# Long and short-range order in tantalum oxide films for the optics of gravitational wave interferometric detectors.

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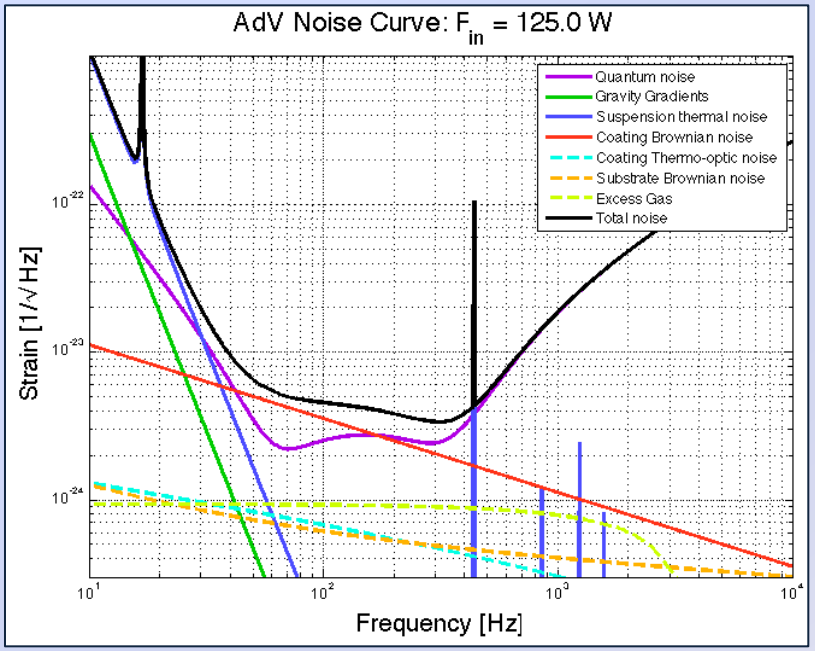
# Coating thermal noise

$$S_x(f,T) \approx \frac{2k_B T}{\pi^2 f} \frac{d}{w^2 Y} \varphi \left( \frac{Y'}{Y} + \frac{Y}{Y'} \right)$$

- The major thermal noise source is the $Ta_2O_5$ film
- This thermal noise seems to be a bulk effect
- Annealing = optical absorption decrease



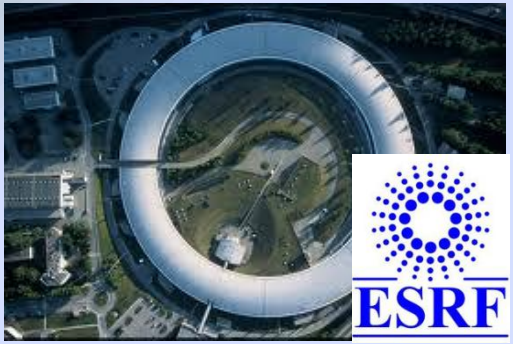

How does the atomic structure of $Ta_2O_5$ film change with the annealing?

# Local atomic structure:

# EXAFS

## (Extended X-Ray Absorption Fine Structure)

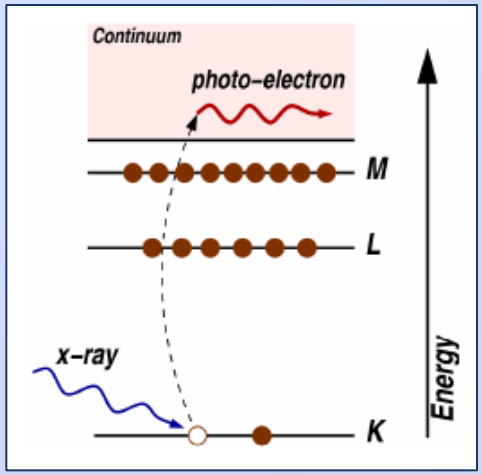
# EXAFS

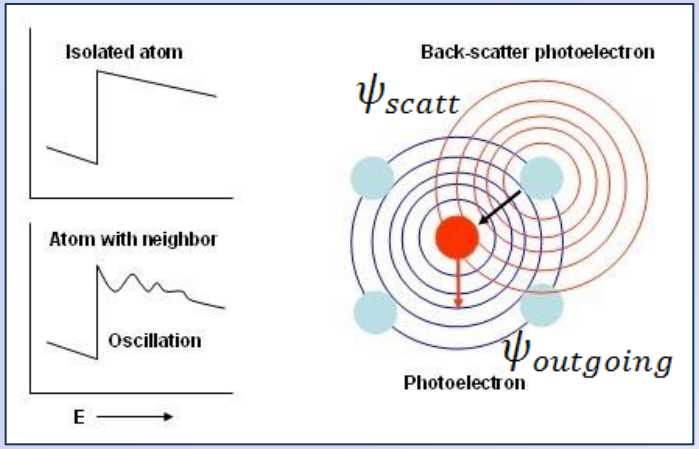



Extended X-Ray Absorption Fine Structure:
local atomic structure.

