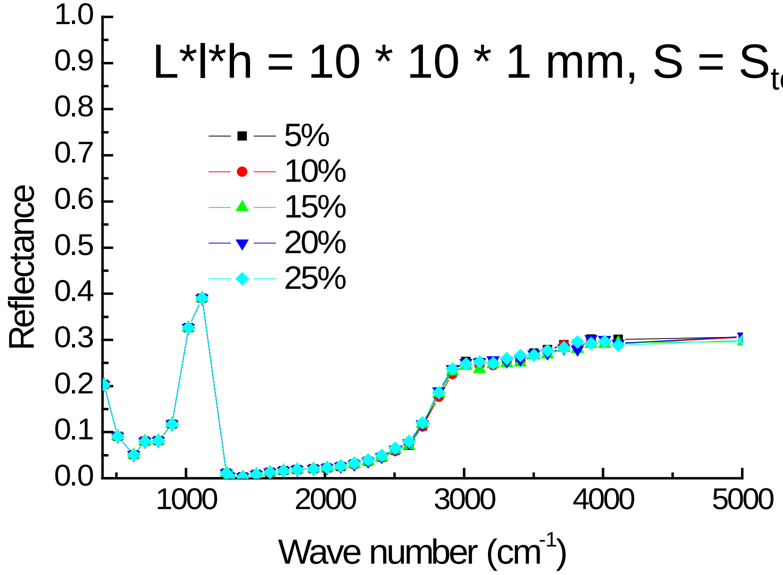


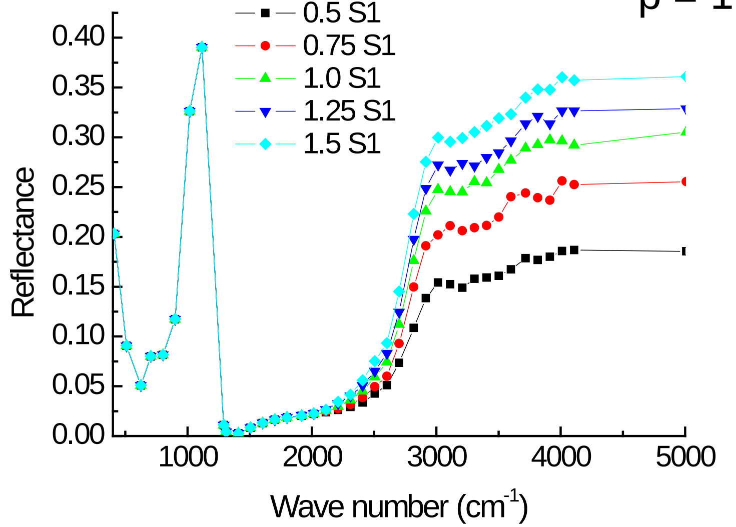
NUMERICAL RESULTS

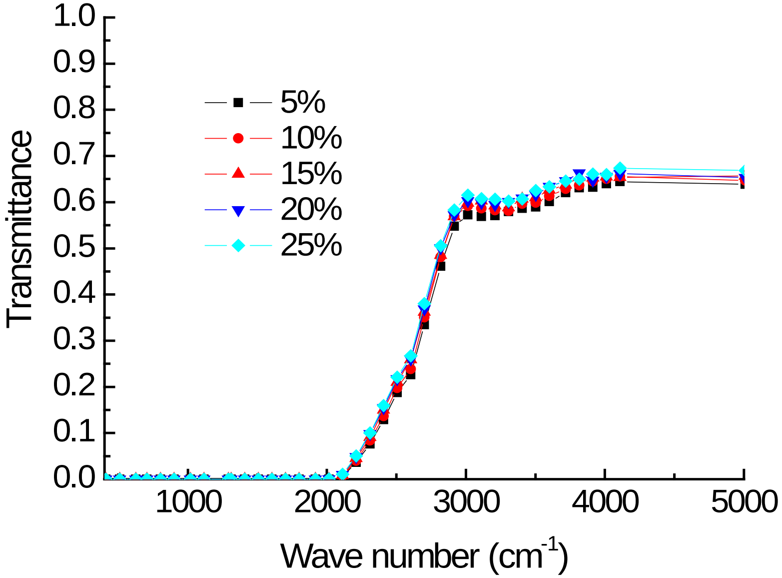
T = 1 300 K,

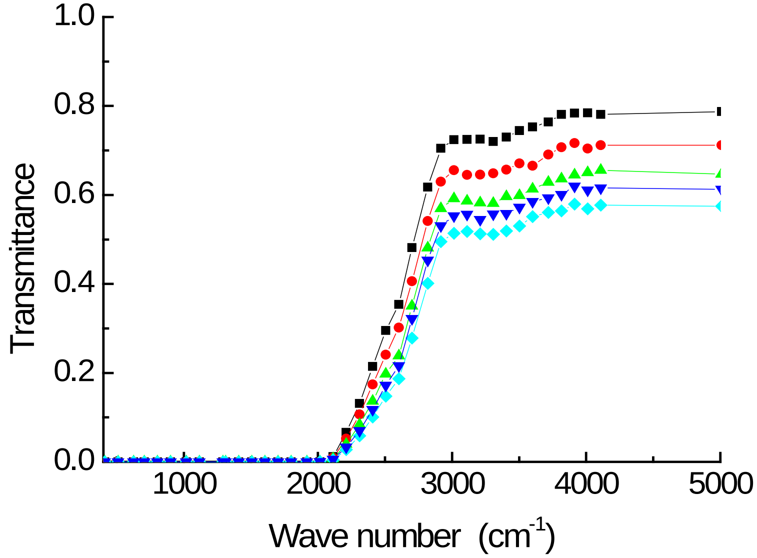
L*l*h = 10 * 10 * 1 mm, S = $S_{tomography}$

