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New results on losses correlation with structure

E. Coillet, V. Martinez, C. Martinet, A. Mermet

Institut Lumière Matière – Lyon, France

M. Granata, V. Dolique, C. Michel, B. Sassolas, G. Cagnoli,

Laboratoire des Matériaux Avancés – CNRS – Lyon, France

LABORATOIRE MATÉRIAUX AVANCÉS

Lyon 1

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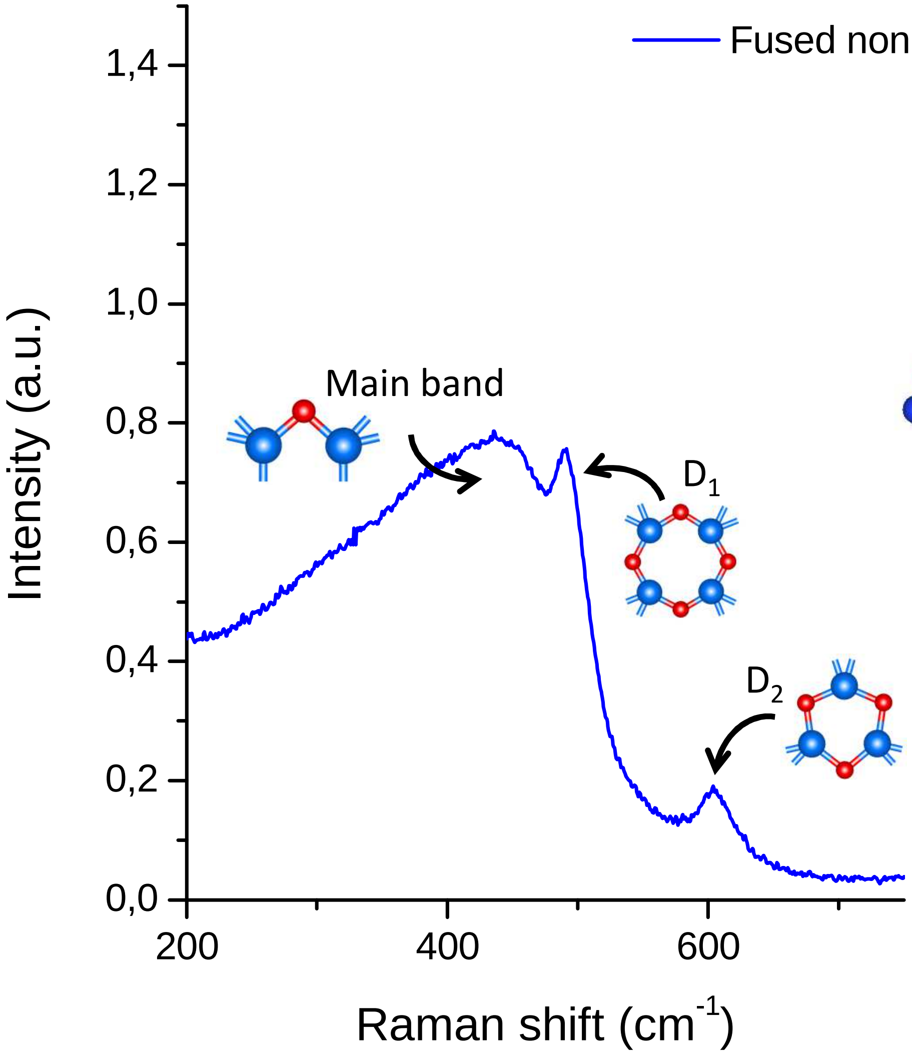
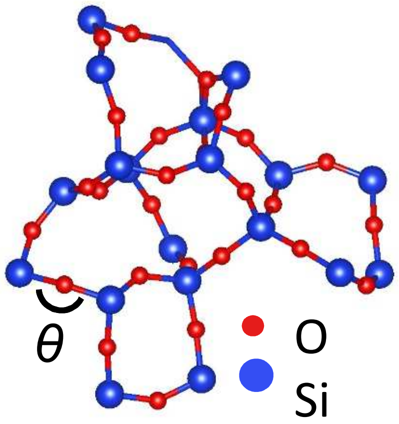
Outline

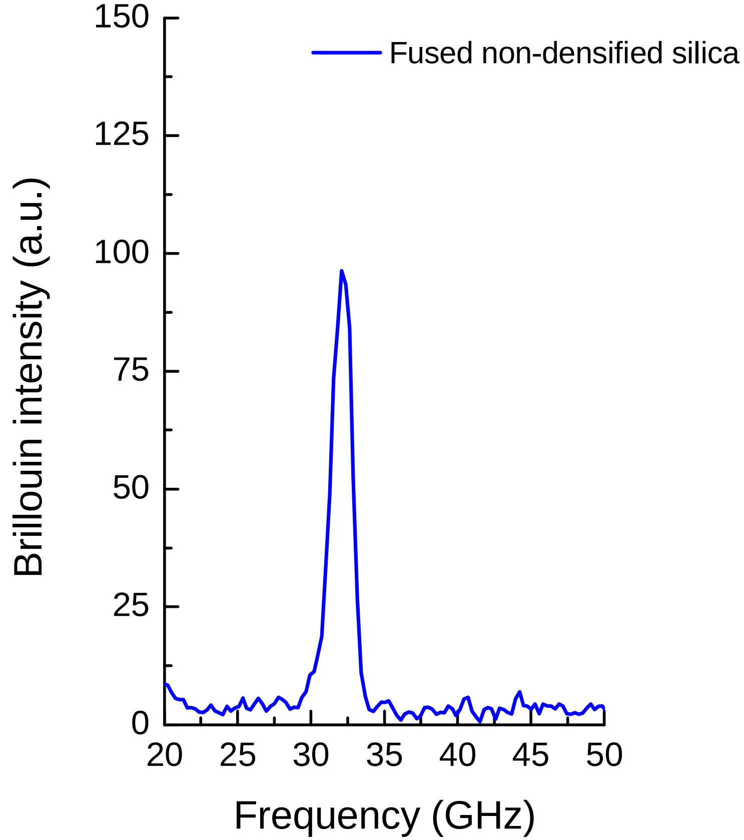
New results on the structure :

I. Silica coatings : Impact of the annealing
II. Silica coatings : Effect of the deposition parameters on the structure
III. Ta_2O_5 : effect of annealing
IV. Comparison between TiO_2 and Ta_2O_5 structures