- High X-Ray flux
- Monochromatic flux
- Tuned flux

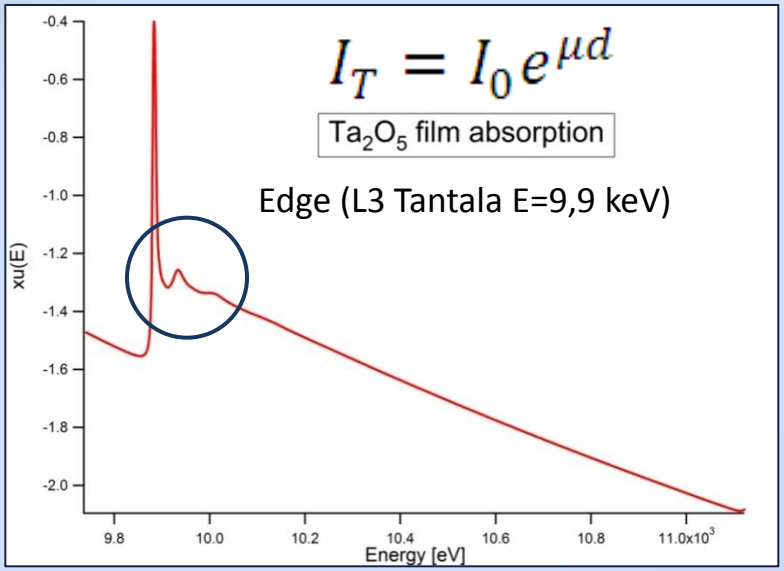
- Very sensitive
- Photo-electric effect
- Absorption coefficient




The absorption coefficient is modulated by neighbor atoms.

# EXAFS




$$\mu(E) \propto |\langle i|H|f\rangle|^2 \qquad |f\rangle = |f_0\rangle + |\Delta f\rangle$$

$$\mu(E) = \mu_0[1 + \chi(E)]$$

$$\chi(E) \propto |\langle i|H|\Delta f\rangle|^2$$

Oscillations:
chemical-physical state of the neighborhood

$$\chi(k) = \sum_j \frac{N_j f_j e^{-2k^2\sigma_j^2}}{kR_j^2} \sin\left[2kR_j + \delta_j(k)\right]$$

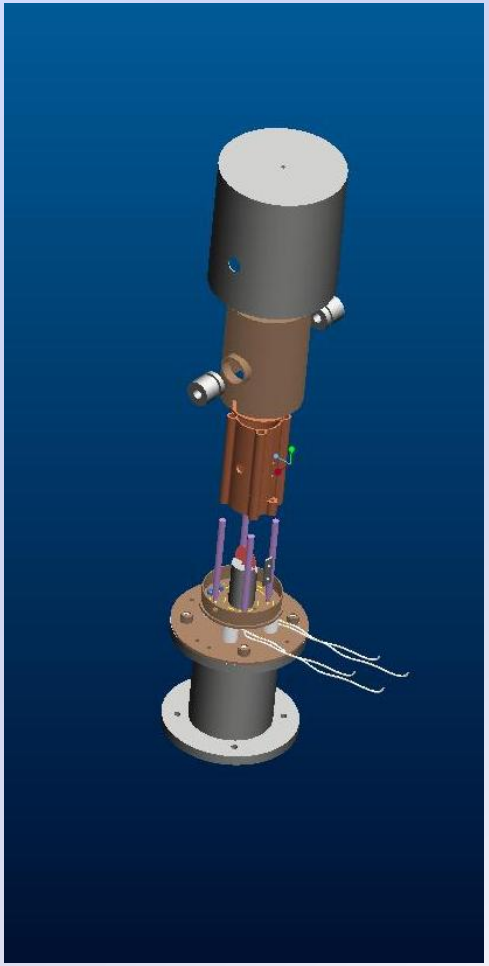
- Peak positions– atomic distances
- Coordination
- Chemical sensitivity

# Experimental setup

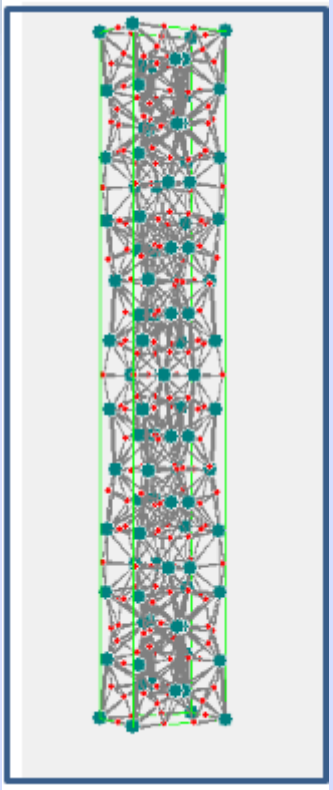
# Samples

$Ta_2O_5$ (2 µm) amorphous films deposited on $SiO_2$ (200 µm) substrates by IBS ( LMA Lyon)

| Sample | Temperature (°C) | Duration (h) |
|---|---|---|
| A | Not annealed | ------ |
| B | 300 | 1 |
| C | 400 | 1 |
| D | 350 | 3 |
| E | 450 | 4 |
| Crystalline powder | ------ | ------ |