p = 10 %

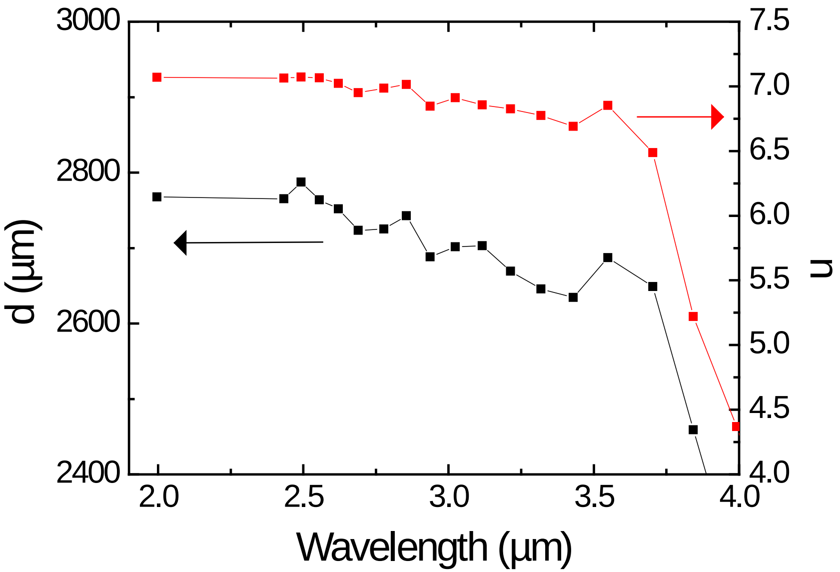


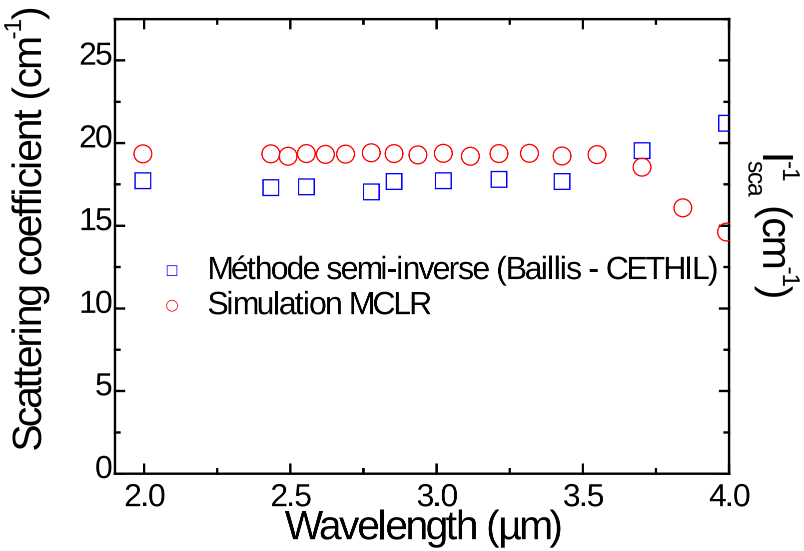


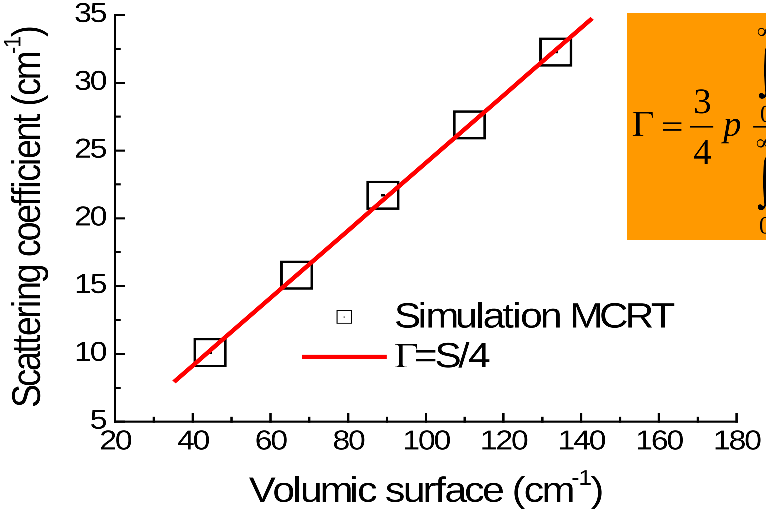




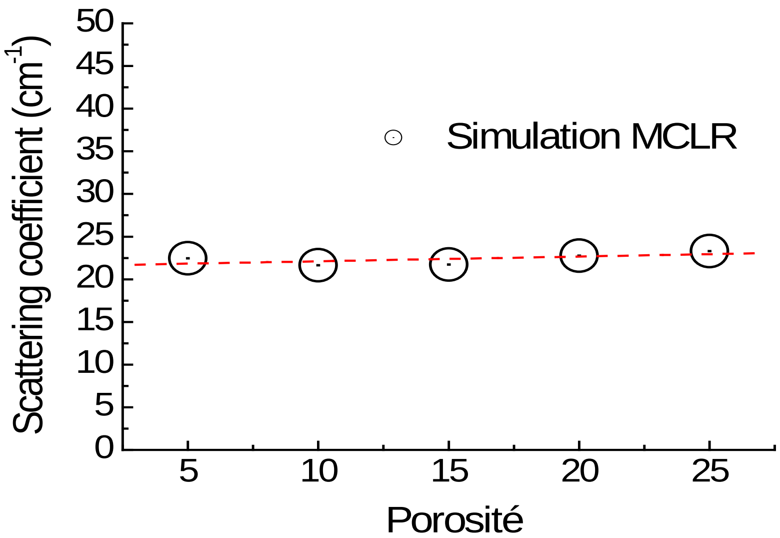
INFLUENCE OF THE VOLUMETRIC SURFACE





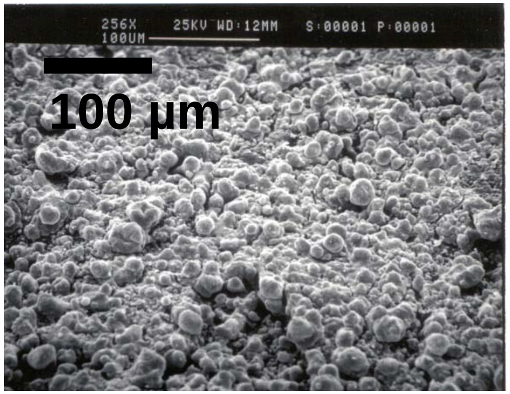


$$\Gamma = \frac{3}{4} p \frac{\int_0^\infty f(r) r^2 dr}{\int_0^\infty f(r) r^3 dr}$$

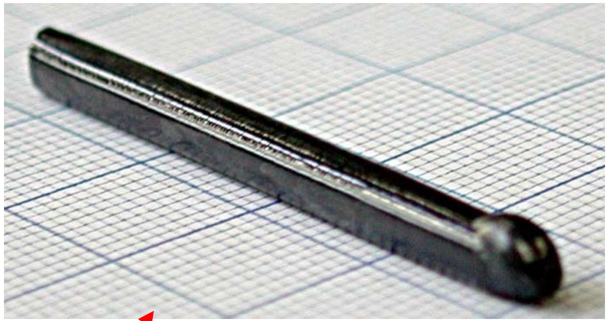


AN OPAQUE MEDIUM

ROUGH COATING OF $Pr_2NiO_{4+\delta}$



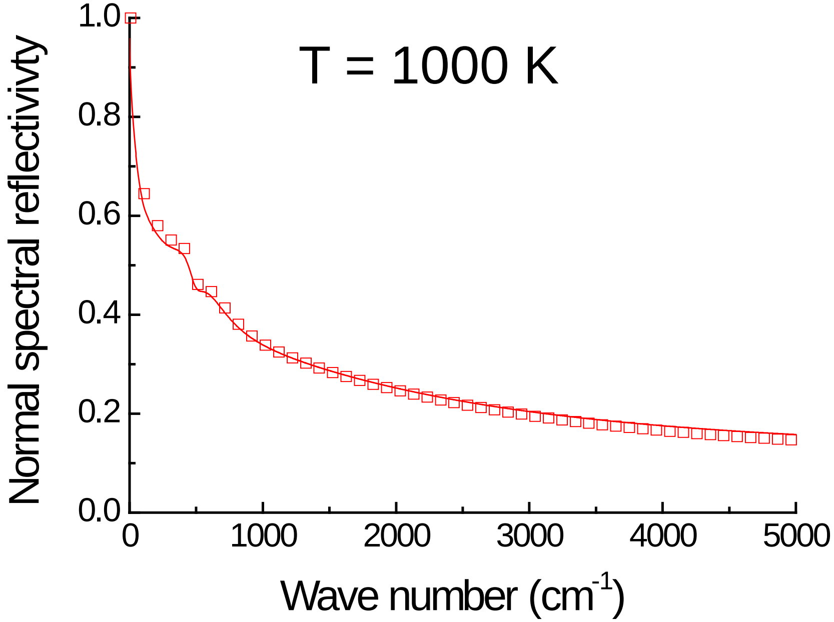
OPTICAL FUNCTIONS OF $Pr_2NiO_{4+\delta}$

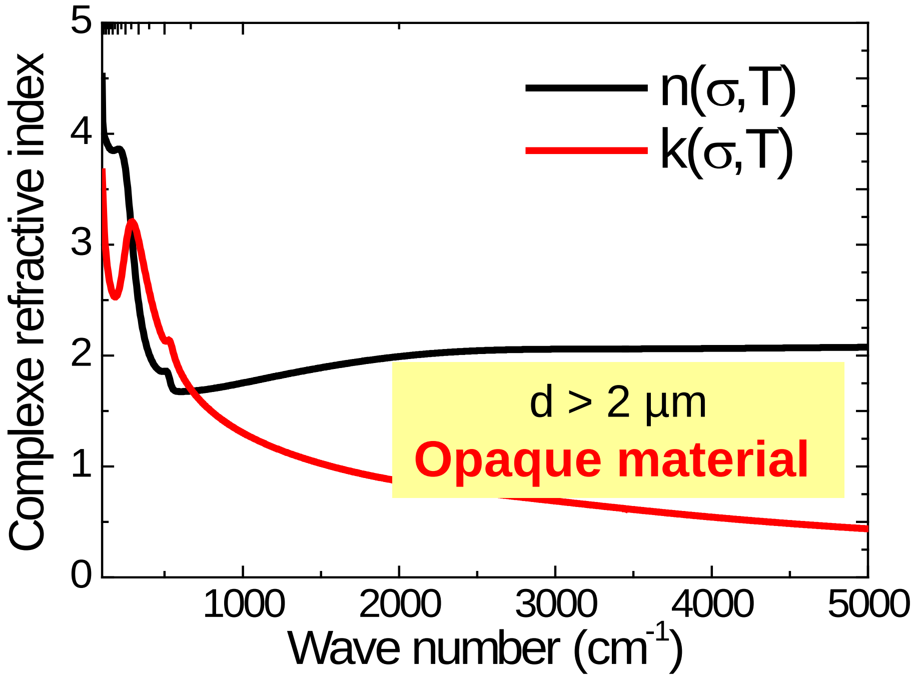


$$\rho(\sigma,T)=\frac{I_{reflected}(\sigma,T)}{I_0(\sigma,T)}=\left|\frac{\tilde{n}(\sigma,T)-1}{\tilde{n}(\sigma,T)+1}\right|^2=\left|\frac{\sqrt{\tilde{\varepsilon}(\sigma,T)}-1}{\sqrt{\tilde{\varepsilon}(\sigma,T)}+1}\right|^2$$

$$\frac{\tilde{\varepsilon}(\sigma,T)}{\varepsilon_\infty}=\prod_j \frac{\Omega^2_{LOj,T}-\sigma^2+i\gamma_{LOj,T}\sigma}{\Omega^2_{TOj,T}-\sigma^2+i\gamma_{TOj,T}\sigma} - \frac{\Omega^2_{pl,T}-\sigma^2+i\gamma_{pl,T}\sigma}{\sigma(\sigma-i\gamma_{o,T})}$$