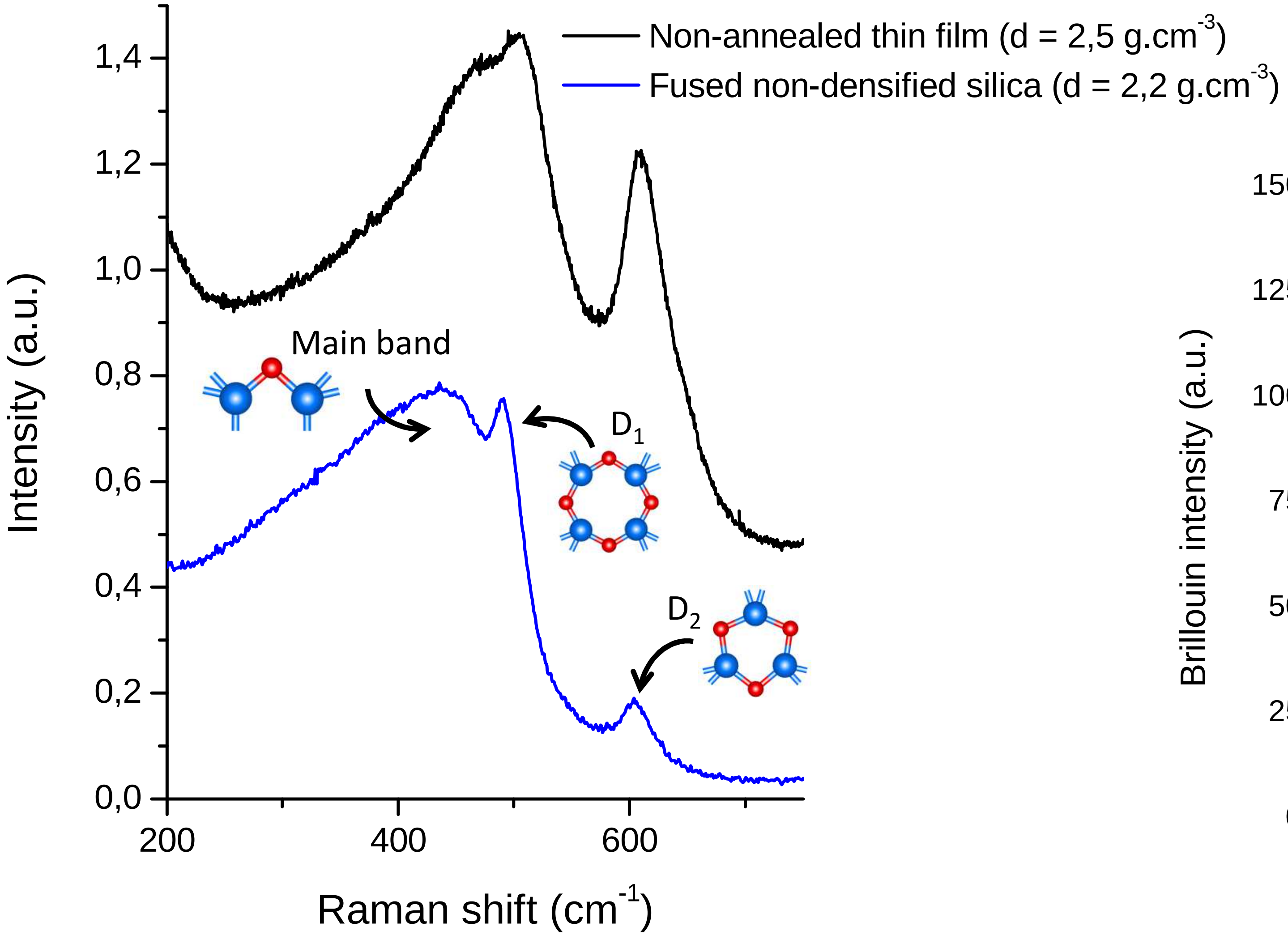
I - Fused silica

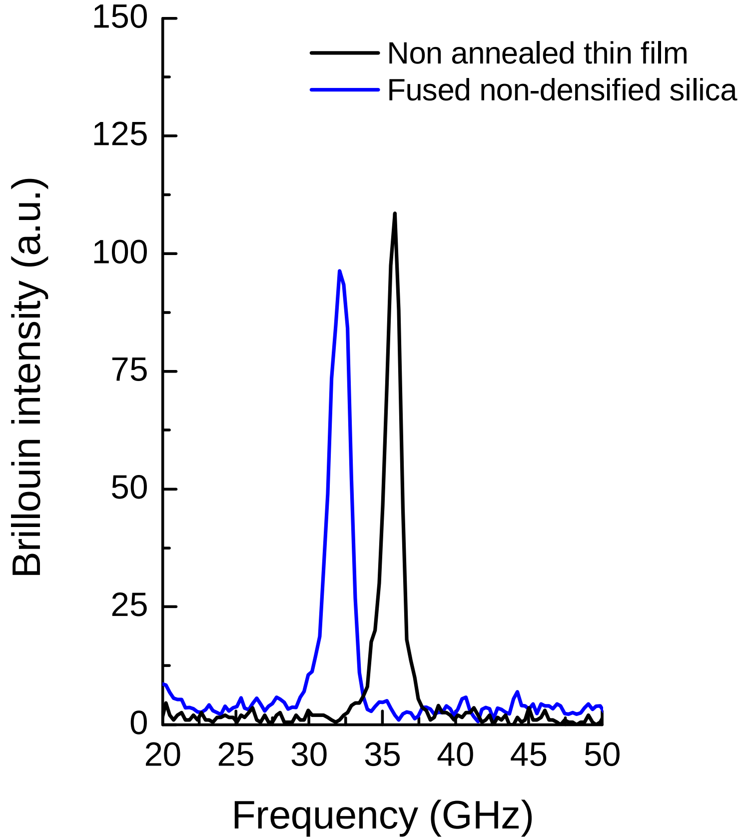






I - IBS silica coatings vs fused





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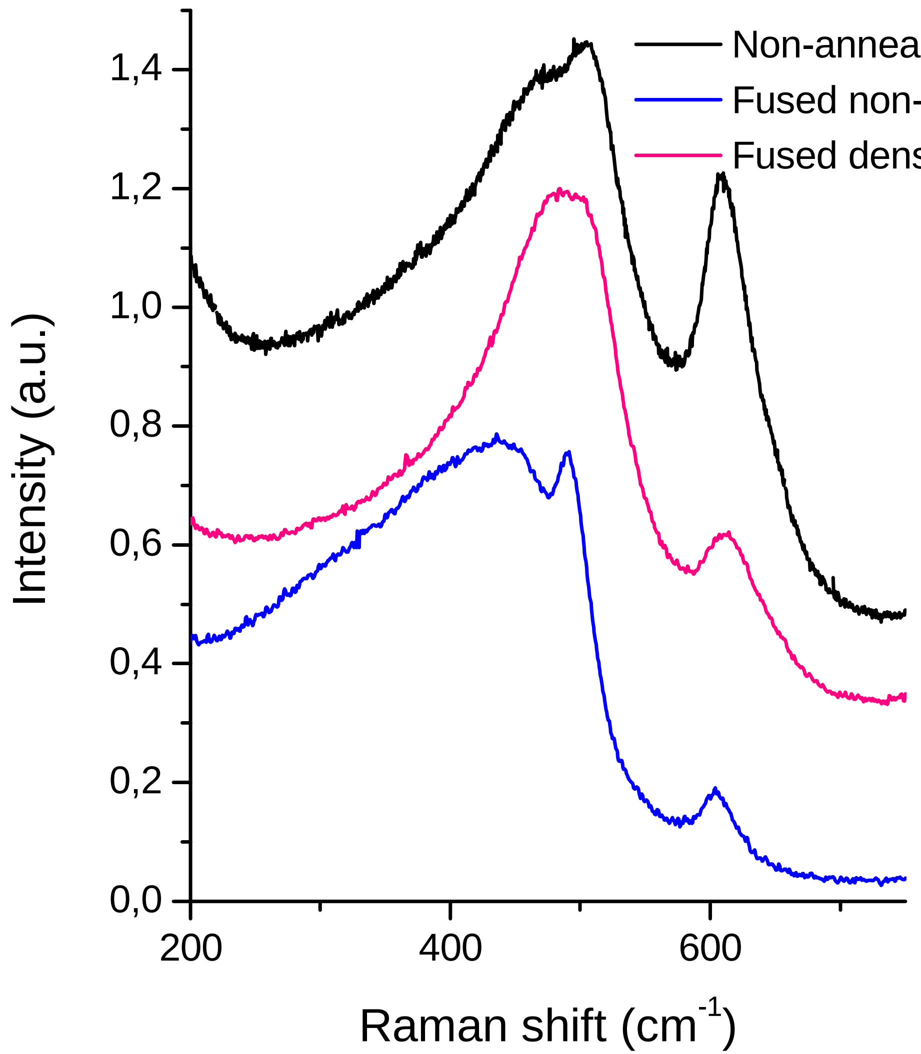
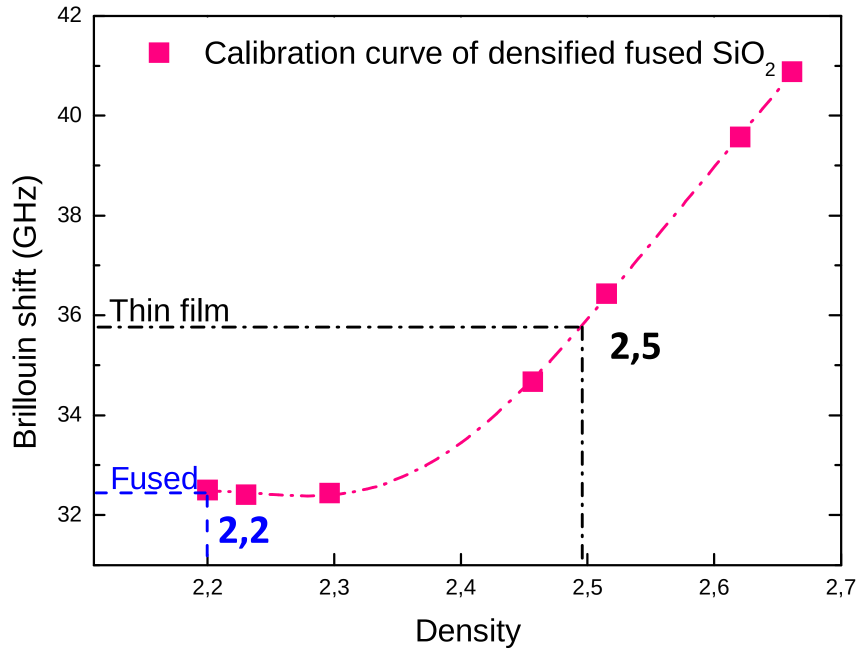
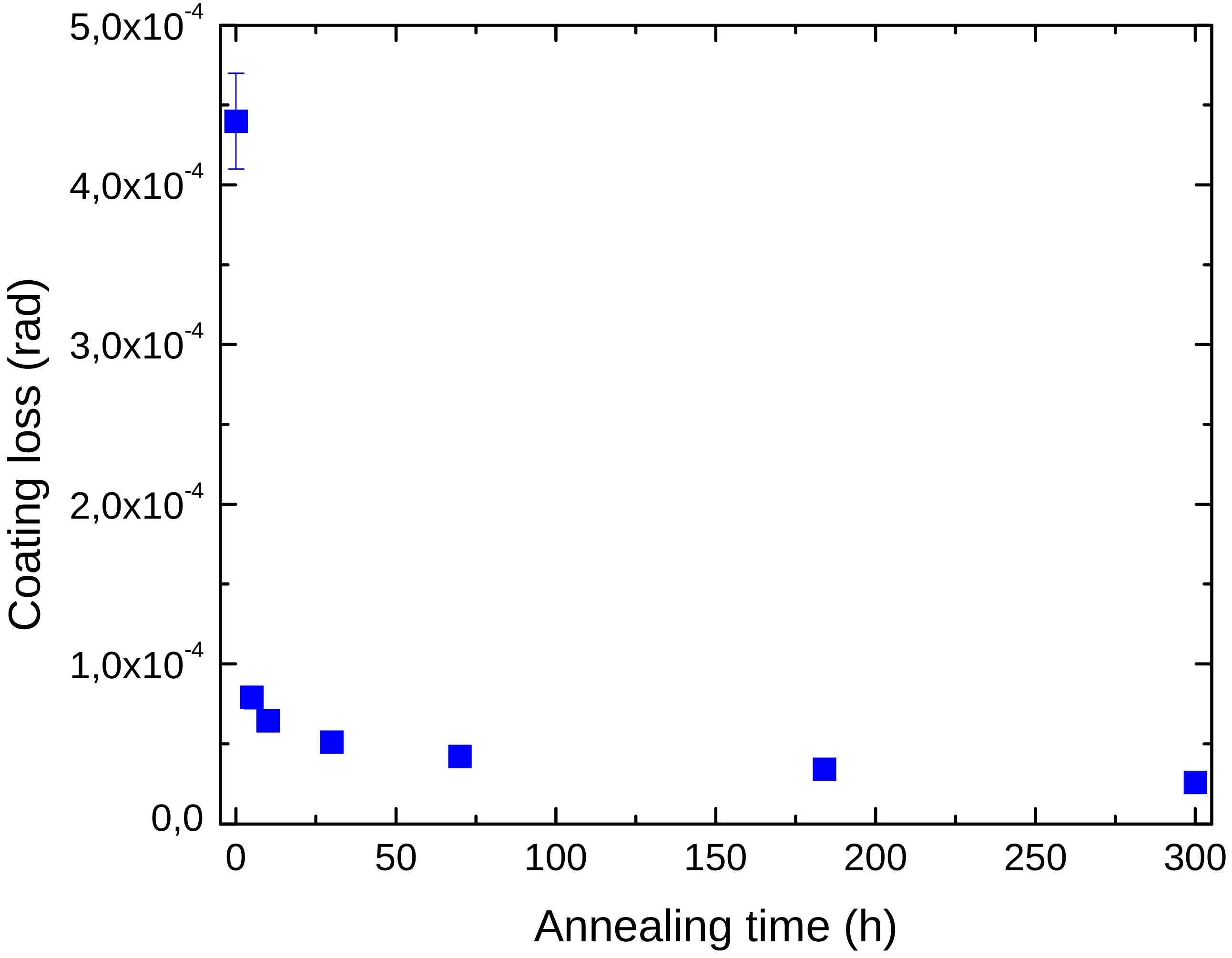




T. Deschamps, Scientific report (2014)

Structure of the Ion Beam Sputtered layers closer to densified silica

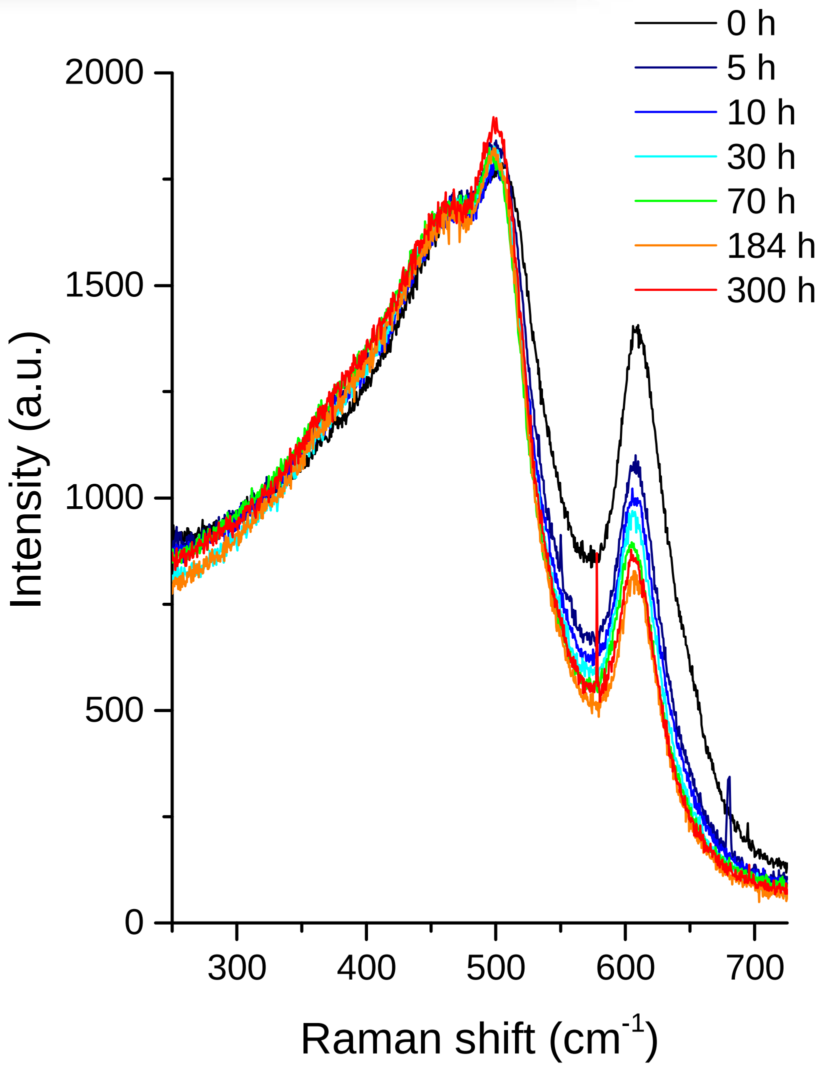
I - Silica coatings : effect of annealing



➡ Link with the structure ?