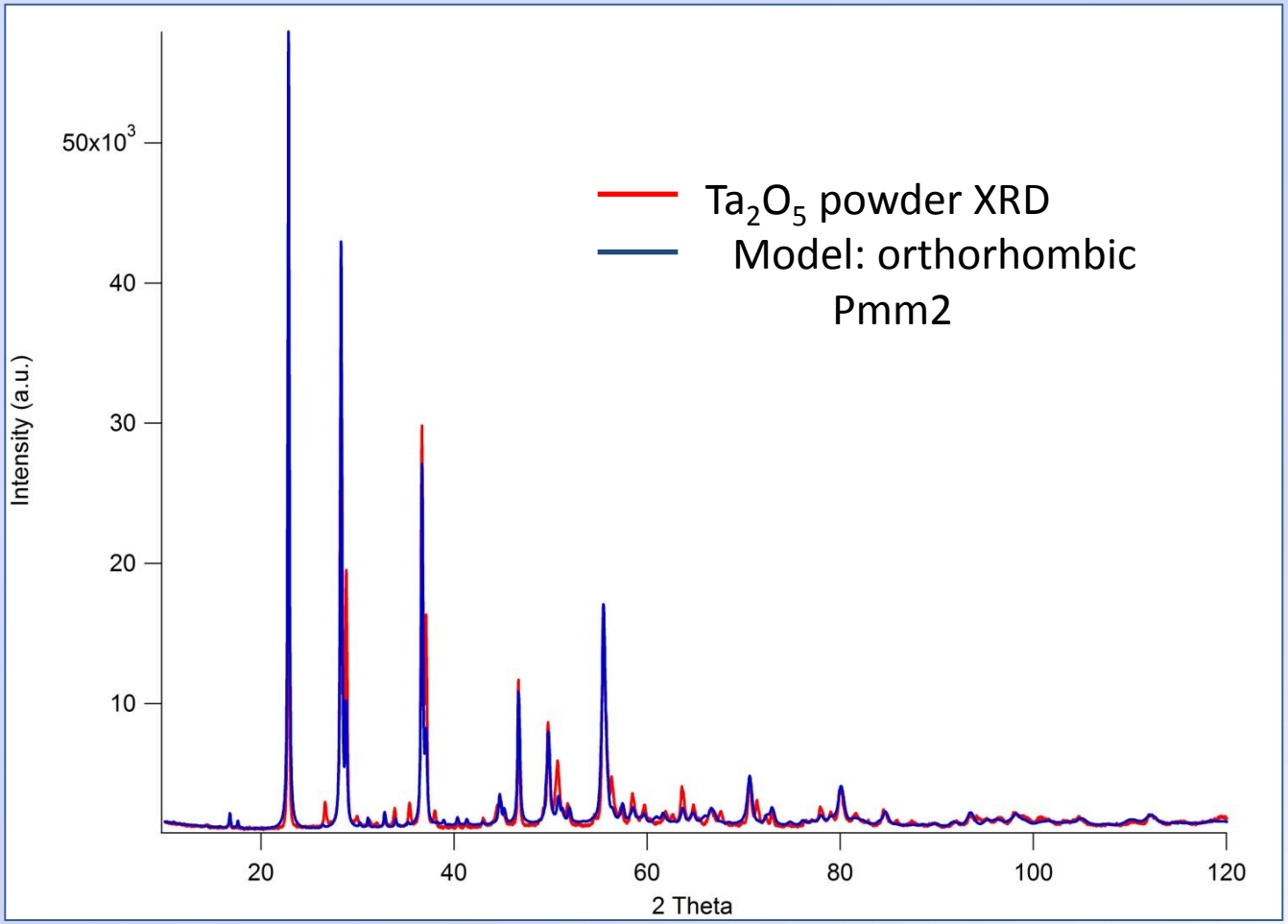


# $Ta_2O_5$ polycristalline powder XRD



Orthorhombic Pmm2
a=6,194 Å
b=3,888 Å
c=40,29 Å

$Ta_2O_5$ polycristalline powder (XRD)