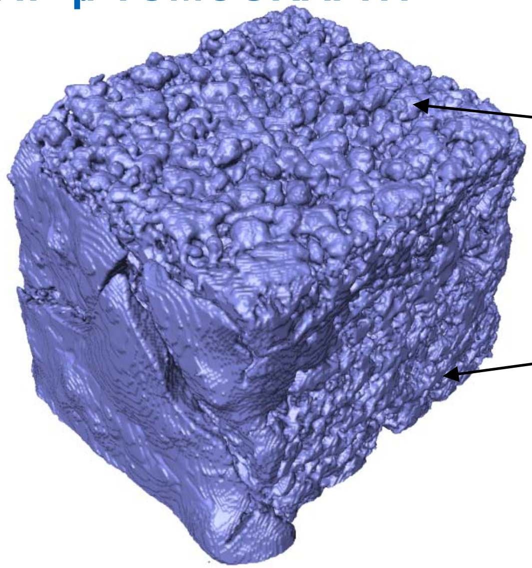
B. Rousseau et al. PRB 2005





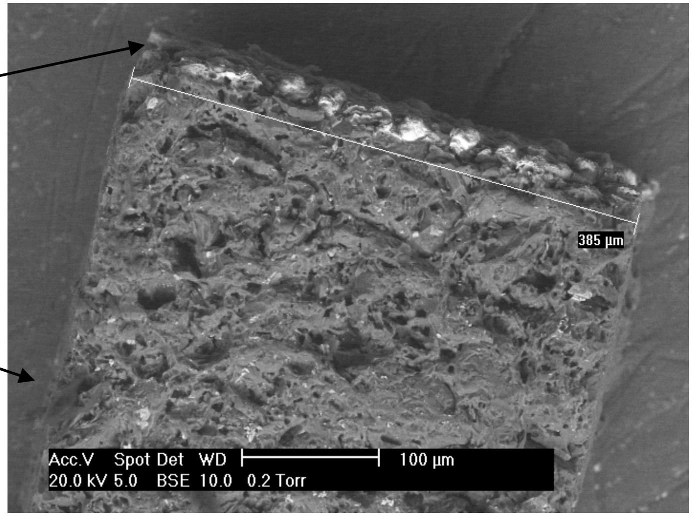
HOW CAN WE EXTRACT THE GEOMETRIC SURFACE?

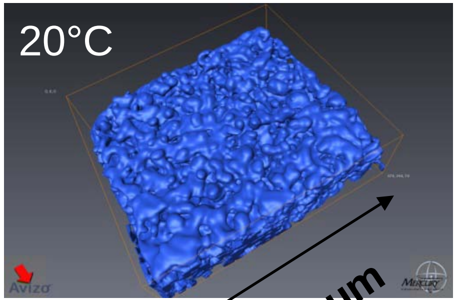
X-RAY µ-TOMOGRAPHY Resolution ~0.7 µm



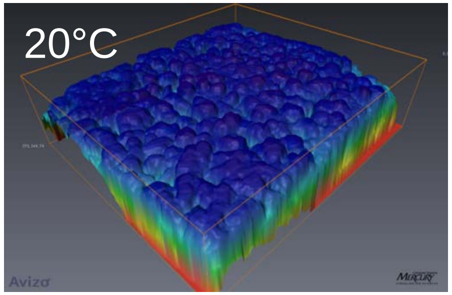
Rough coating
$Pr_2NiO_{4+\delta}$

Alumino-silicate tile

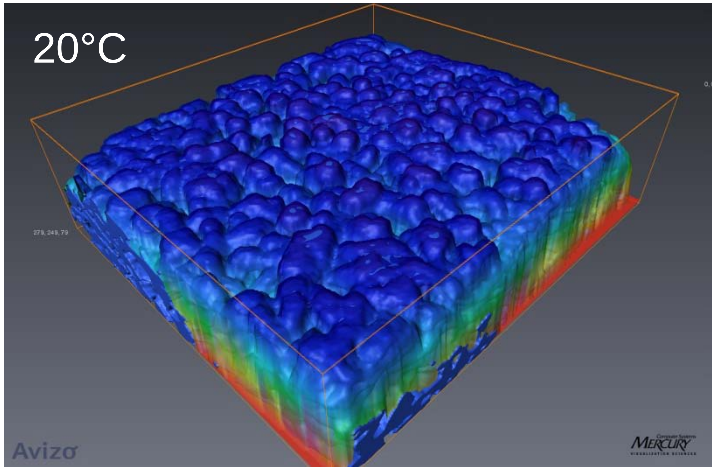




200 µm



HEIGHT CARD ON A REGULAR GRID [280×250]



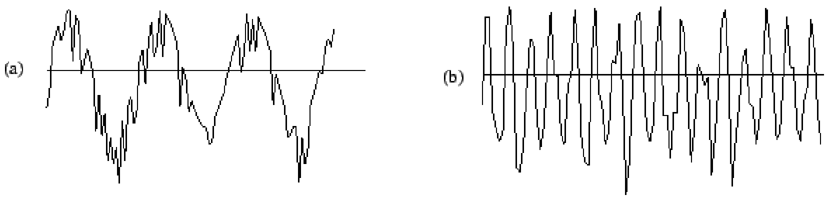
STRATEGY OF SIMULATION ?

Statistical parameters

$$R_z(u) = \frac{\left(\langle Z(x,y)\rangle \langle Z(x+u,y)\rangle\right)}{\langle Z(x,y)^2\rangle}$$

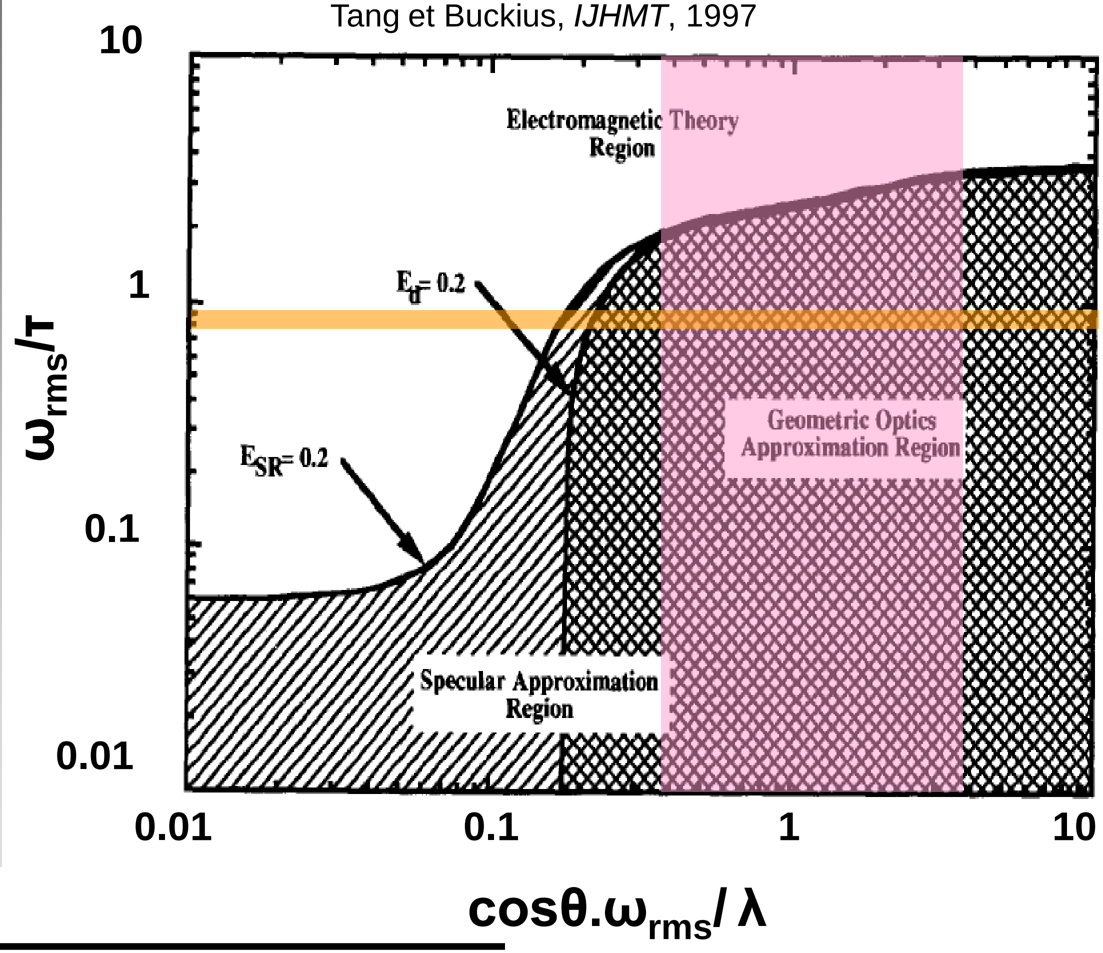
$$\omega_{rms} = \sqrt{\langle Z(x,y)^2\rangle}$$