I - Silica coatings : effect of annealing

Annealing at T = 500 °C << T_g



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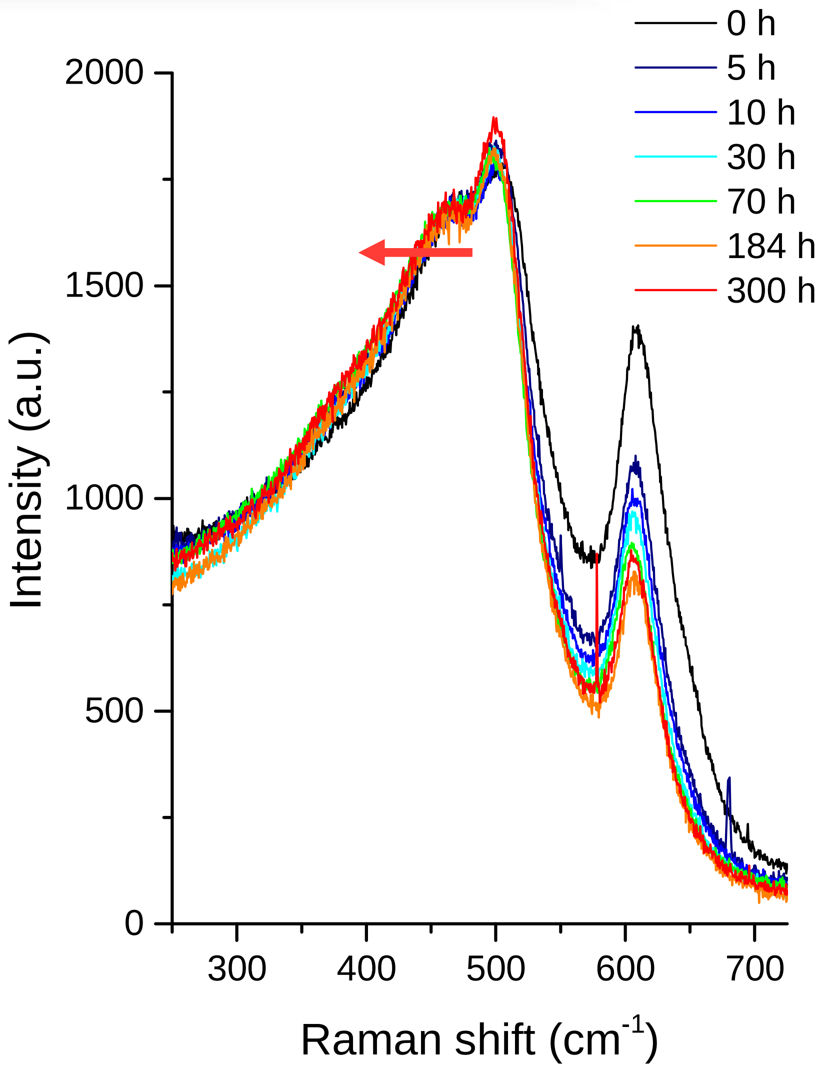

Shift of the main band position towards lower frequencies

⇨ Larger inter-tetrahedral angles

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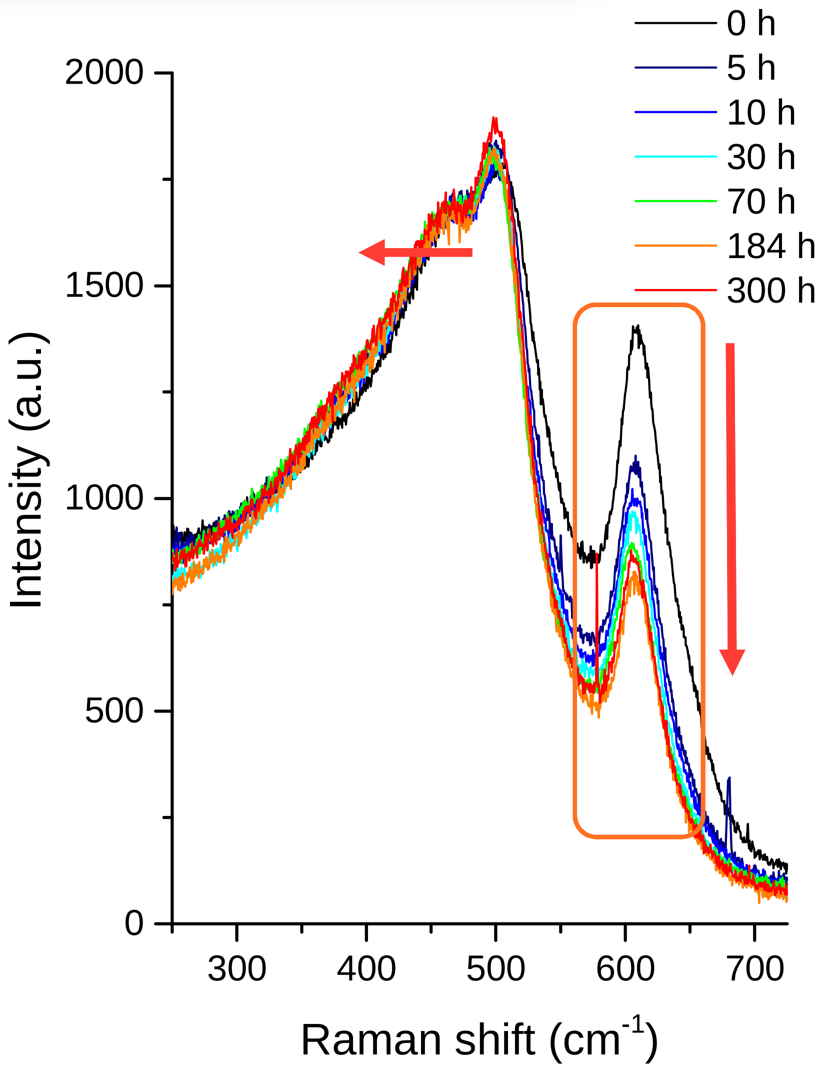

Shift of the main band position towards lower frequencies

⇨ Larger inter-tetrahedral angles

Decrease of the D_2 intensity

⇨ Less 3-membered rings

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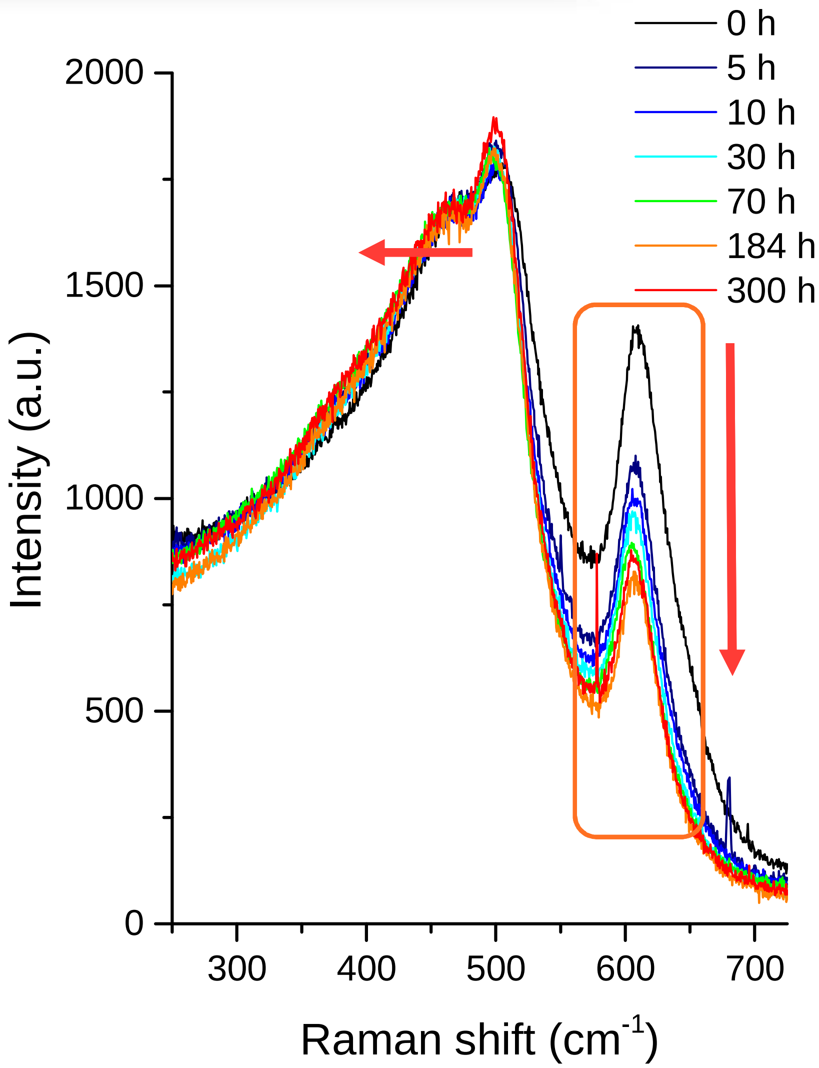

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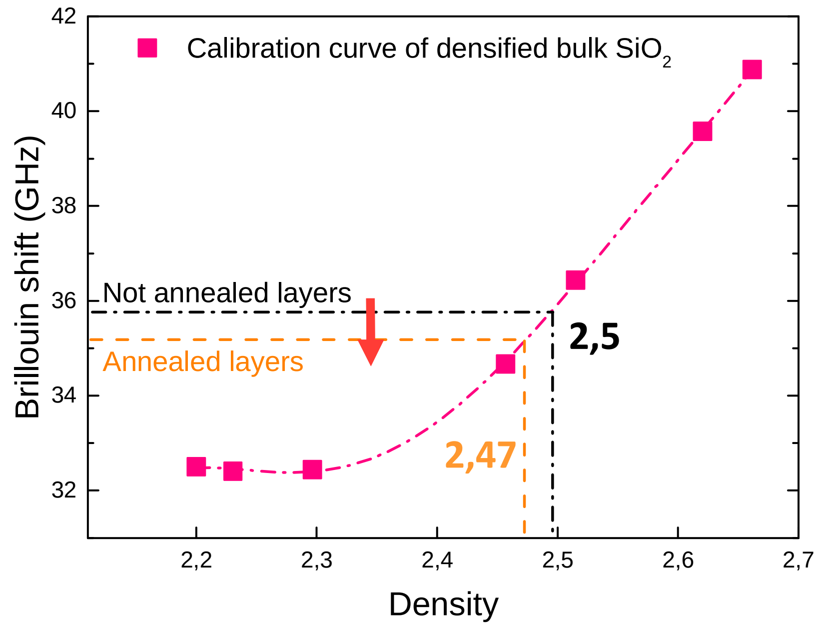

T. Deschamps, Scientific report (2014)

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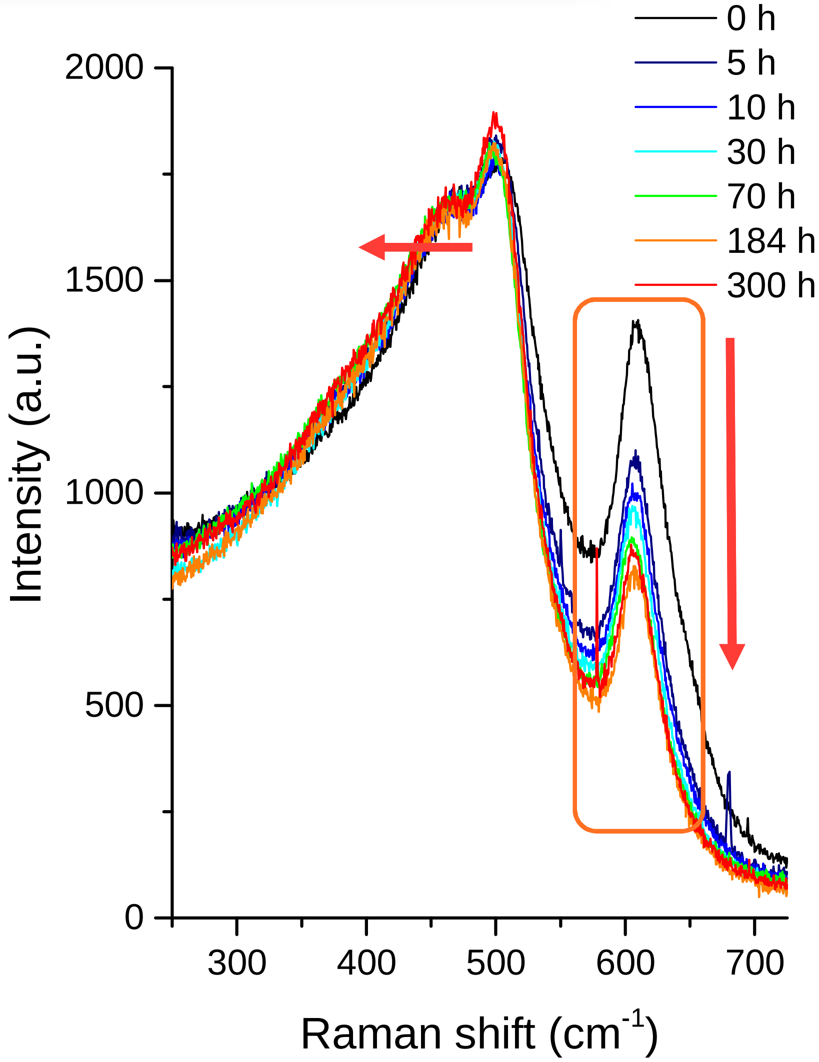