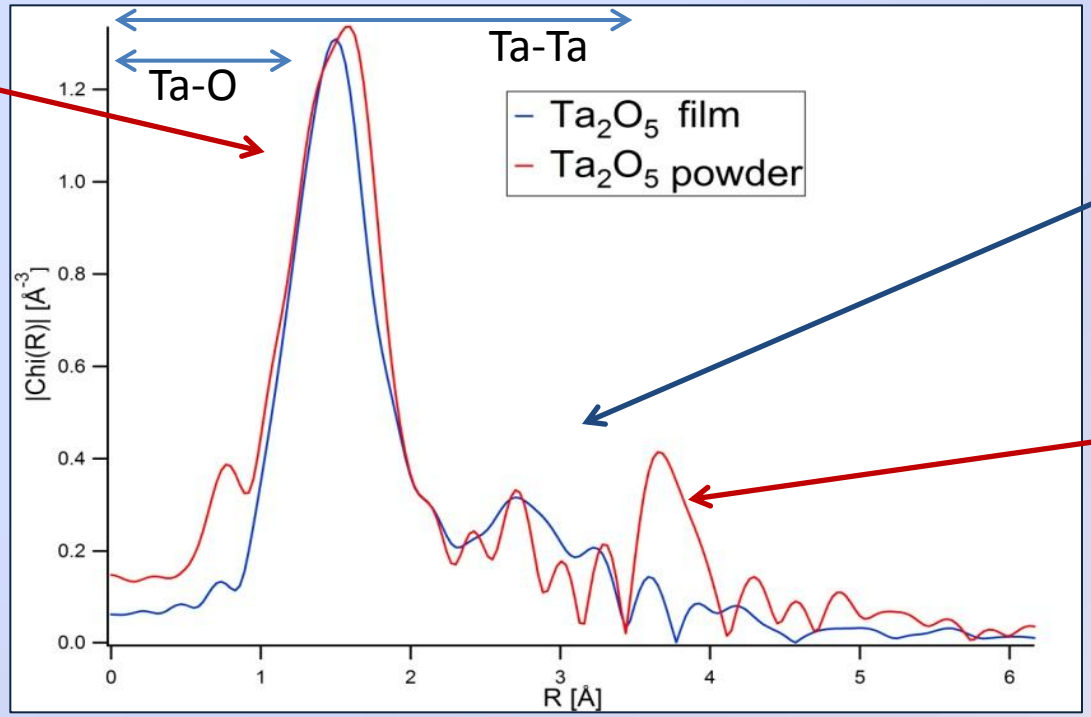


# Data analysis

# EXAFS

Powder vs. amorphous local structure

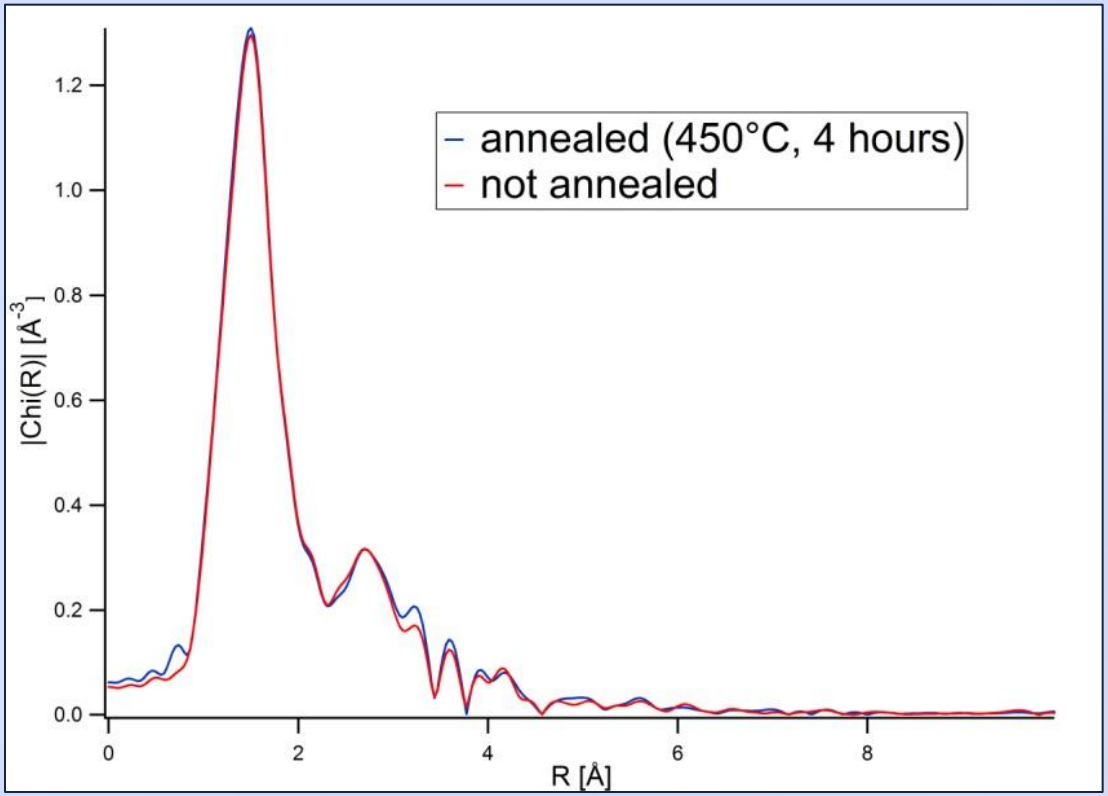
I shell:
Ta-O bond




Amorphous :
short range
order