$$\tau = R_z\left(e^{-1}\right)$$



Light Matter Interaction

Tang et Buckius, *IJHMT*, 1997



300 K

ω_{rms} =5. 5 µm

τ = 8.4 µm

500 K

ω_{rms} = 5.7 µm

τ = 8.7 µm

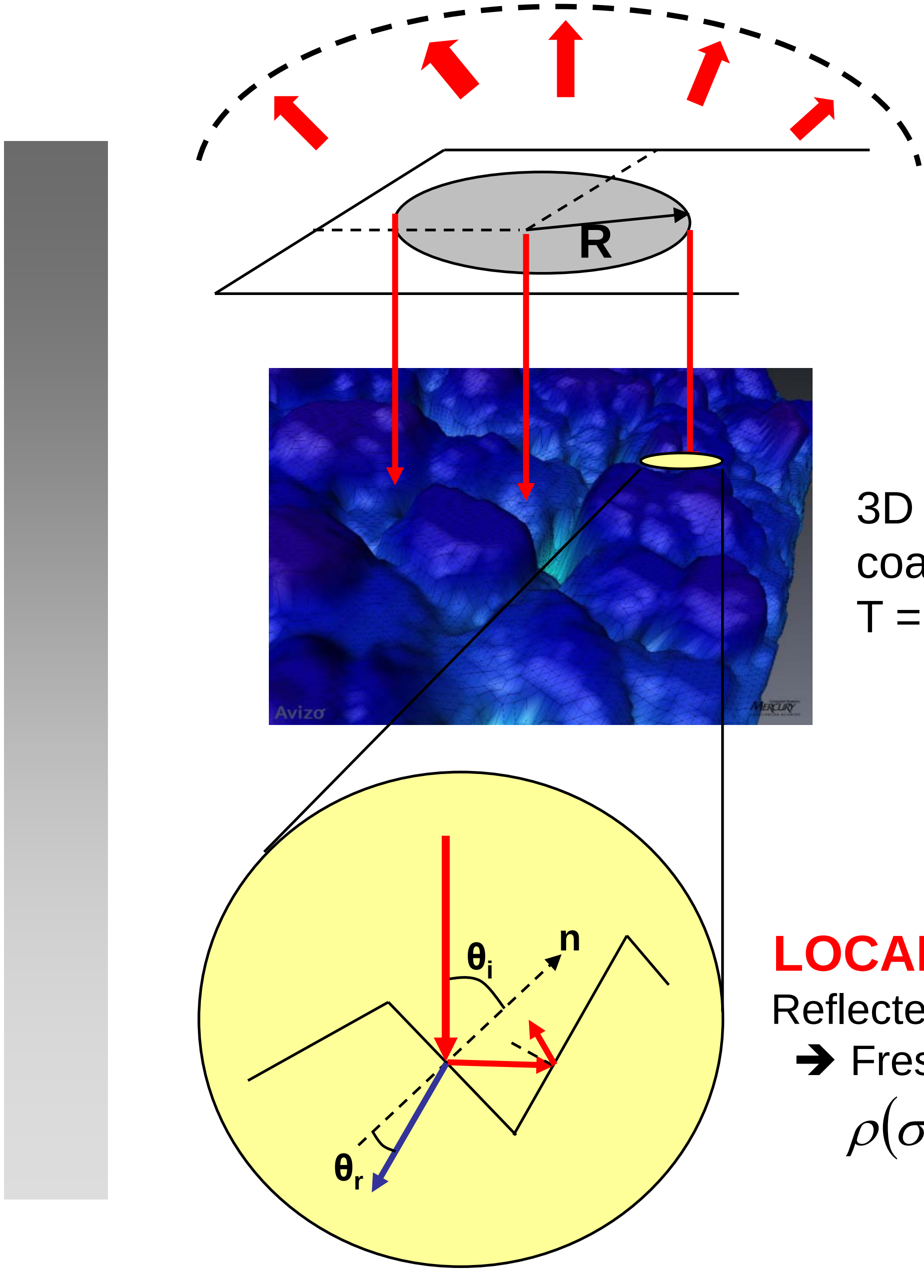
900 K

ω_{rms} =5. 6 µm

τ = 8.3 µm

Geometrical optics

MODELLING : ROUGH SURFACE



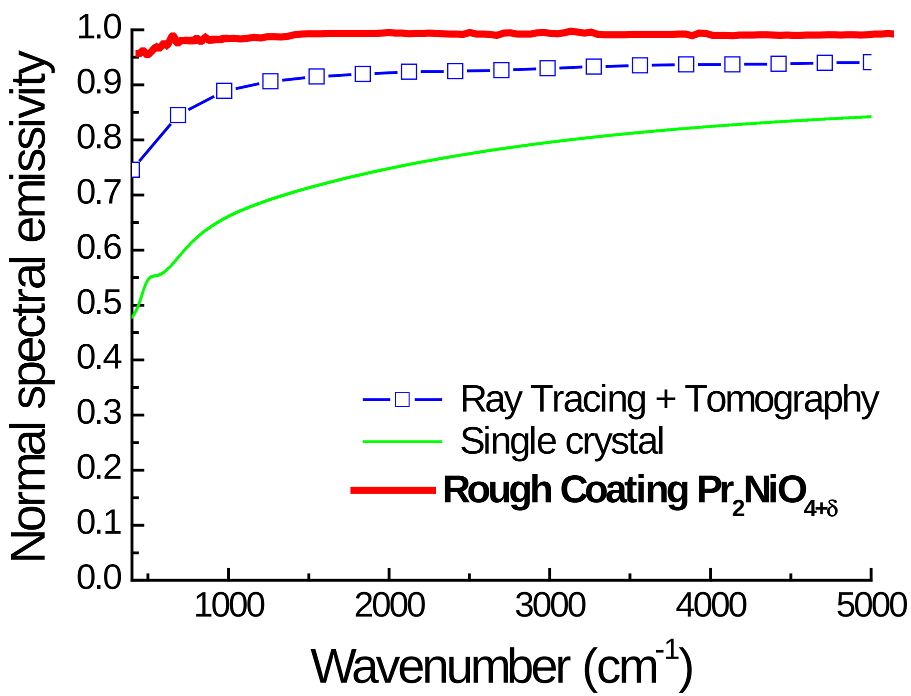
To reproduce an experiment where :

$$E = 1 - \hat{R}$$

Large number (10^6) of rays issued from an infrared parallel beam are thrown onto the numeric surface

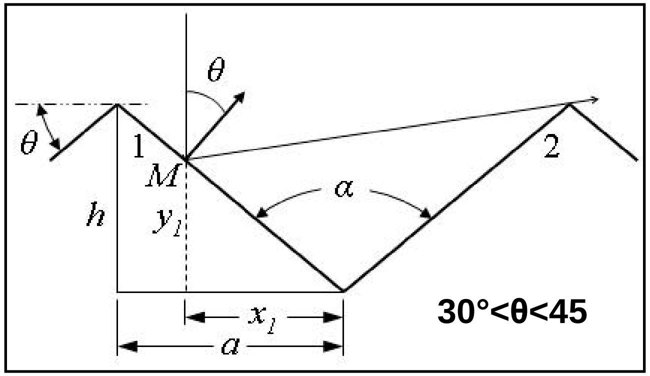
3D image of the
coating surface
T = 900 k