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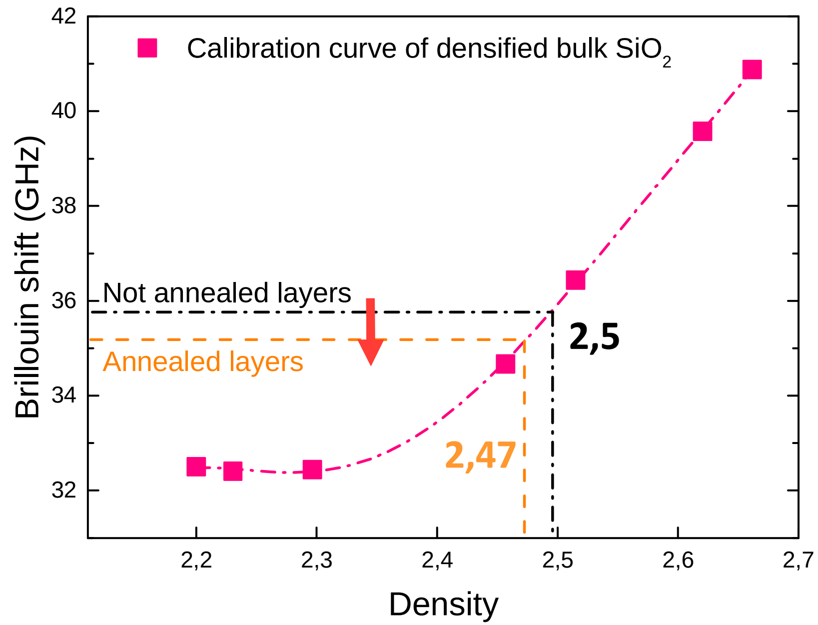
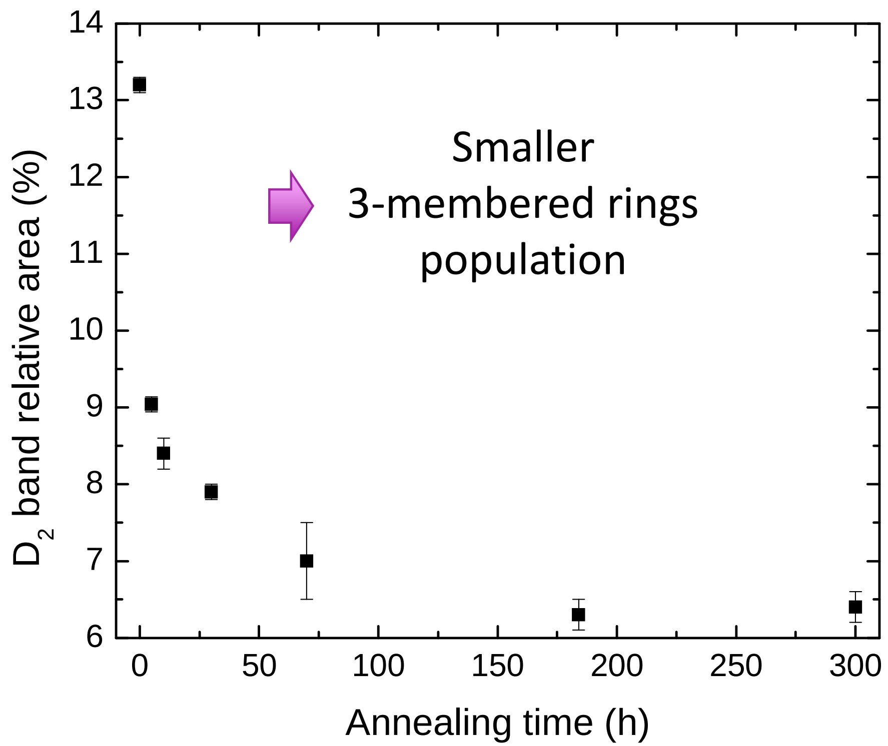
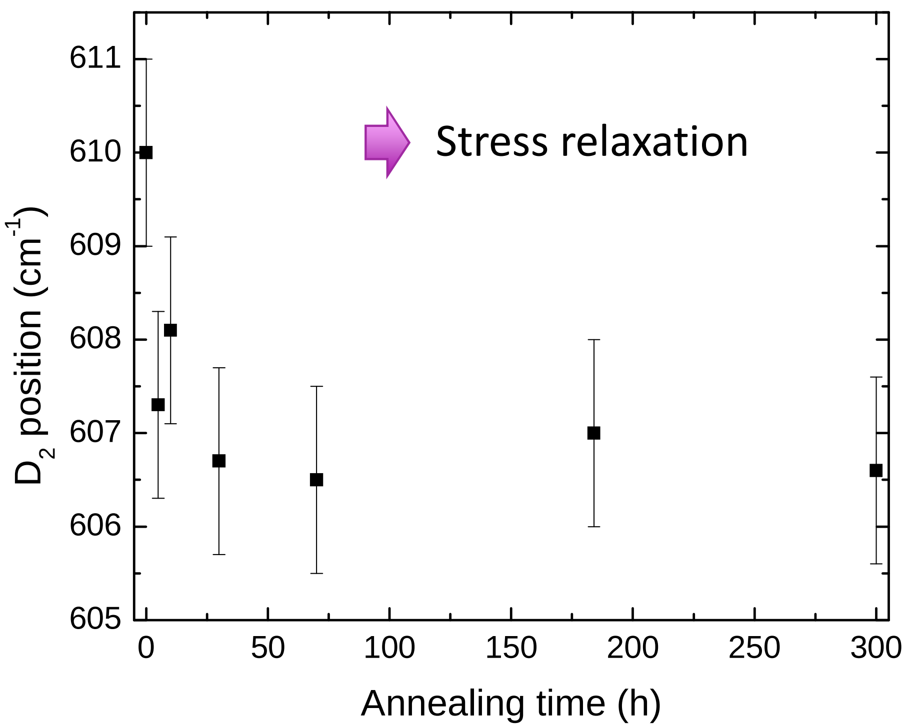


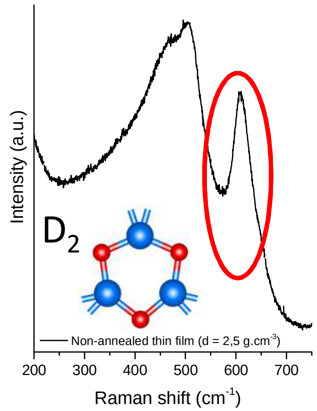
T. Deschamps, Scientific report (2014)

Relaxation of the structure with annealing toward a less dense thin film

Evolution of the Raman signatures





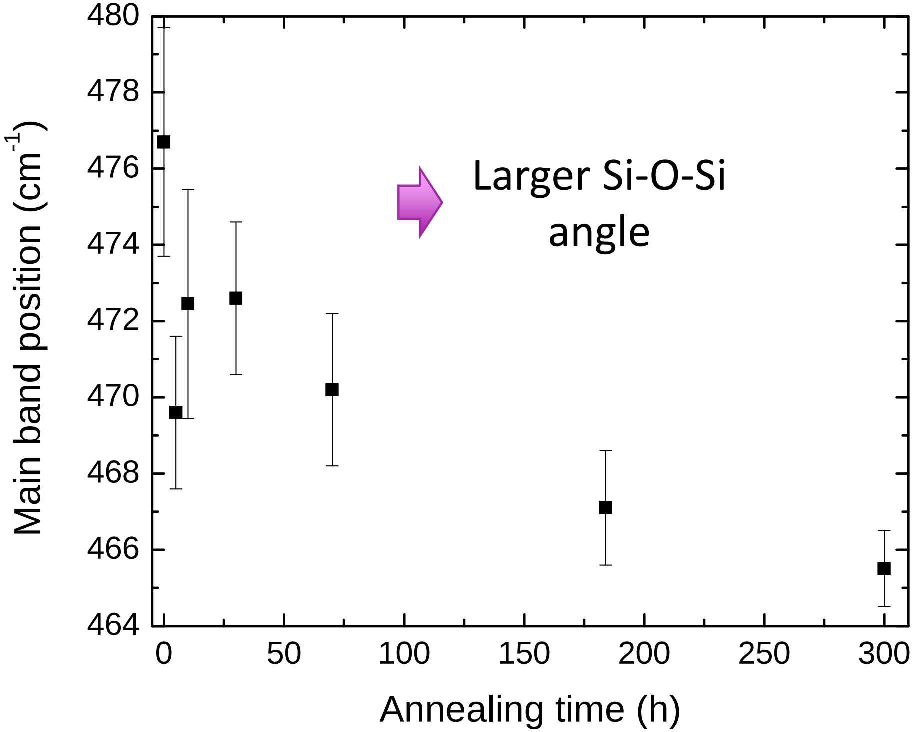


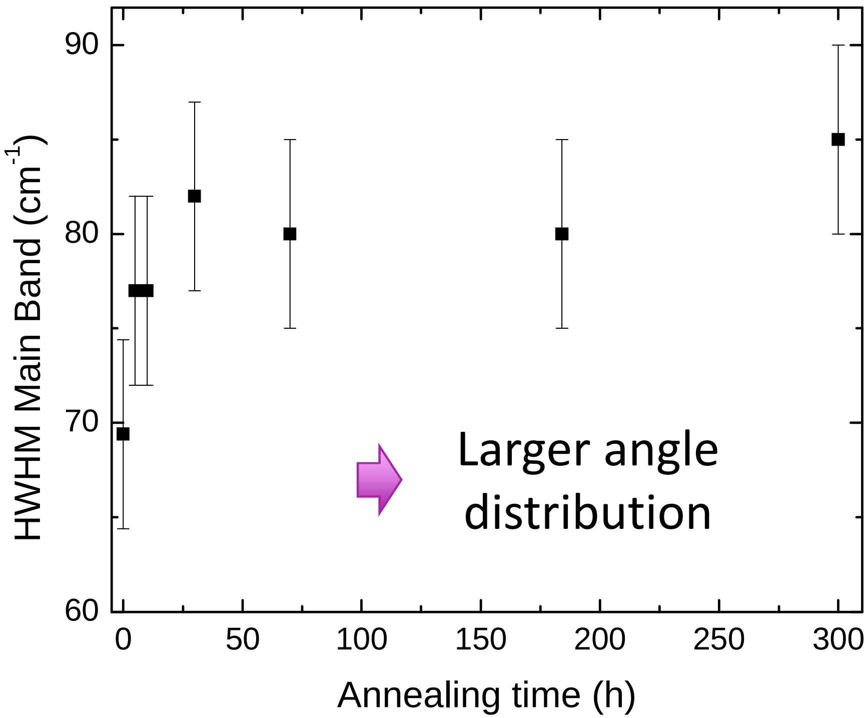
Fused SiO_2 :

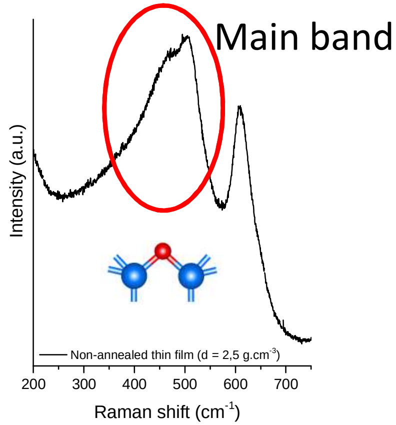
- **D2 band area = 3%**
- **D2 band position = 606 cm^{-1}**
- **Main band position = 435 cm^{-1}**
- **Main band HWHM = 110 cm^{-1}**