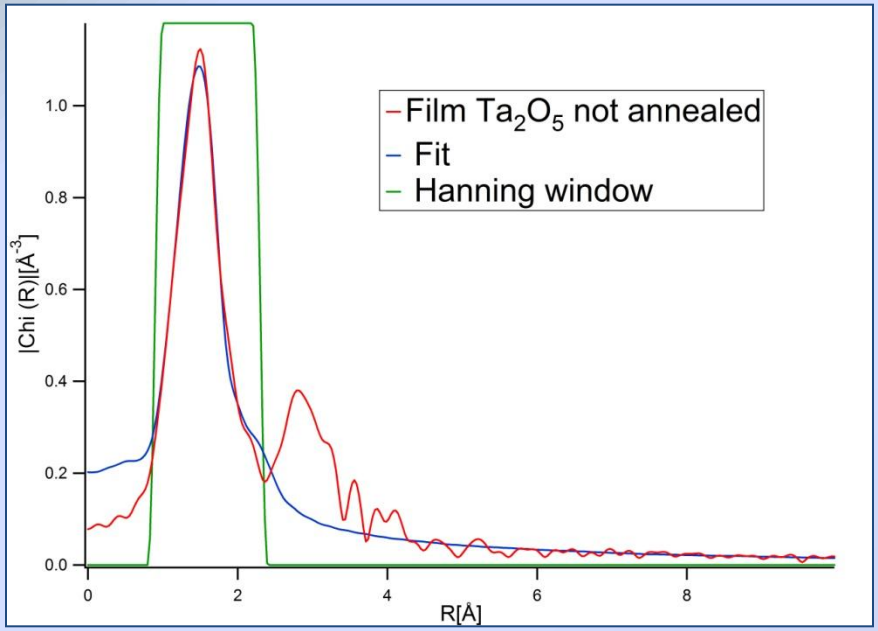
Powder:
long range
order

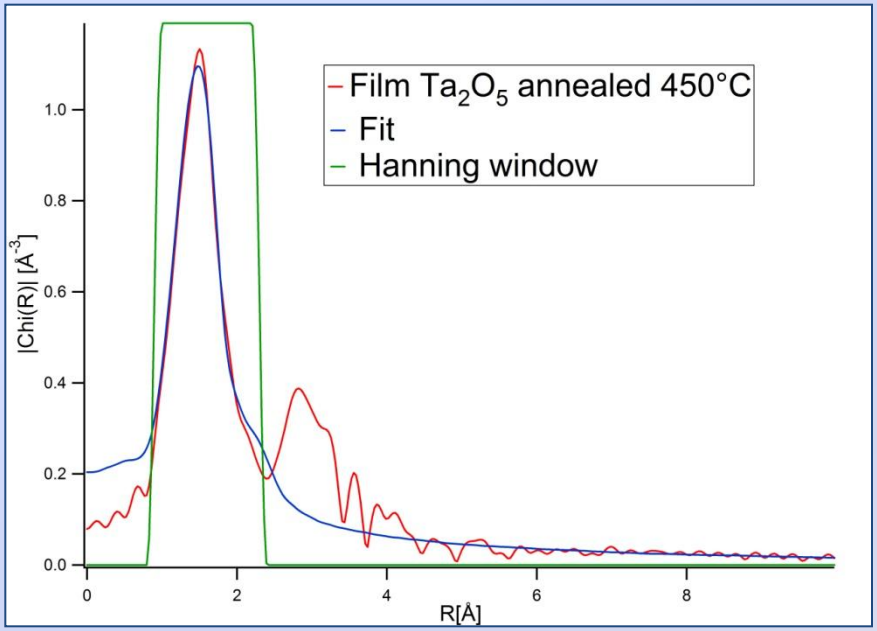
# EXAFS: amorphous films




EXAFS measurement on “A” and “E” samples:
no apparent significant differences.