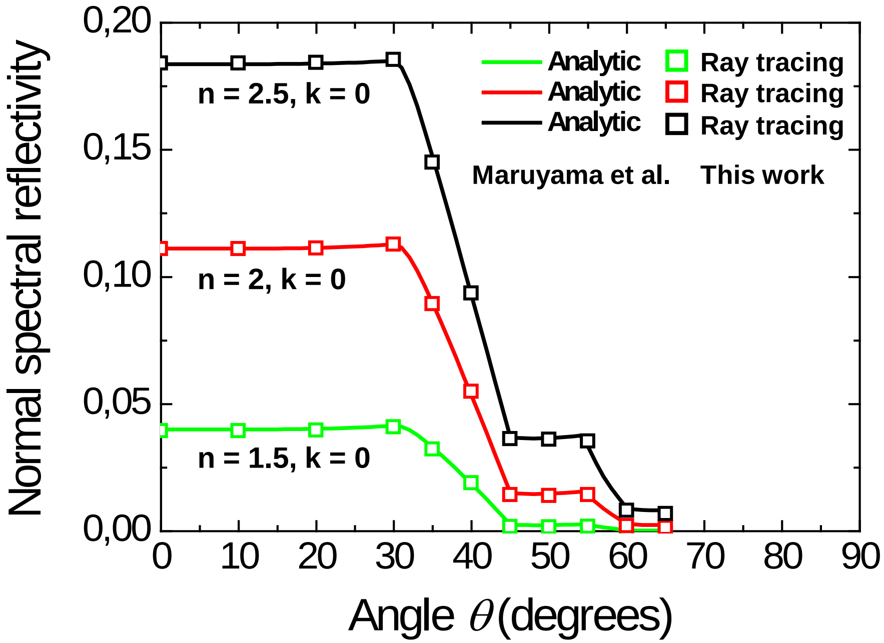
LOCAL SC
Reflected Inte
➔ Fresnel 's
$\rho(\sigma, T, \theta_i$



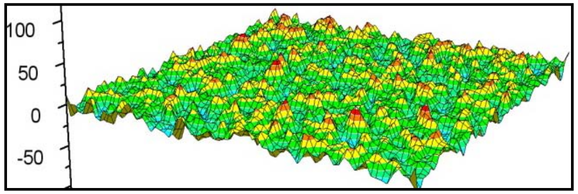
RAY TRACING VALIDITY : LITERATURE COMPARISON

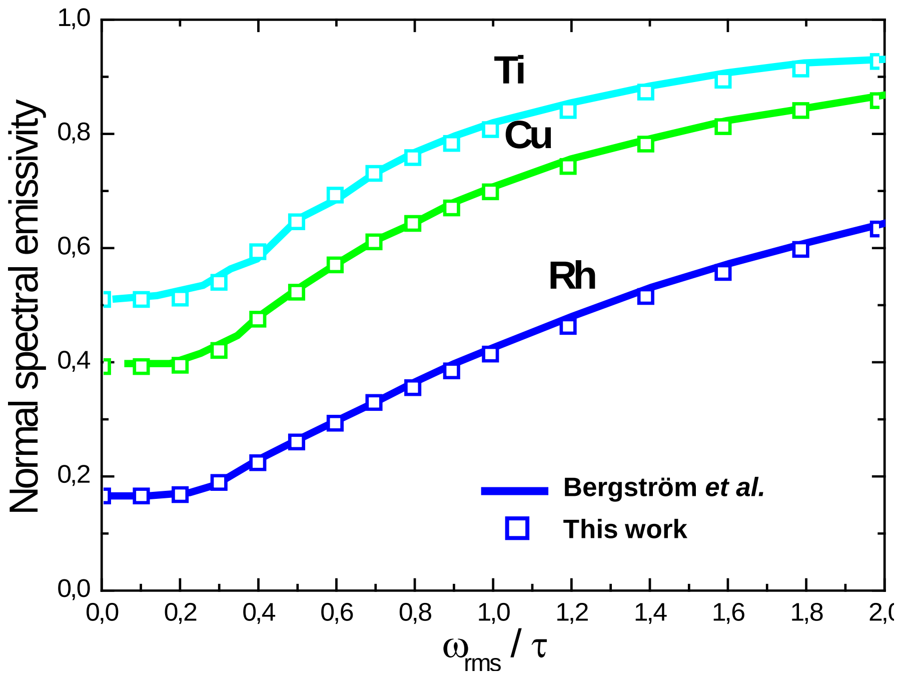
2D-surface with V-groove cavities:
An analytic model
(Sacadura, IJHMT, 1972 & Maruyama et al., *SEMSC*, 2004)



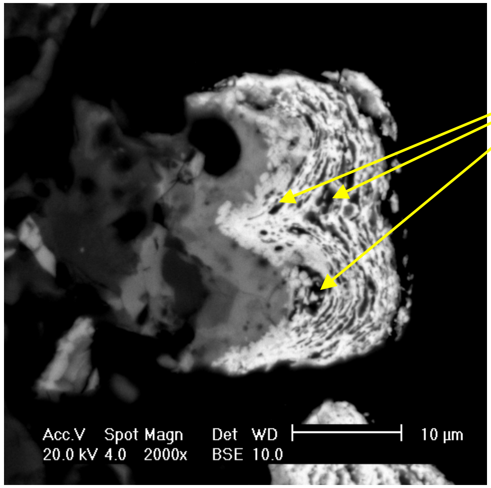


3D-random rough surface (gaussian):
Literature-ray tracing data
(Bergstrom et al., JAP, 2008)





EFFECT OF THE INTERNAL MICROSTRUCTURE



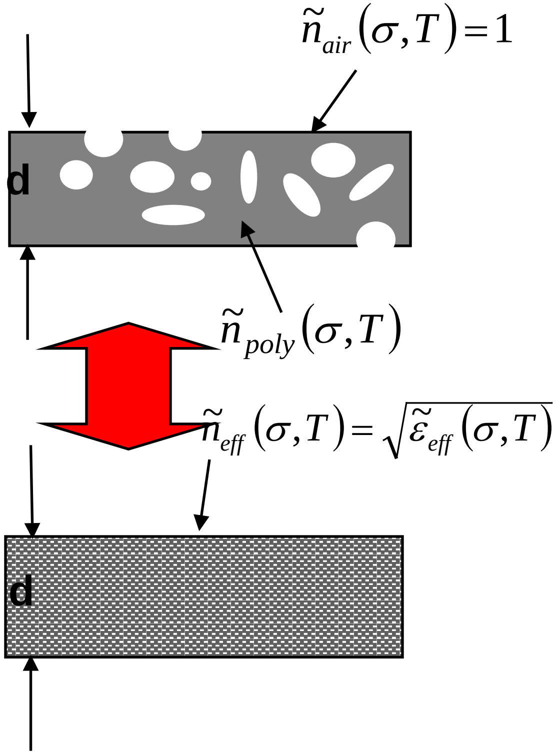
pore : 50 -200 nm

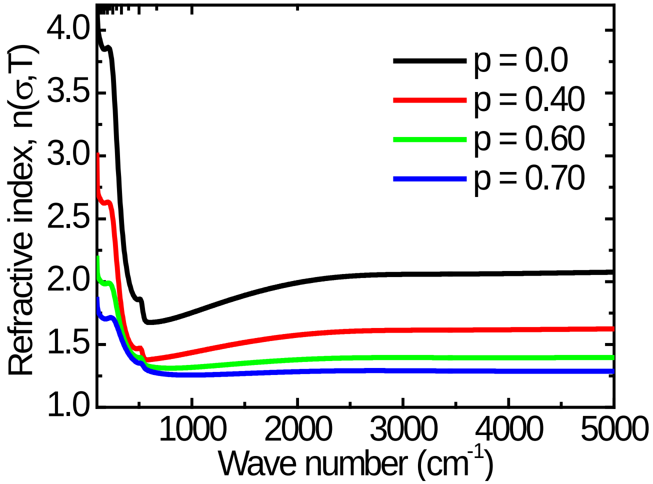
$d_{pore} << \lambda_{infrared}$ (2-20 µm)