I - Silica coatings : effect of annealing

Evolution of the Raman signatures







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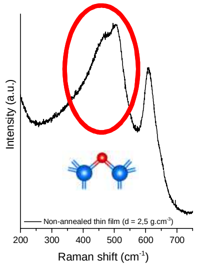
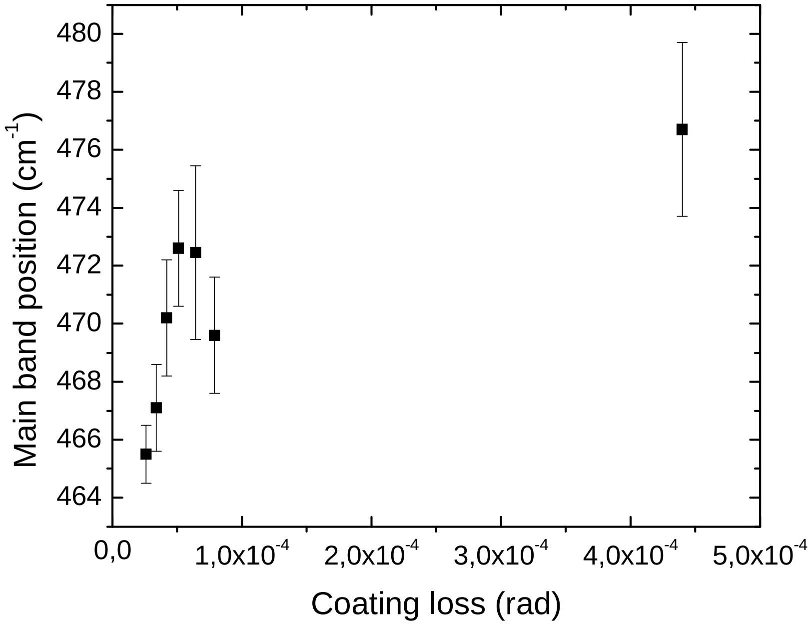
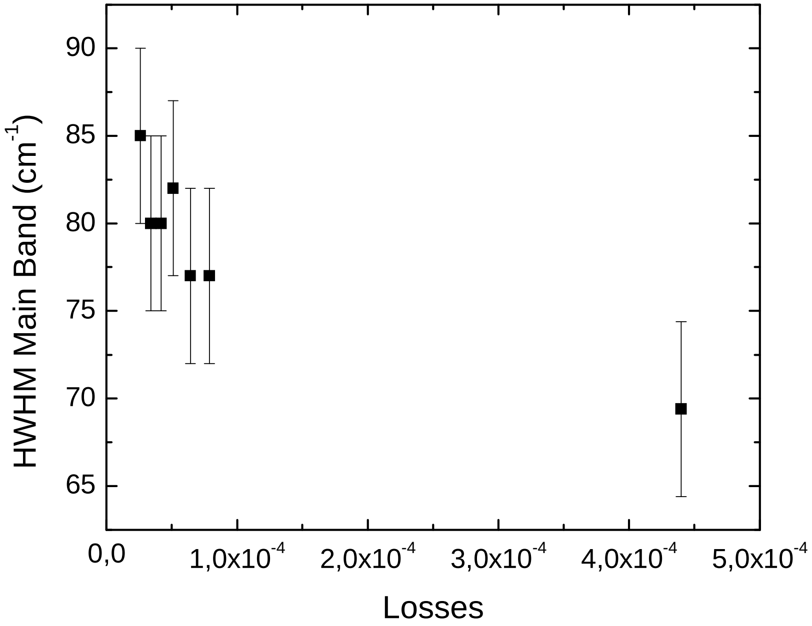
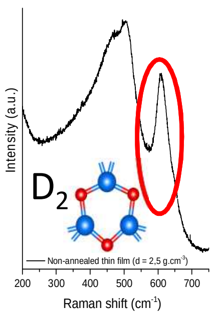
I - Silica coatings : effect of annealing

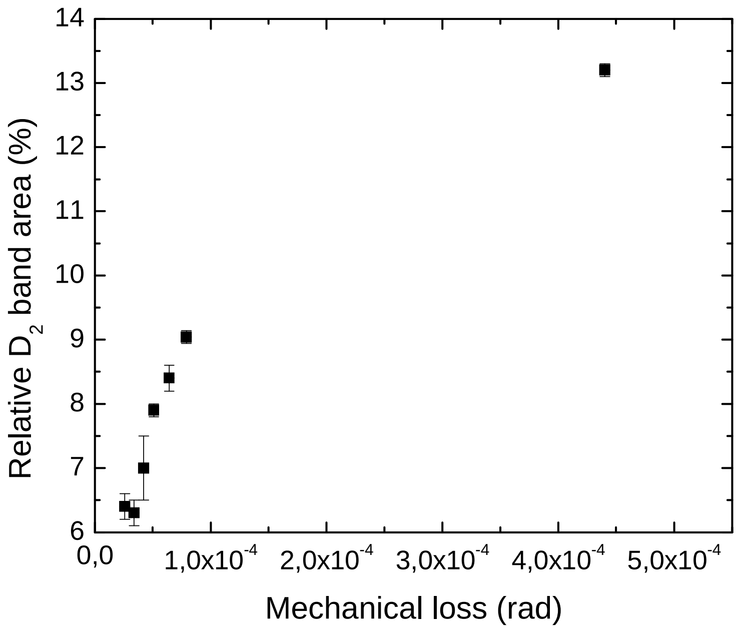
Link between coating loss and structure











Clear correlation between the 3-membered rings population and the coating loss

I - Silica layers : Annealing

Link between coating loss and structure

- Denser structure of the layers compare to fused silica
- Annealing leading to a more relaxed structure and loss decrease

<u>Origin of the loss by modelisation</u>

- *Anderson et al* :
  lateral motion of O perpendicularly to Si-O bonds
- *Hamdan et al (2014)* :
  tetrahedral chain rearrangement via rotation and stretching of Si-O bonds (10 to 100 atoms)

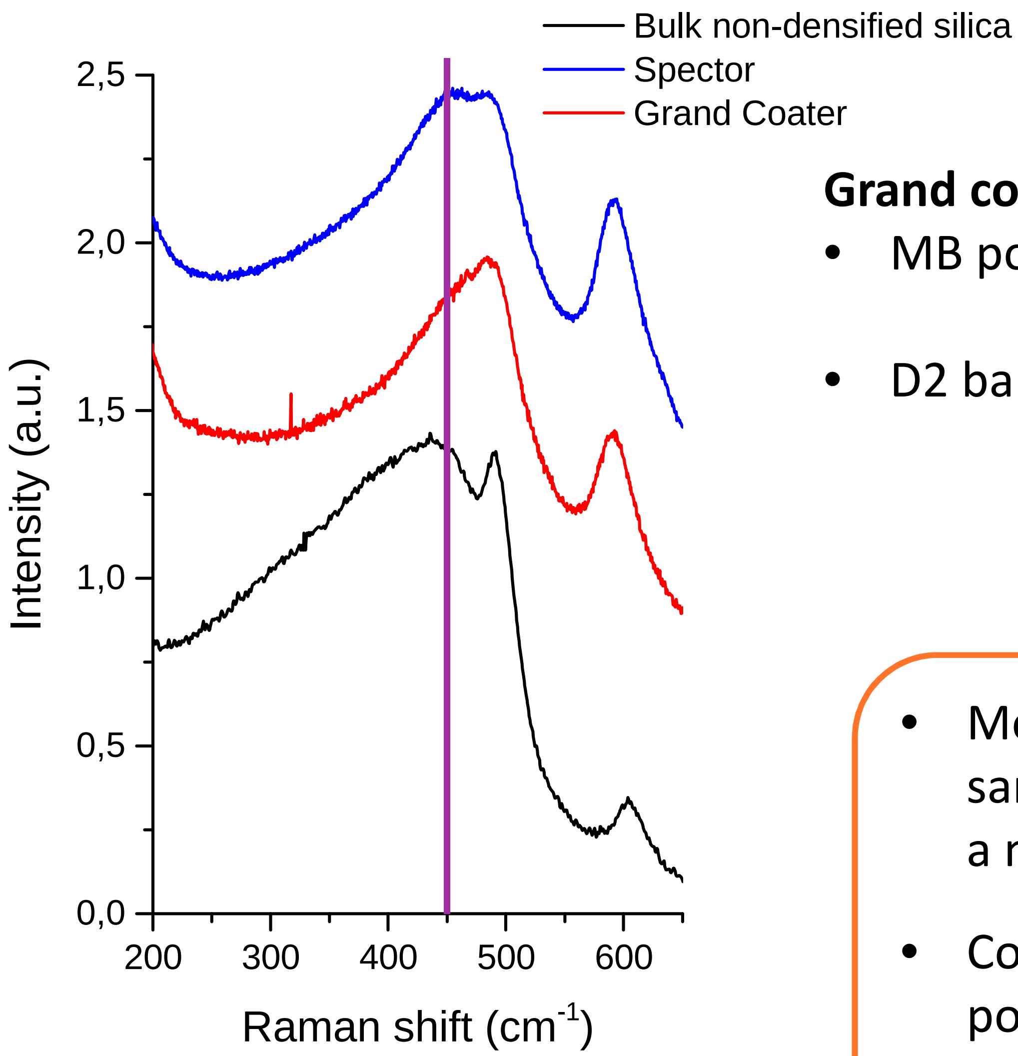
➡ Structural modifications needing low activation energy : available at T << T_g

<u>Info given by Raman spectroscopy</u>

- *D_2 band : 3-membered rings breathing mode*
  - Area decrease : smaller 3-fold population -> stress relaxation

➡ Relation between 3-fold rings and two level systems (TLS) energy landscape ?

II - Effect of the deposition parameters on the structure



Grand coater compared to Spector :

- MB position Grand Coater **>** Spector
  - ⇨ Smaller inter tetrahedral angles
- D2 band area Grand Coater **<** Spector
  - ⇨ Smaller 3-membered ring population

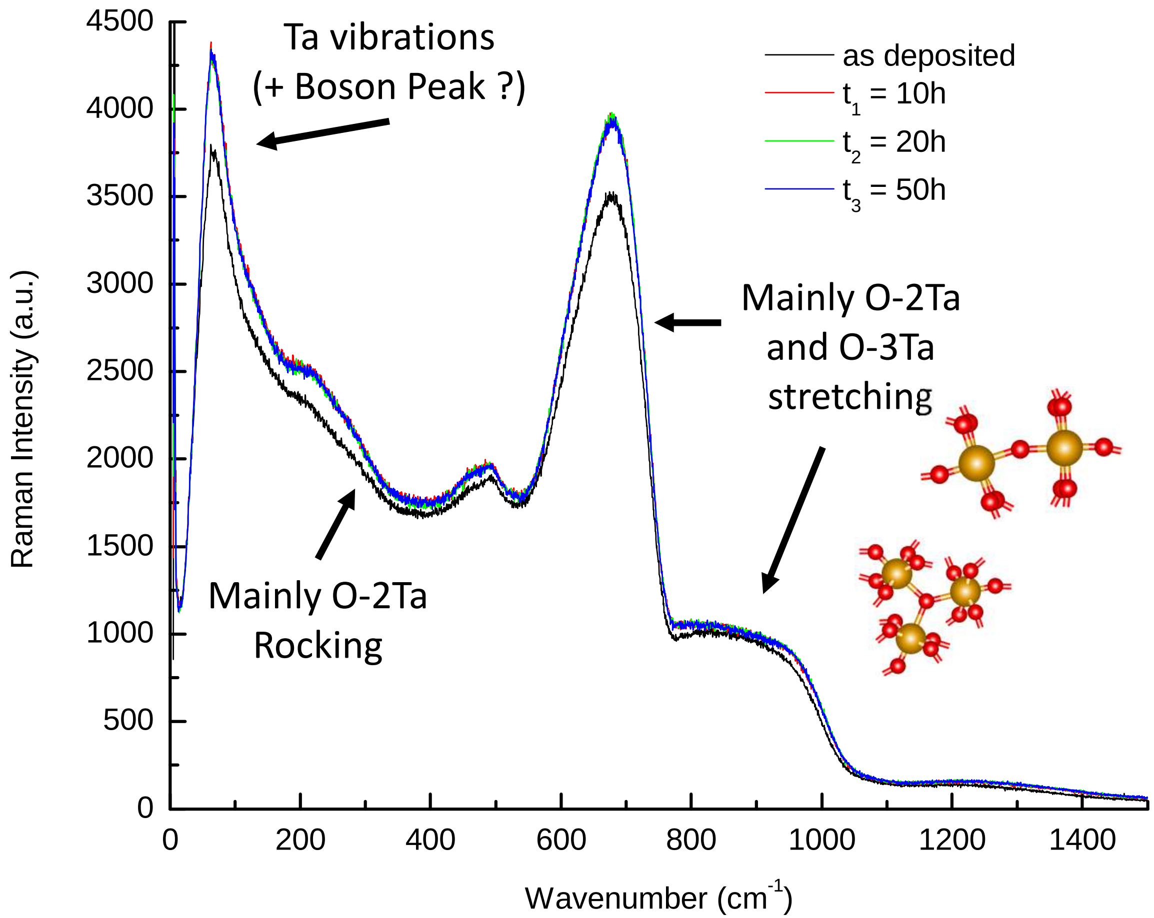
- Mechanical loss of Grand Coaster sample lower than Spector : linked with a more "relaxed" structure
- Correlation between 3-membered rings population and mechanical losses as seen with annealing.