# EXAFS: analysis



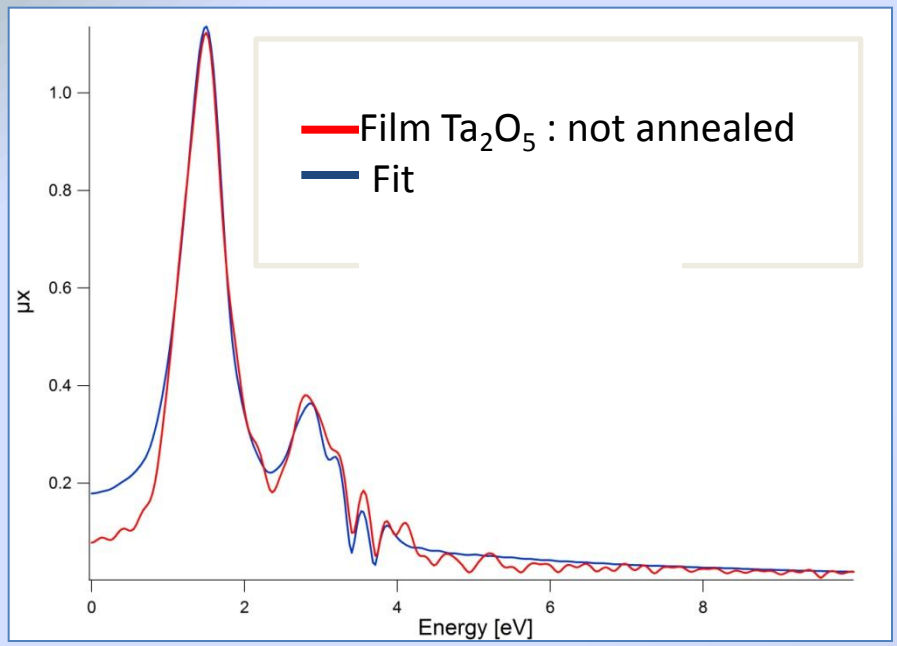



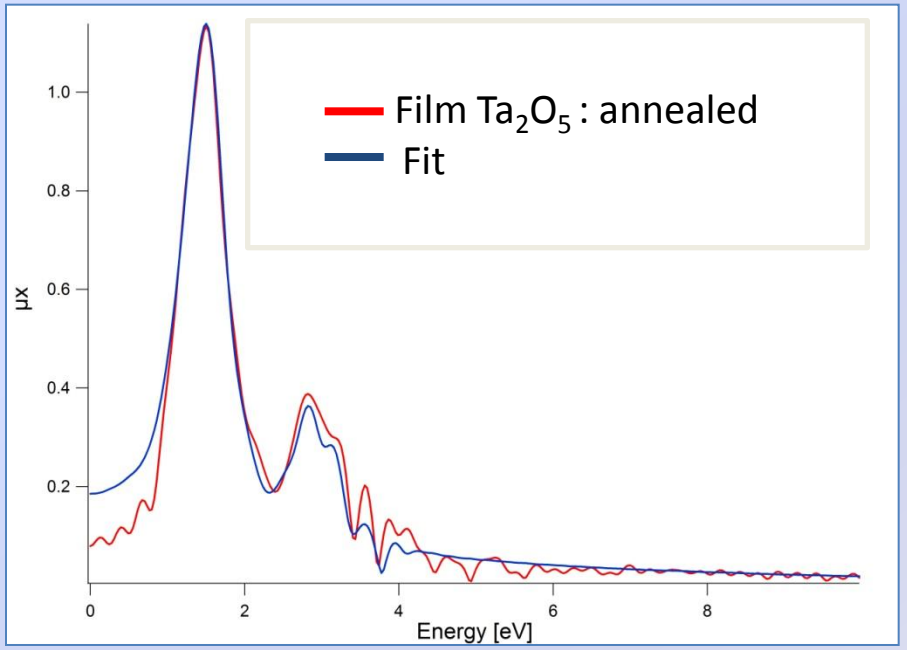

Analysis :
first coordination shell

Limiting the analysis at the first shell, the two samples show the same structure.

| Parameter | Sample "A" | Sample "E" |
|---|---|---|
| Amplitude | 0,93±0,02 | 0,96±0,05 |
| $E_0$ [eV] | -2,7±0,5 | -2,5±0,5 |
| D_r [Å] | 1,873±0,004 | 1,871±0,004 |
| $\sigma^2$ [Å$^2$] | 0,0078±0,0003 | 0,0082±0,0003 |

# EXAFS: analysis




Analysis :

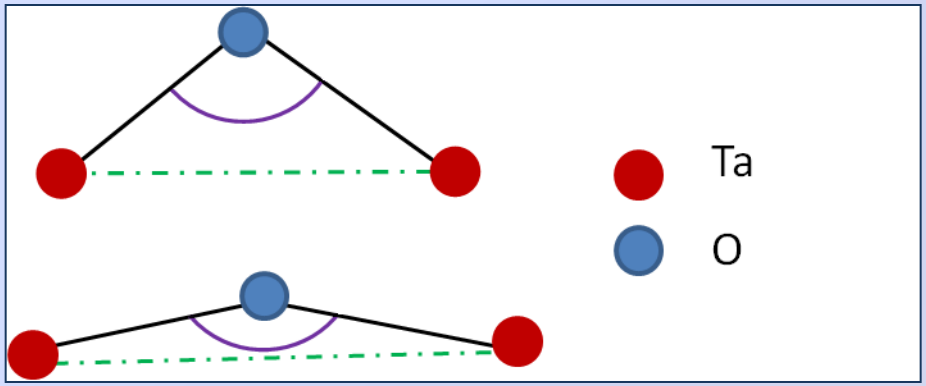
•Structure: orthorhombic Pmm2

Significant differences in the Ta-Ta distance.