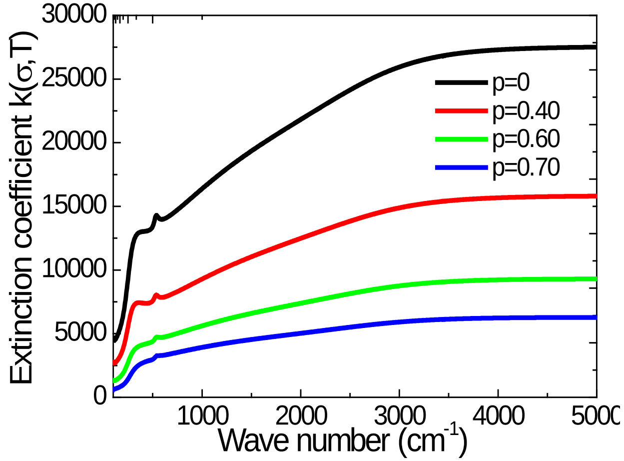
$$(1-p)\frac{\tilde{\varepsilon}_{poly}(\sigma,T)-\tilde{\varepsilon}_{eff}(\sigma,T)}{\tilde{\varepsilon}_{eff}(\sigma,T)+y_{poly}\left(\tilde{\varepsilon}_{poly}(\sigma,T)-\tilde{\varepsilon}_{eff}(\sigma,T)\right)}+p\frac{\tilde{\varepsilon}_{pore}(\sigma,T)-\tilde{\varepsilon}_{eff}(\sigma,T)}{\tilde{\varepsilon}_{eff}(\sigma,T)+y_{pore}\left(\tilde{\varepsilon}_{pore}(\sigma,T)-\tilde{\varepsilon}_{eff}(\sigma,T)\right)}=0$$

Effective Medium Approximation

D.E. Apnes, optical properties of thin films, Thin Solid Films 89 (1982) 249

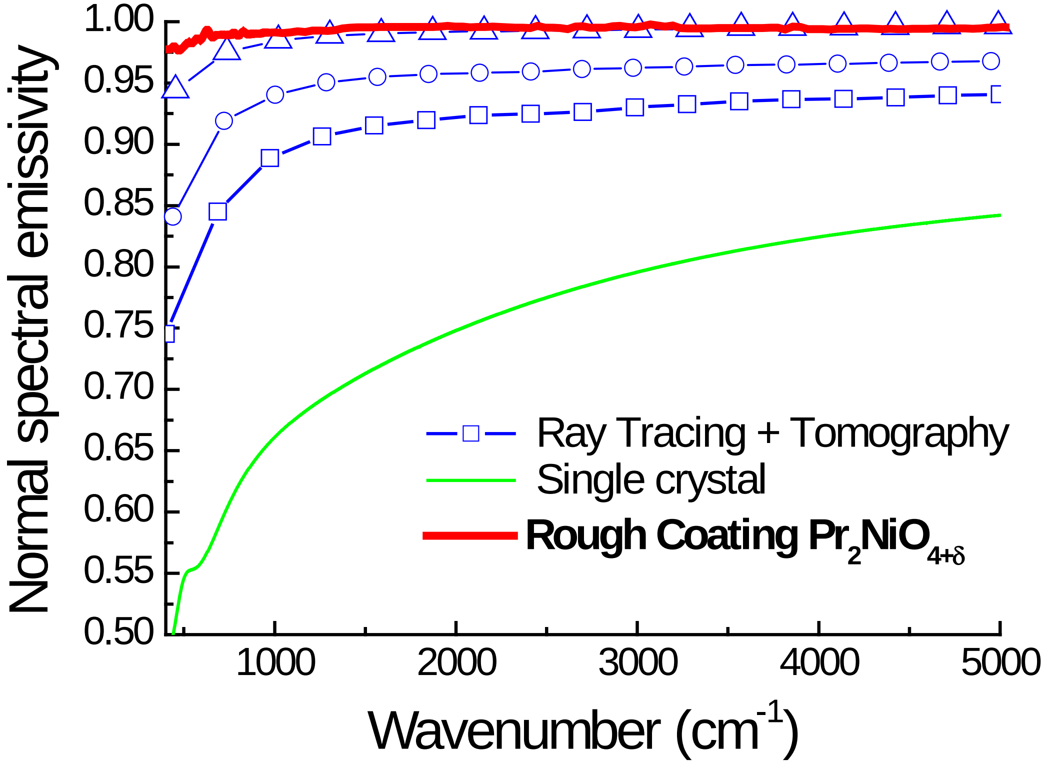


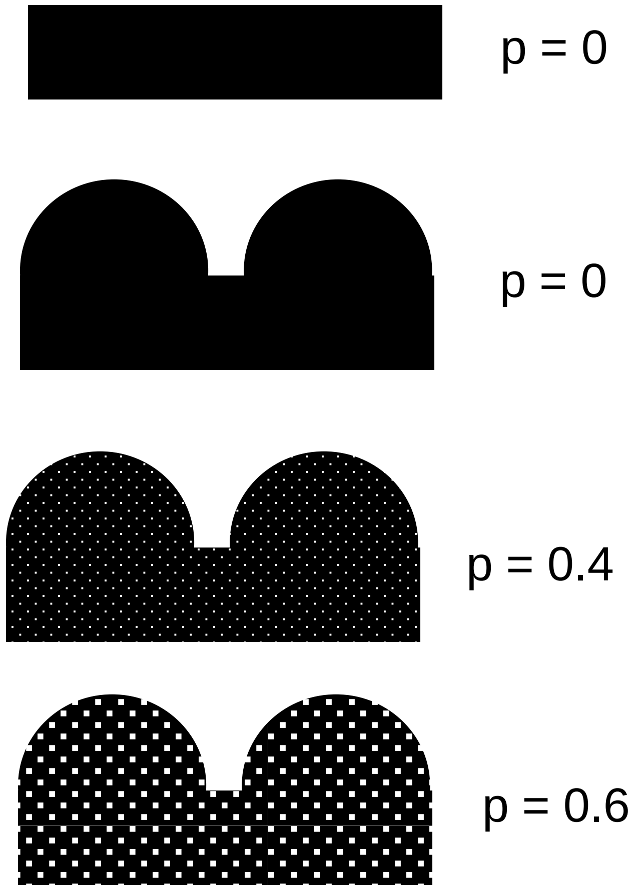


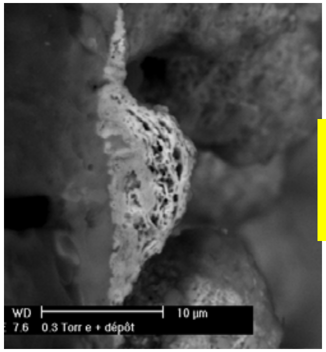


p =70% d> 11 µm (opaque)