II – Silica coatings

- Structural relaxation of the amorphous silica coating with annealing towards less dense glass
- Correlation between the mechanical losses and the 3-membered rings population
- Important impact of deposition parameters on the amorphous silica layers

What about Ta_2O_5 layers ?

III - Ta_2O_5 coatings : Evolution with annealing



Average coordination number in Ta_2O_5 :

Tantalum	%	Oxygen	%
Coord. 4	0.5	Coord. 2	69.9
Coord. 5	28.5	Coord. 3	30.1
Coord. 6	69.4		
Coord. 7	1.6		

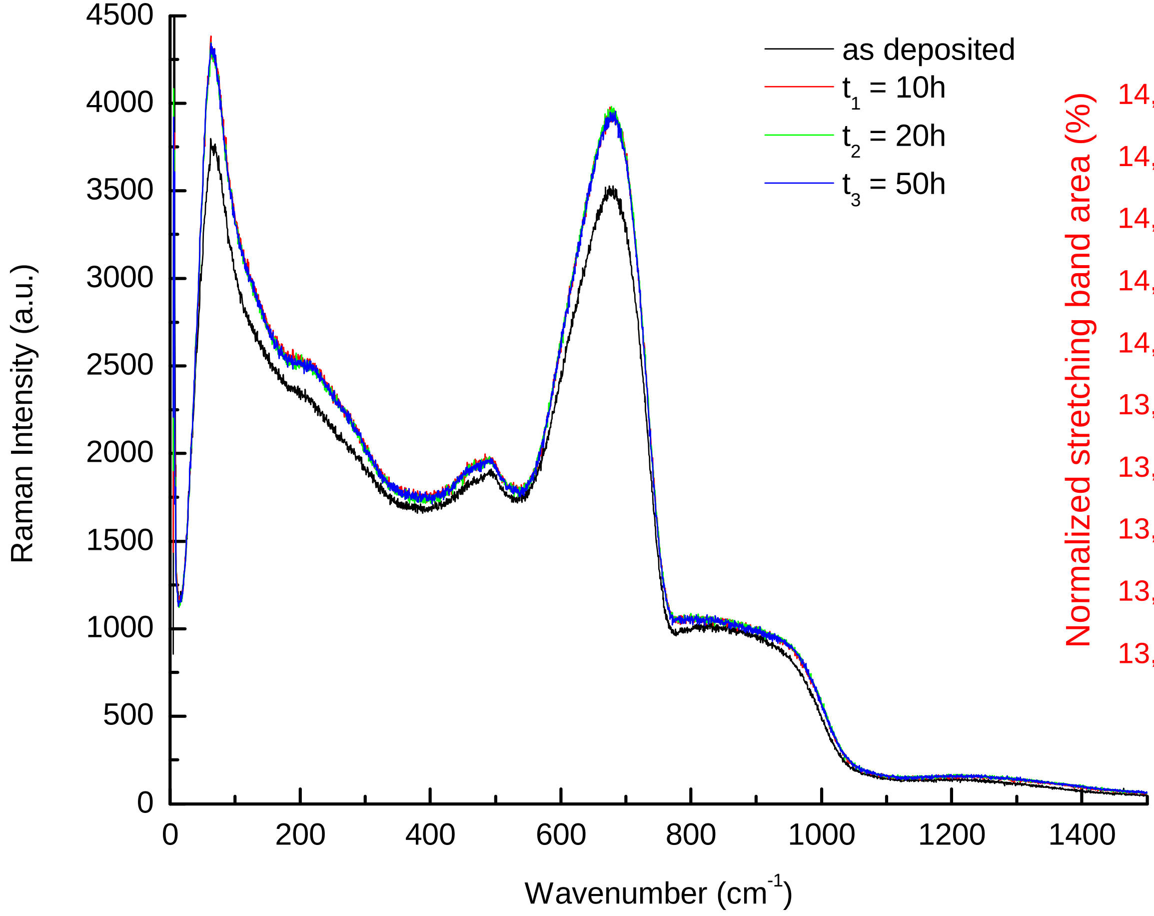
Coordination and band attribution done by the simulation group at the ILM.

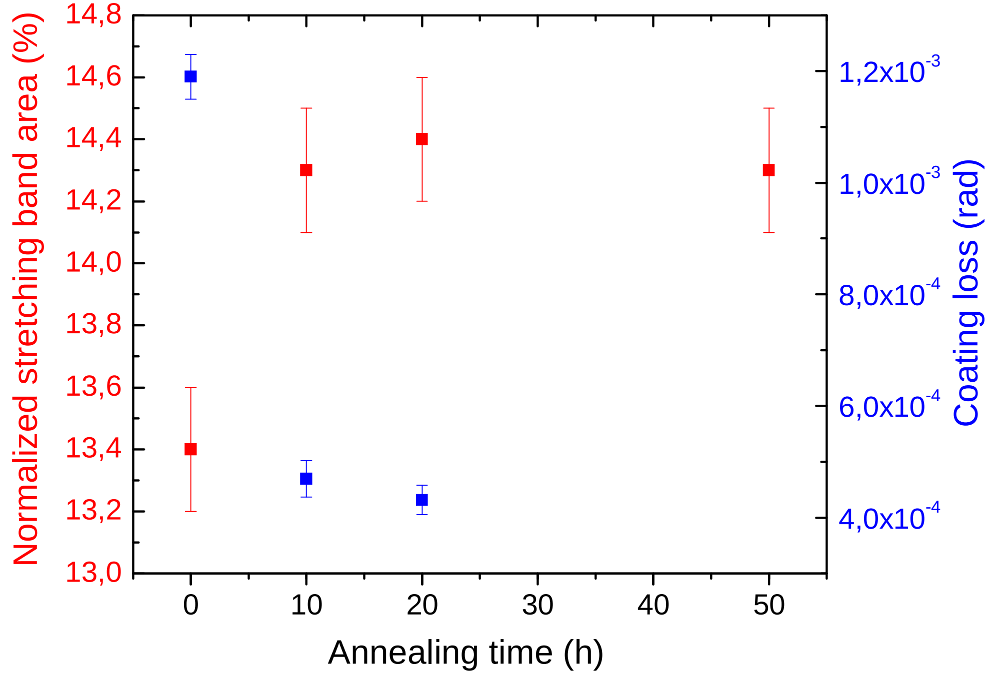
T. Damart et al., JAP **119** (2016)

Glass unknown in the fused state

III - Ta_2O_5 coatings : Evolution with annealing

T = 500 °C





- Similar evolution with coating loss
- Less structural evolution visible on the Raman spectrum than in silica glass

Need to better understand the structure and its possible evolutions

IV - Comparison between TiO_2 and Ta_2O_5 structures

<u>Amorphous TiO_2 structure close to that of Ta_2O_5</u>

Damart et al., JAP (2016) Ta_2O_5

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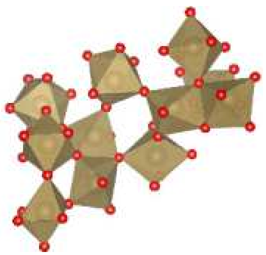
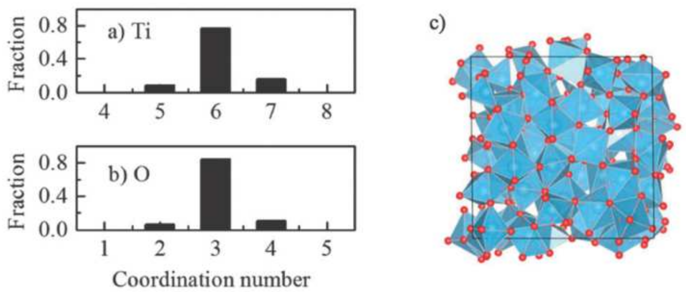
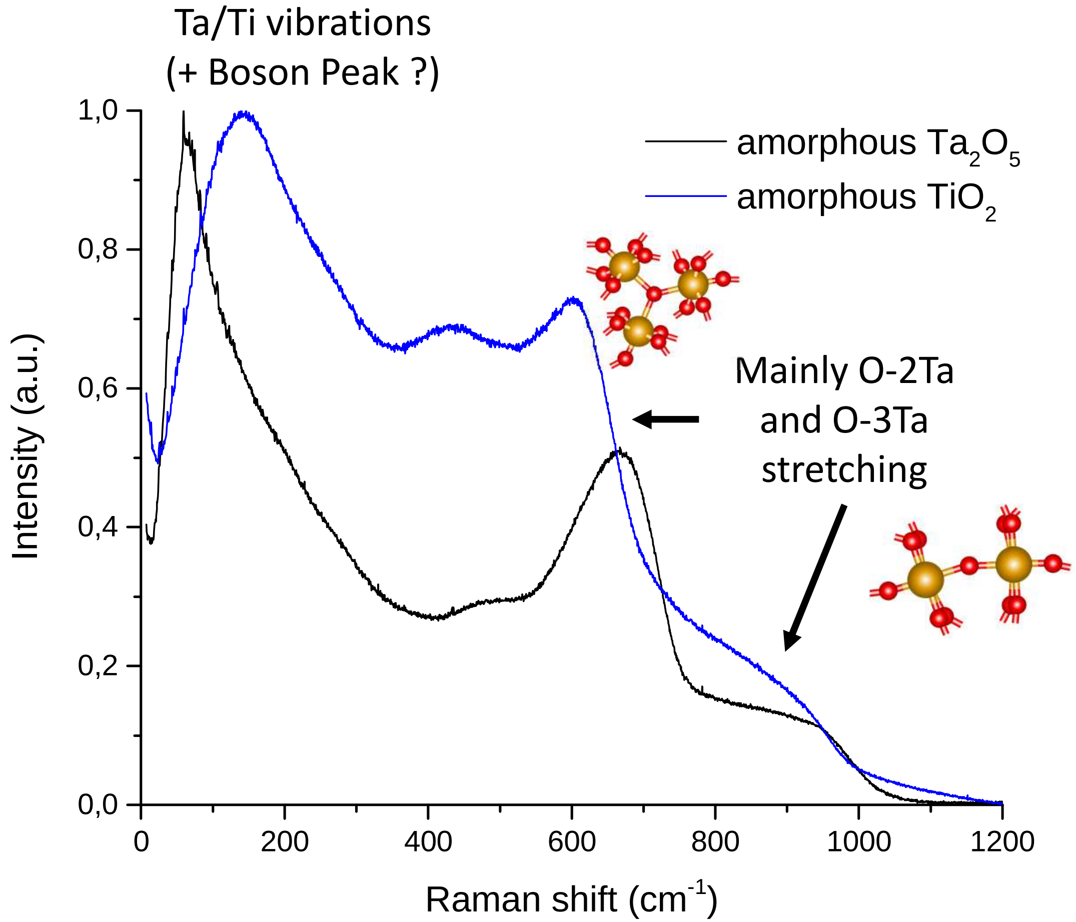