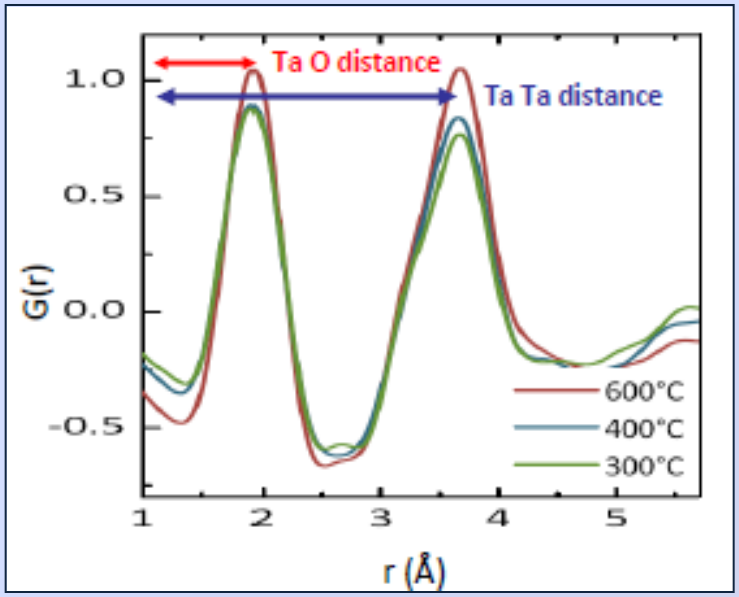
| Coordination shell | Distance [Å] (sample "A") | Distance [Å] (sample "E") |
|---|---|---|
| Ta-O | 1,93±0,05 | 1,93±0,04 |
| Ta-Ta | 3,8±0,2 | 3,1±0,1 |
| Ta-O | 3,39±0,02 | 3,44±0,01 |
| Ta-Ta | 3,6±0,2 | 3,3±0,1 |

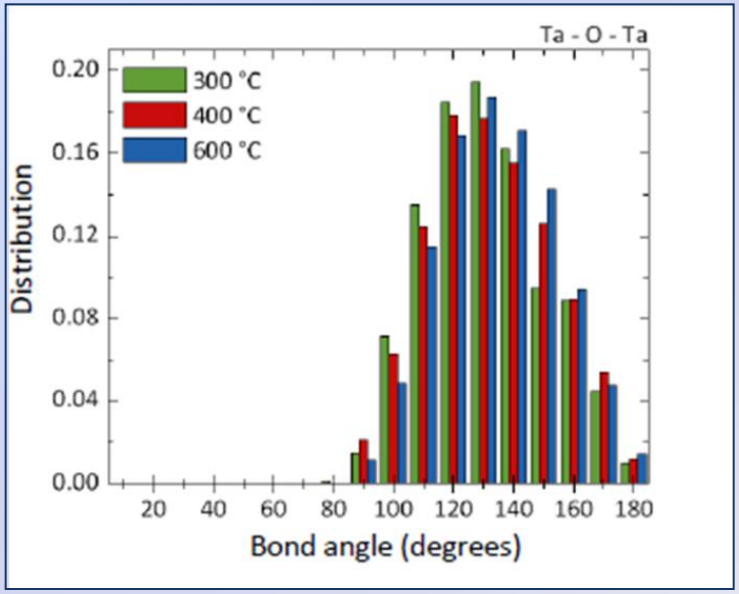
# EXAFS: analysis

- Change in the bond-angle (Ta-O-Ta)
- Several configurations of bond-angles




Martin et al. (2011):