HYBRID MODEL : RAY TRACING+EMA



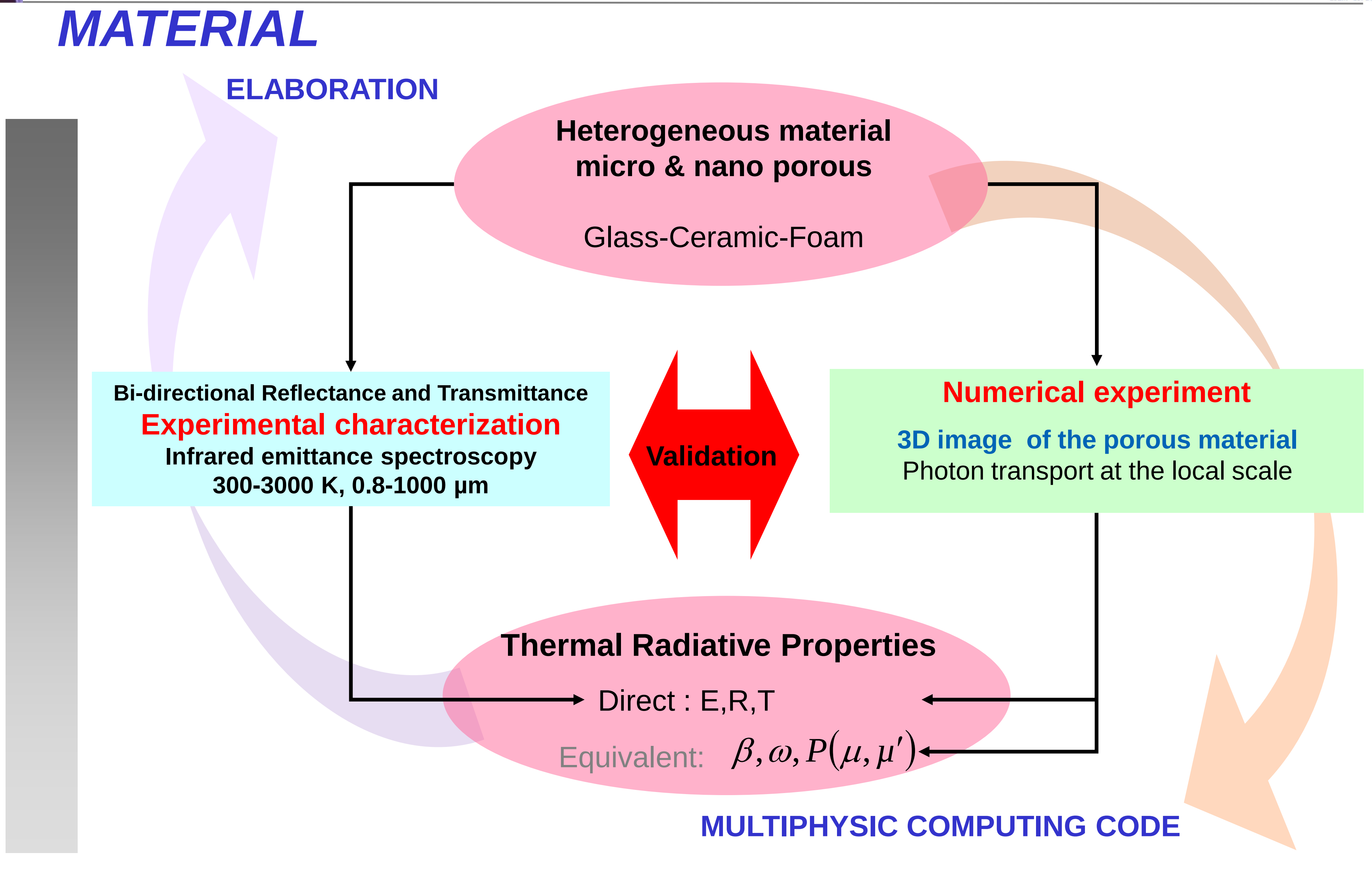




ESTIMATION OF THE POROSITY OF A COLLECTION OF GRAINS?