Pham et Wang, PCCP (2015) TiO_2





Cristalline phase associated with a-TiO_2 : anatase

Conclusion

Understand the link between the mechanical losses and the structure

- Vibrational spectroscopies : useful tool to probe the structural evolution of thin films
- Correlation between mechanical losses and the 3-membered rings population
- Importance of the deposition parameters on the structure and on the mechanical losses

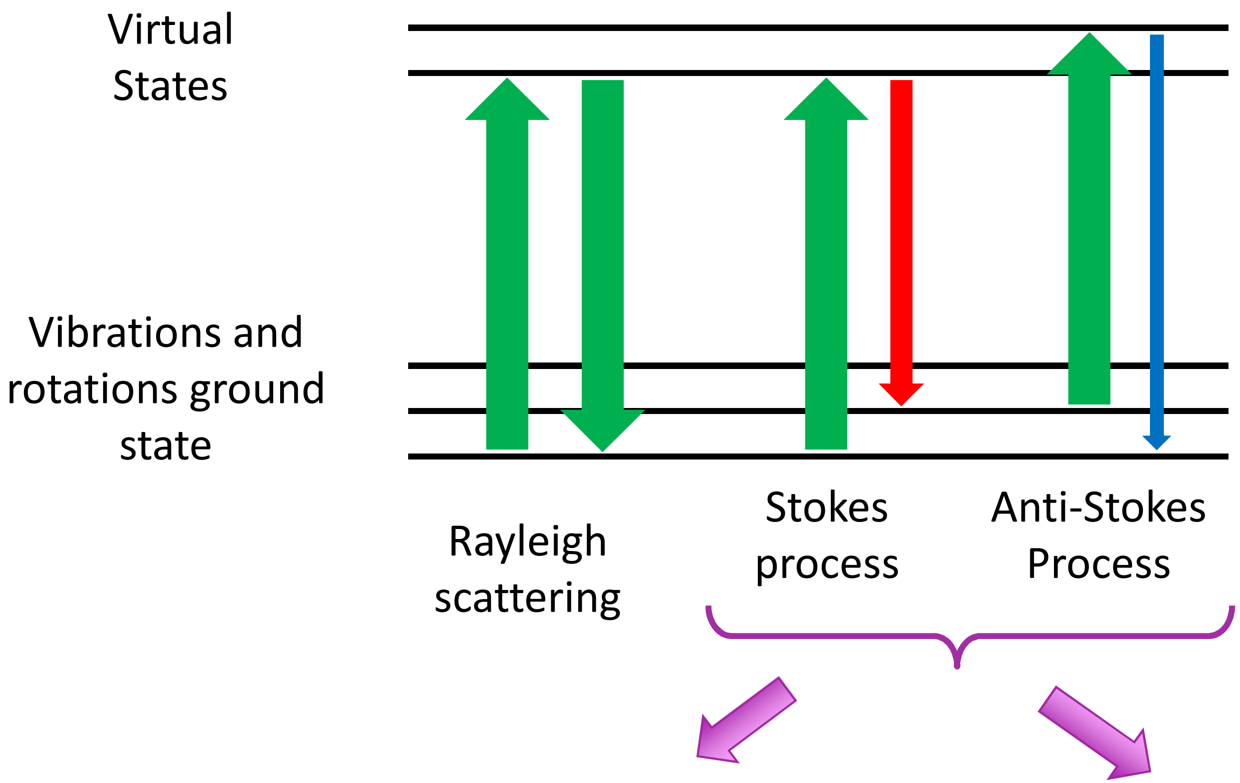
Perspectives :

- Effect of different doping on the structure
- Effect of the deposition temperature

Vibrational spectroscopies

RAMAN BRILLOUIN

Based on **inelastic scattering** of a **monochromatic** incident radiation



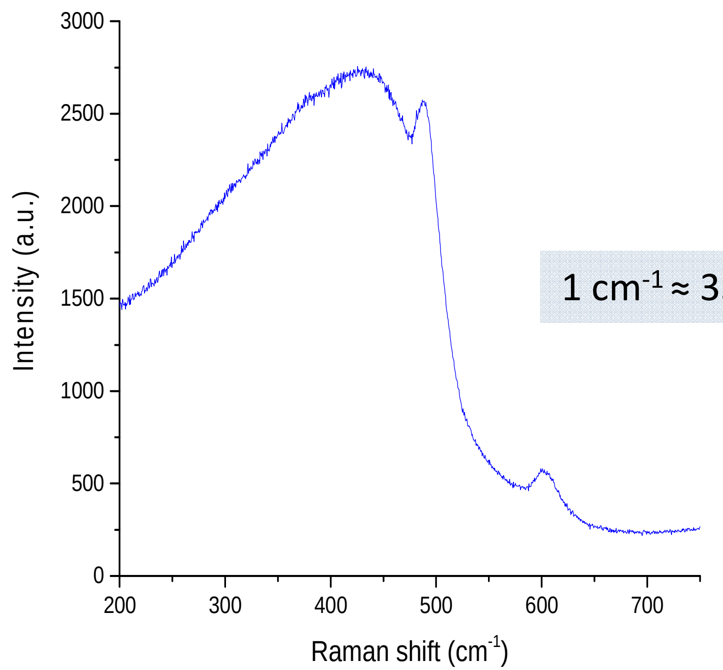
Raman scattering arises from fluctuations of polarizability

Brillouin scattering arises from fluctuations of dielectric susceptibility

Vibrational spectroscopies

Raman spectroscopy

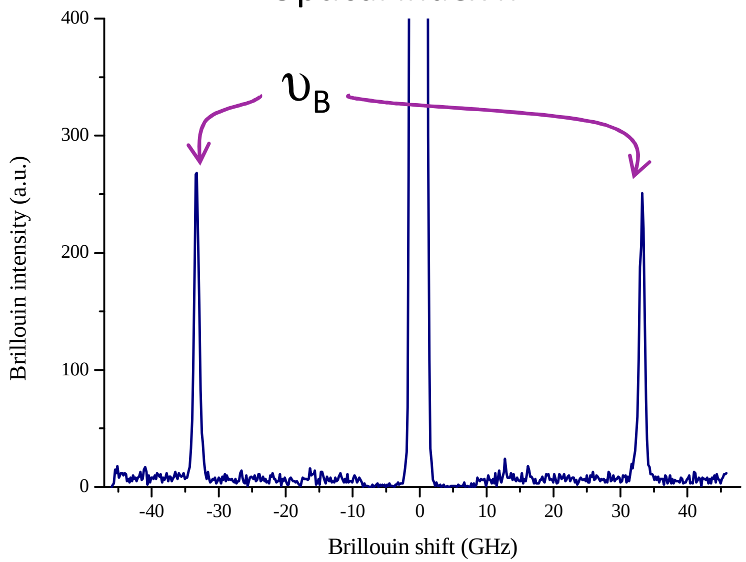
- Optical Modes
- Frequency shift ν > 10 cm^{-1}
- Structural information at short and medium range order (1-20 Å)



Brillouin spectroscopy

- Acoustic Modes
- Frequency shift ν ≈ 1 cm^{-1}
- Continuous media
- Macroscopic properties :
  - Sound velocity V_L
  - Elastic moduli
  - Density d
  - Optical index n

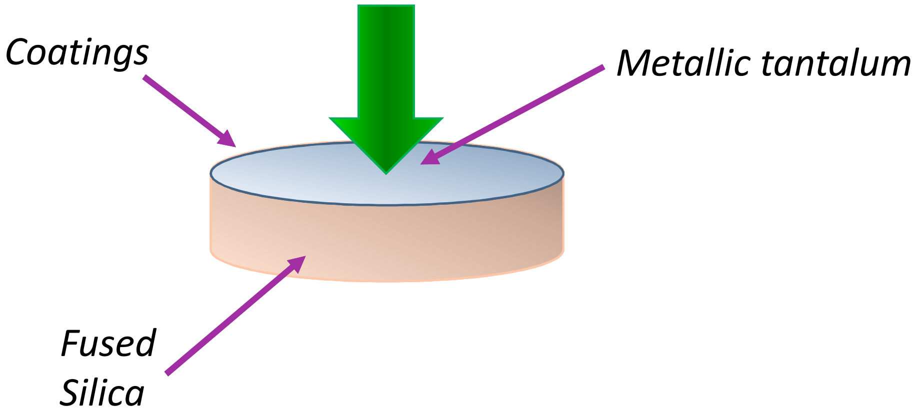
$$V_L = \frac{\lambda_0 \upsilon_B}{2n}$$



Both give information on the structural evolution f(Temperature, Pressure)

Experimental

- Monolayers of SiO_2 or Ta_2O_5 around 1 and 3 µm thick
- Deposited by Ion Beam Sputtering at the LMA in Lyon
- Mechanical losses and vibrational spectra measured on the same layers



Tantalum oxide layers

Average coordination number in Ta2O5

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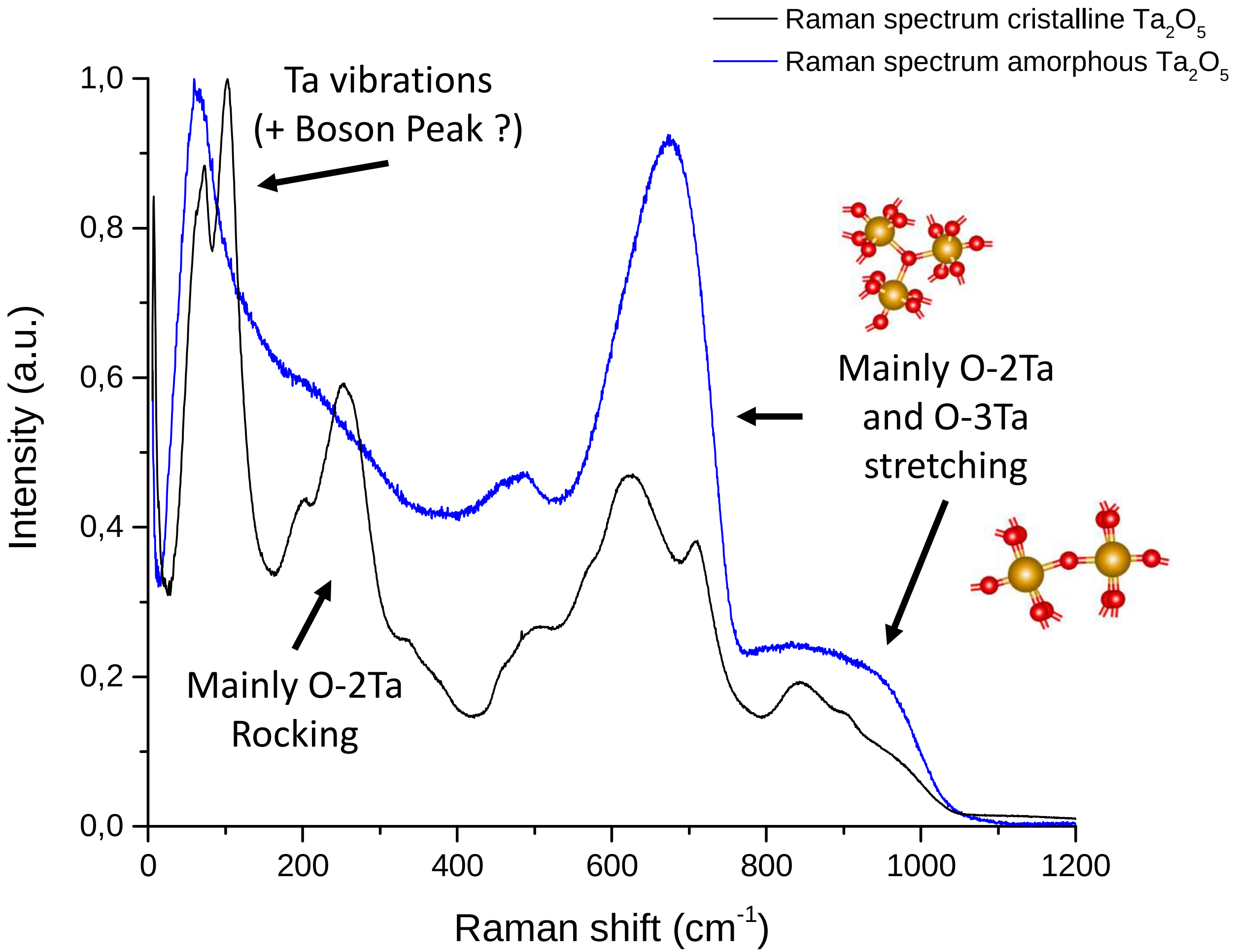
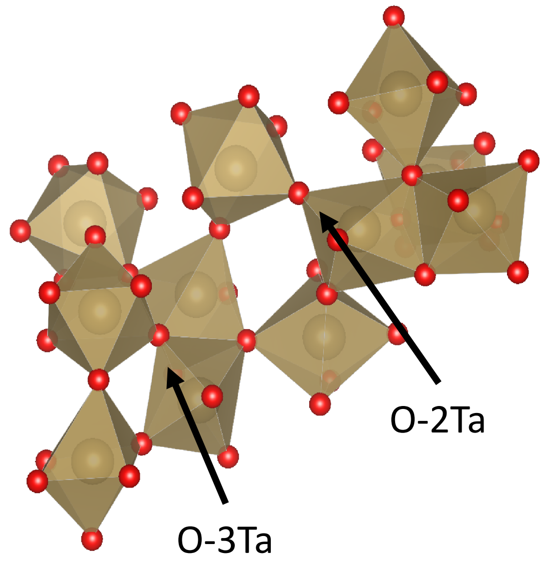