Thèse Hector Gomart, Université d'Orléans, 2008

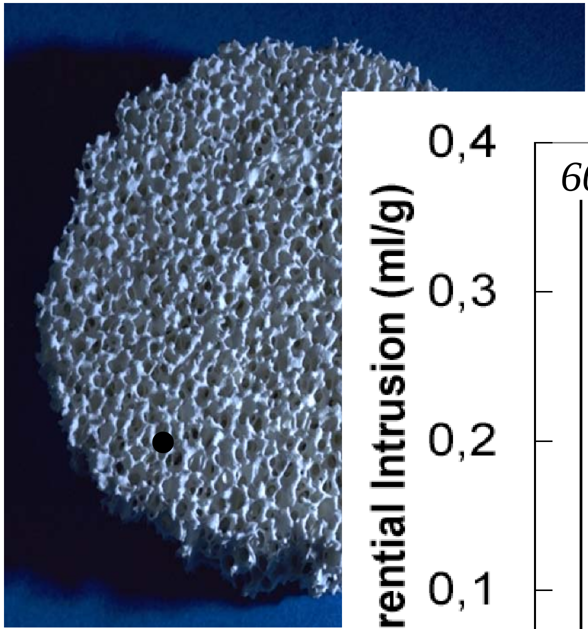
STRATEGY OF PREDICTION



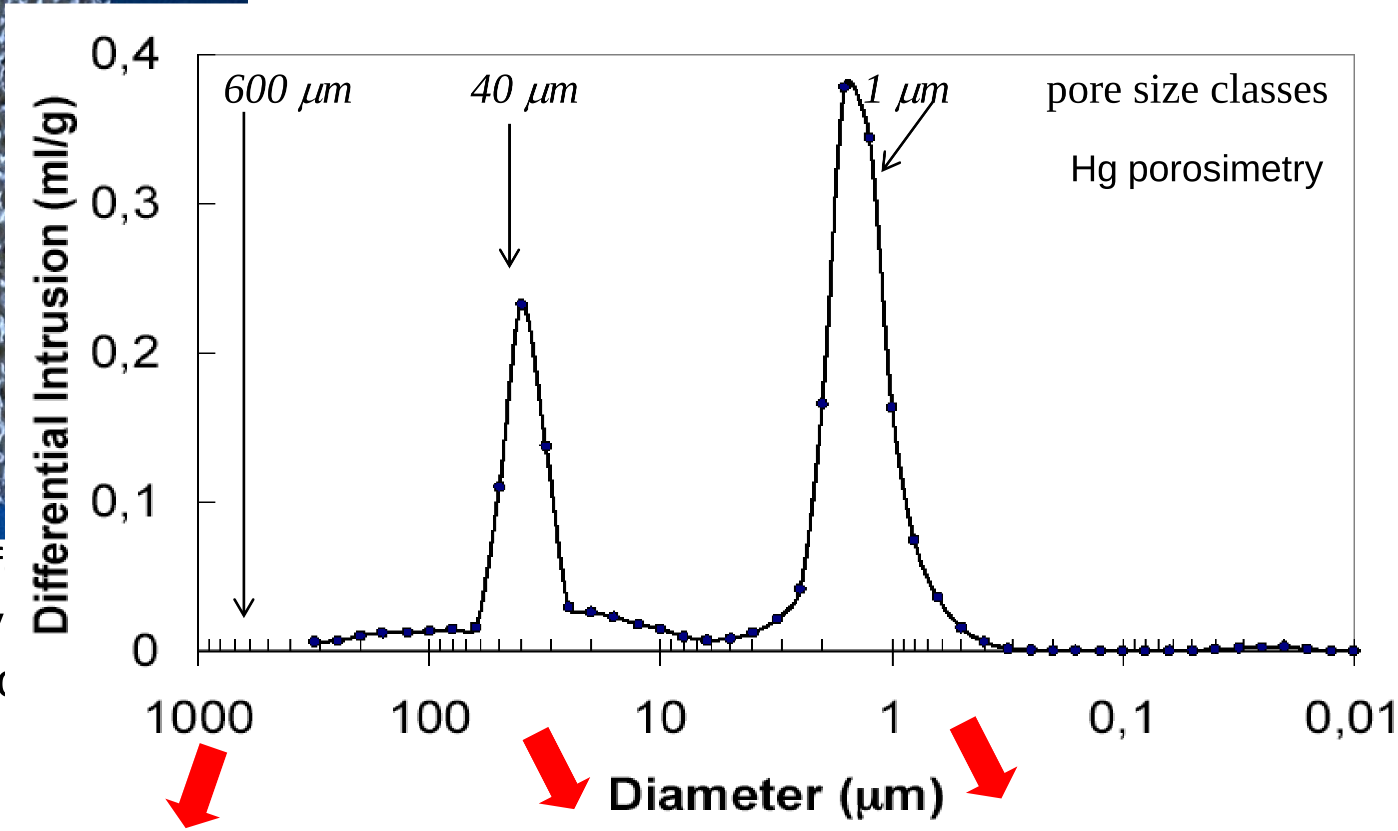
ENERGY

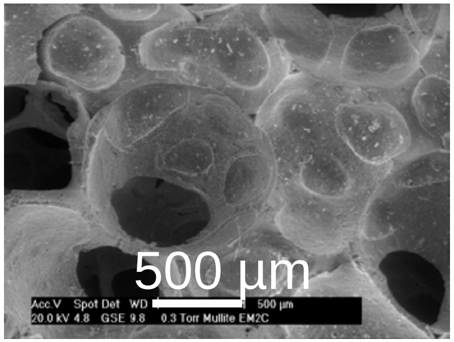
A MORE COMPLEX SAMPLE :MULLITE FOAM

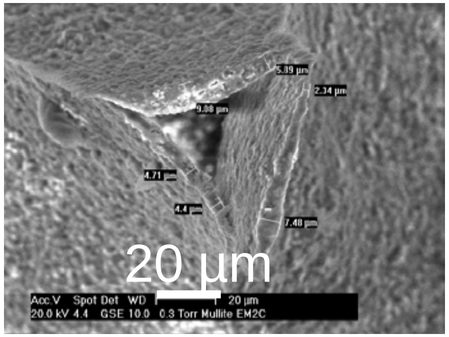
WORK PERFORMED WITH EM2C & CETHIL

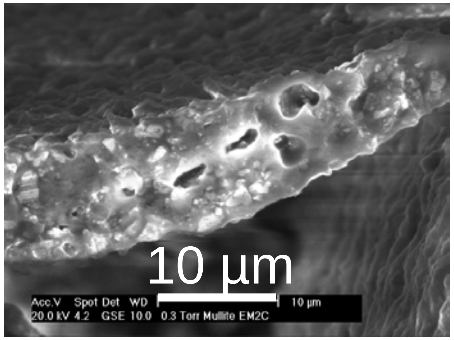


Mullite f
(porosity
for catalytic c



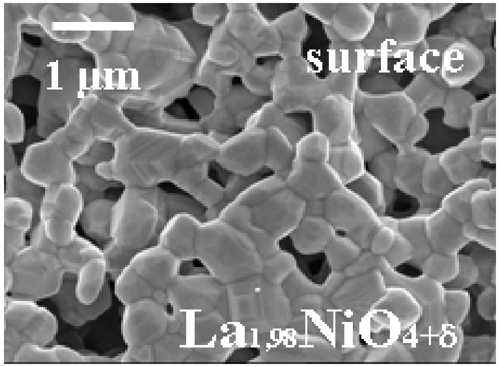


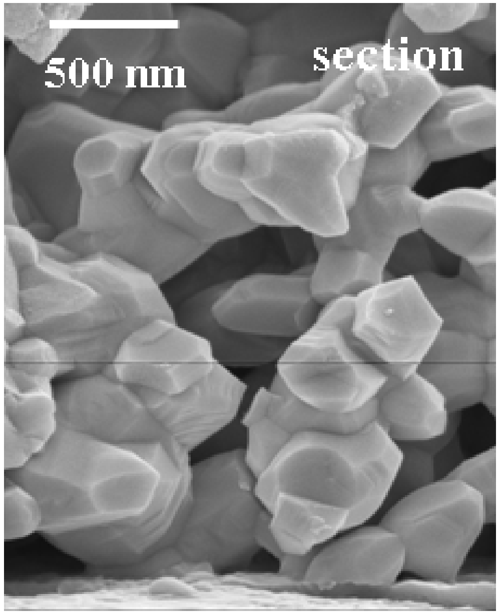


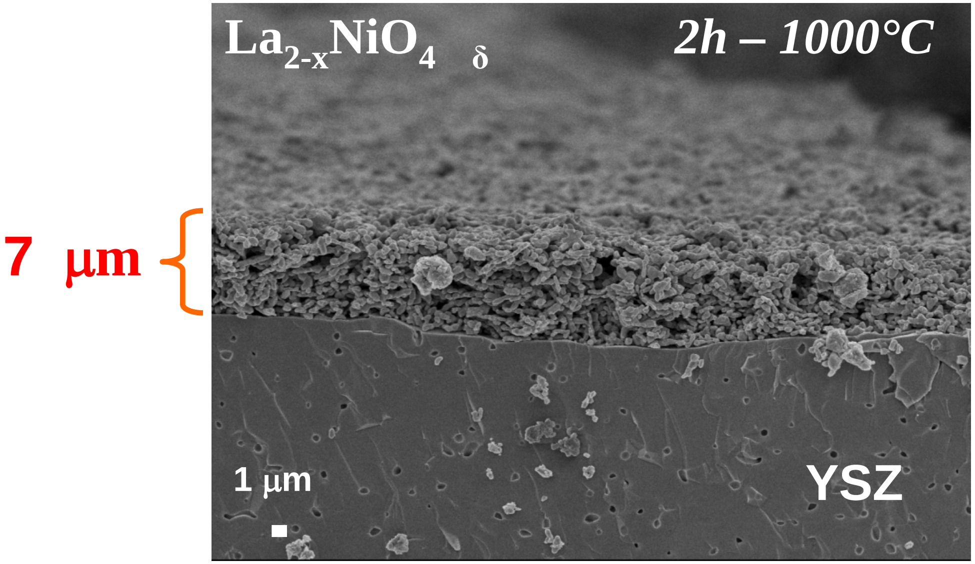


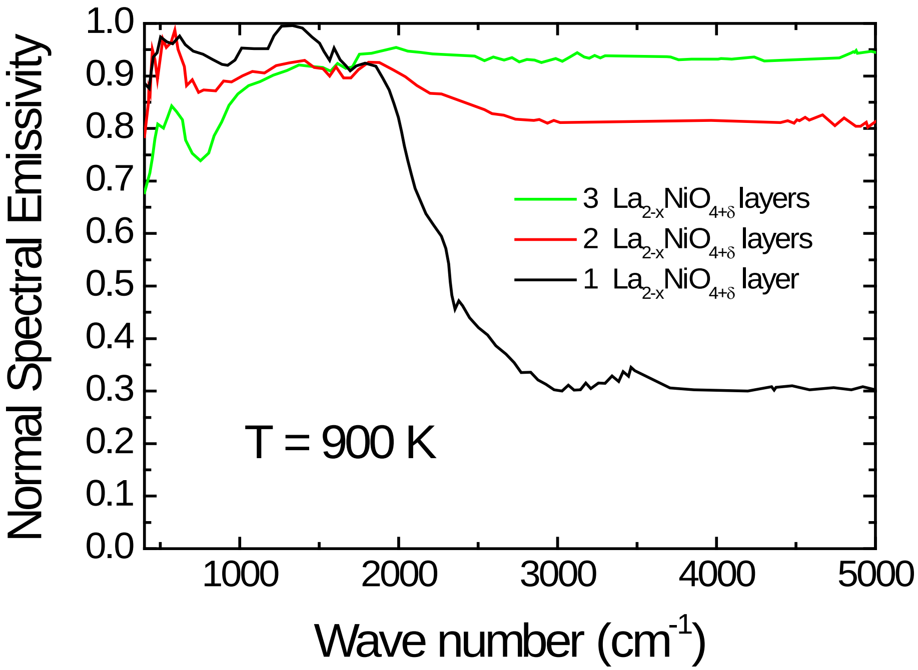
SOFC CATHODE

MIEC cathode







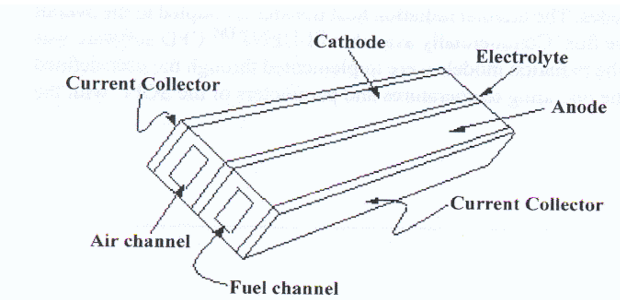


HEAT TRANSFER IN SOFC?

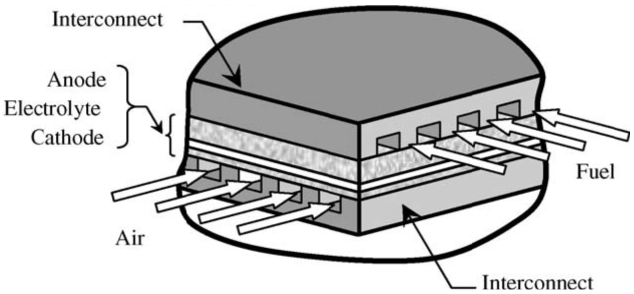
Thermo-mechanical failures in the ceramics used in the design of SOFC

Local temperature gradient at the interface of each component

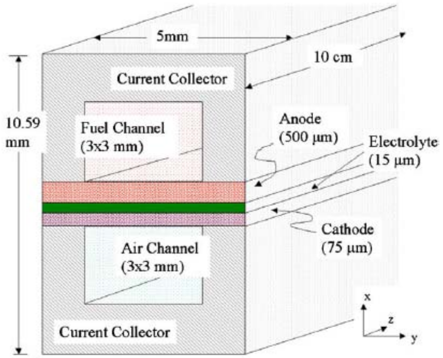
Prediction of the temperature field in the cell (ceramics+interconnects)



Murthy et al., J. Power Sources 2006



K.J. Daum et al. , J. Power Sources (2006)



Damm et al., Transaction of the ASME, 2005