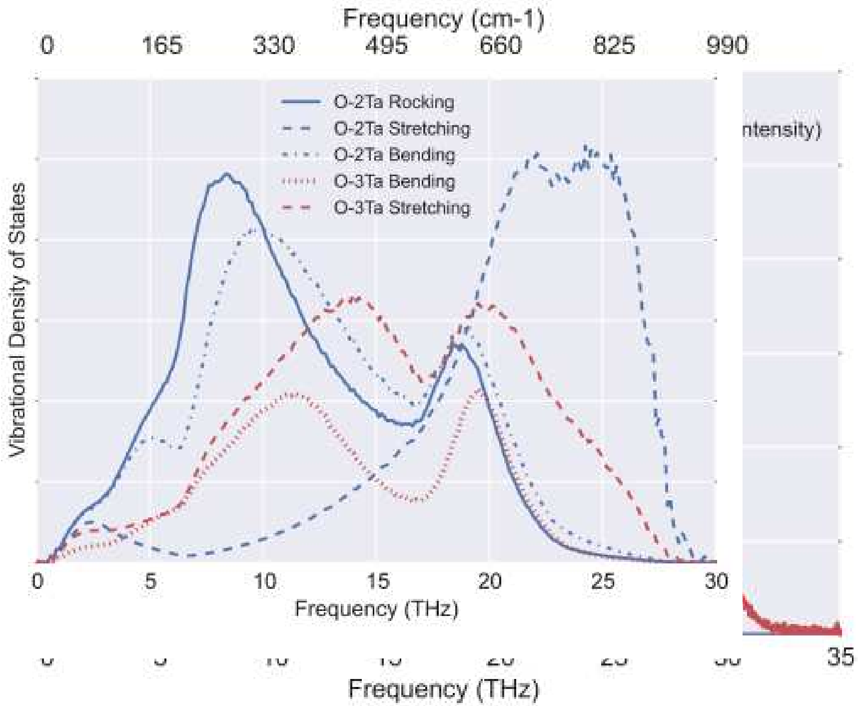
Glass unknown in the fused state

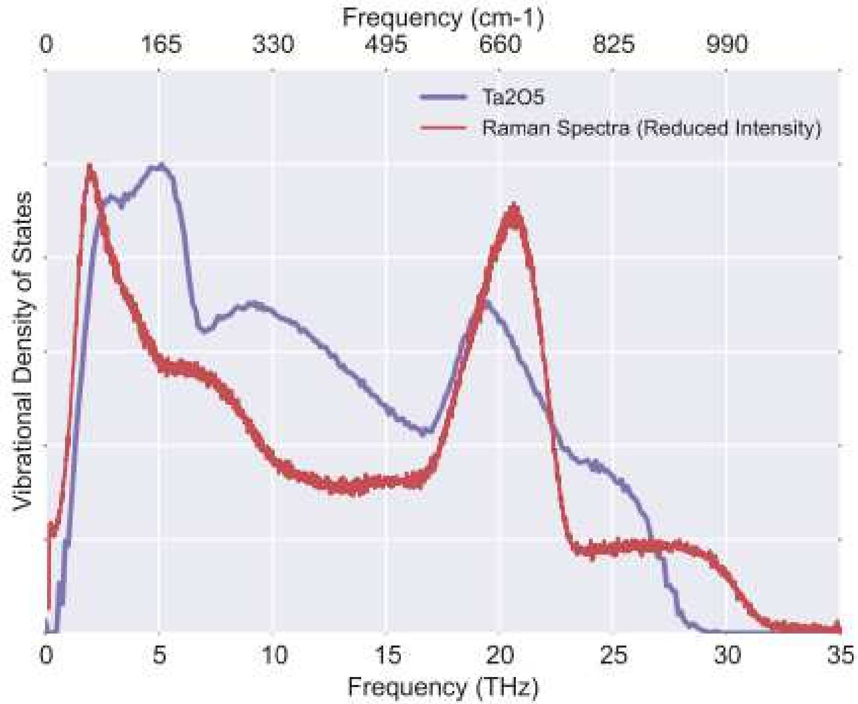
*T. Damart et al., JAP **119** (2016)*

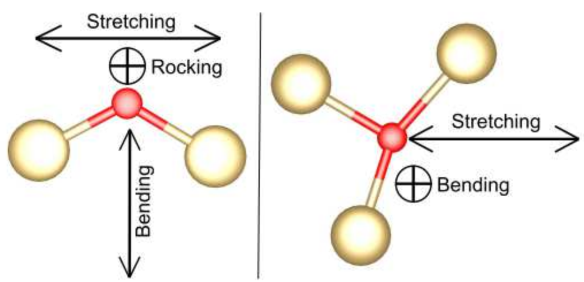
Tantalum oxide layers

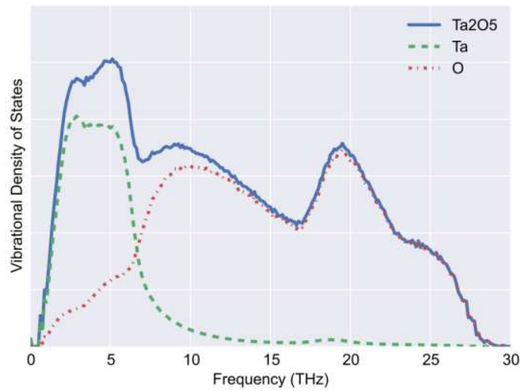
Numerical Study of the Structural and Vibrational Properties of Amorphous Ta_2O_5 and TiO_2-doped Ta_2O_5

T. Damart,[1] E. Coillet,[1] A. Tanguy,[2] and D. Rodney[1]

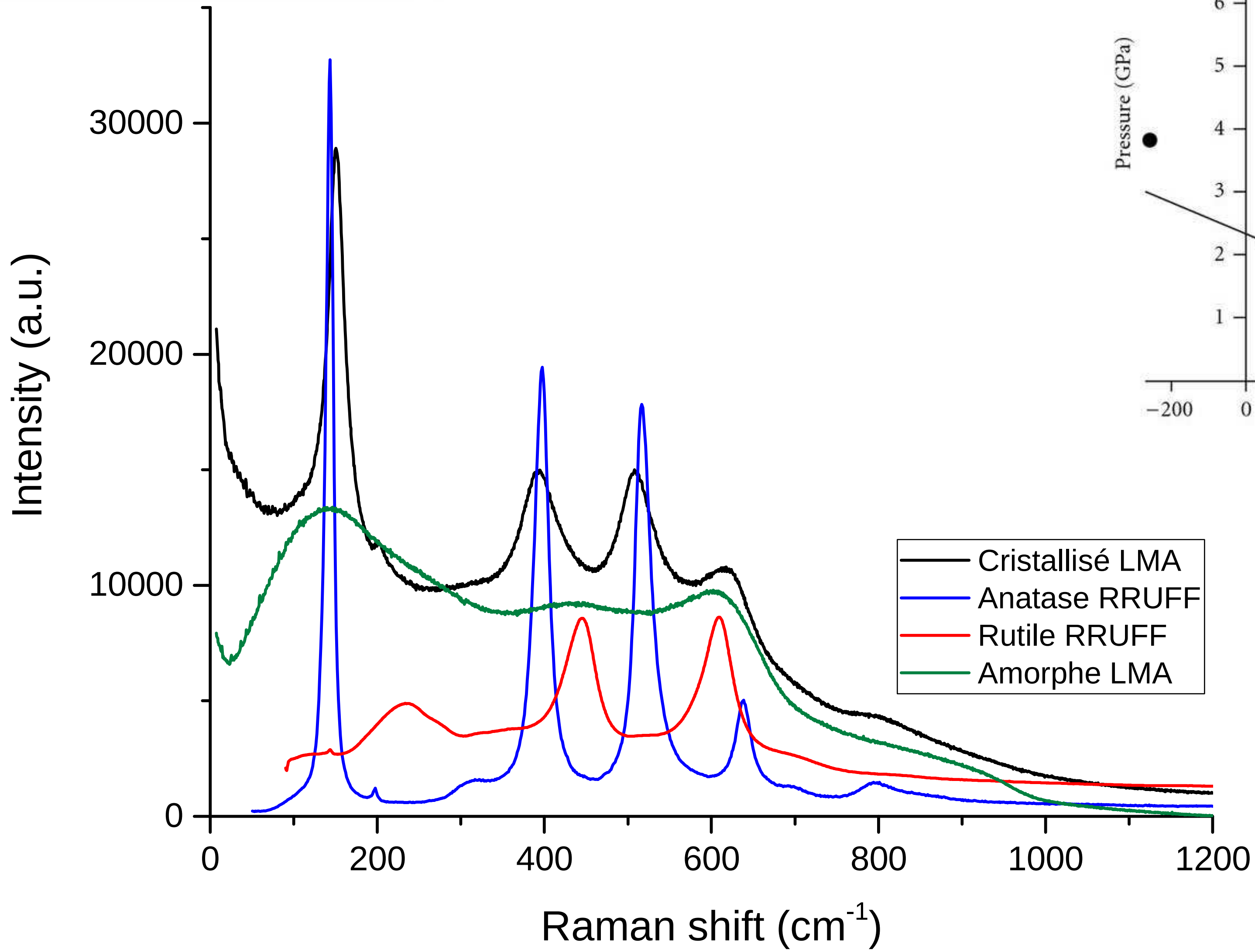


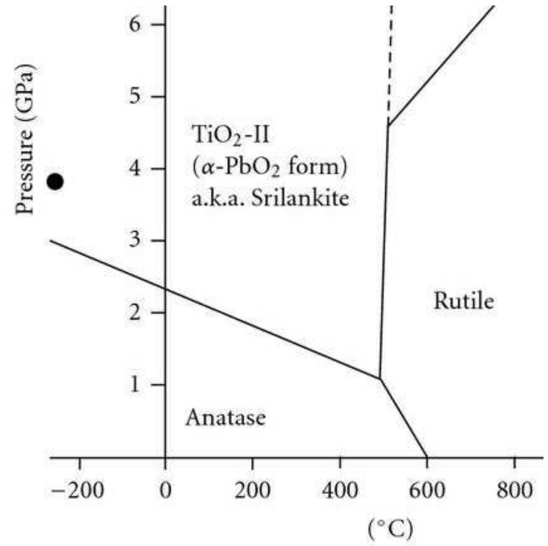






Cristallisation TiO_2





Cristalline layers TiO_2 => Anatase

Coordination Anatase :

- Ti 6 (octahedra)
- O 3 (trigonal planar)