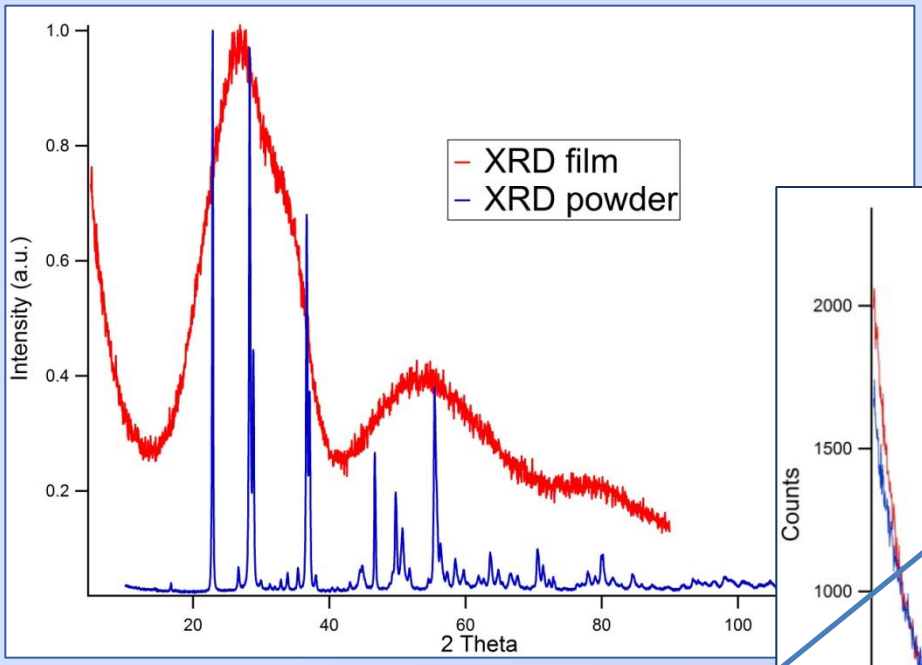


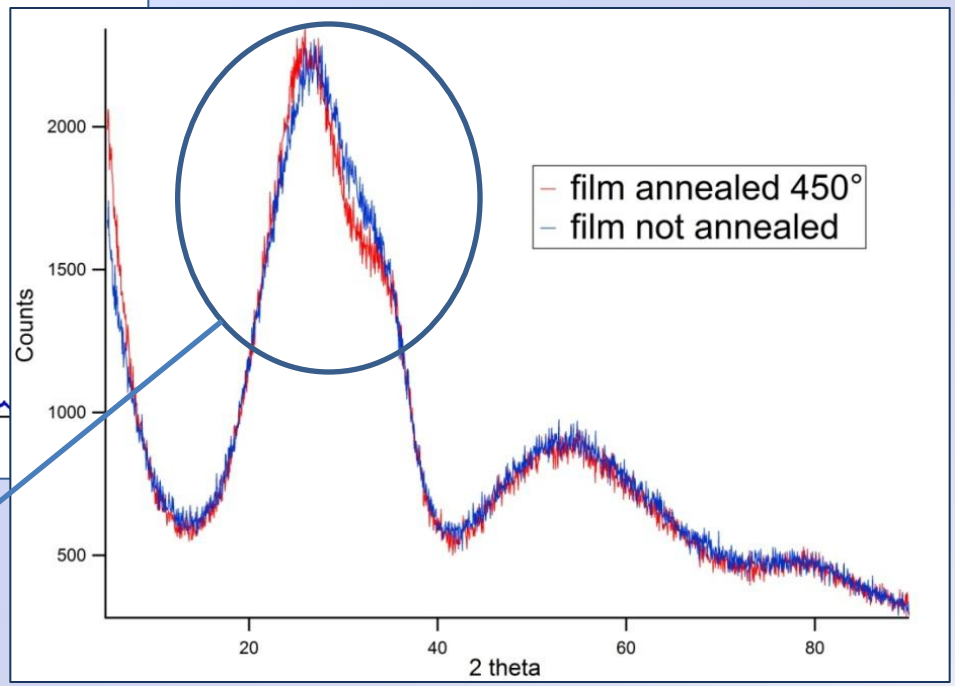



# X-Ray Diffraction and Ellipsometry

# XRD: amorphous samples

X-Ray Diffraction:
atomic structure of the material .



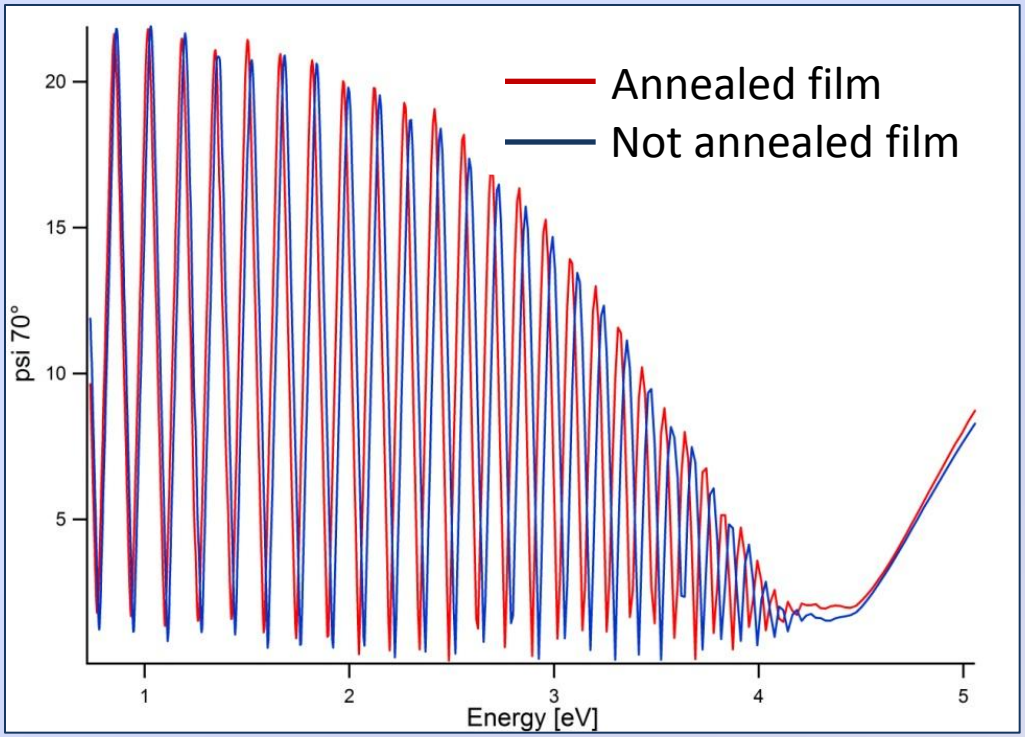

The diffraction pattern of the annealed sample is sharper than the not annealed one

More detailed structure = more ordered structure

# Ellipsometry

Ellipsometry:
Optical properties and surface sensitivity.

$$tg(psi) = \frac{|R_p|}{|R_s|}$$



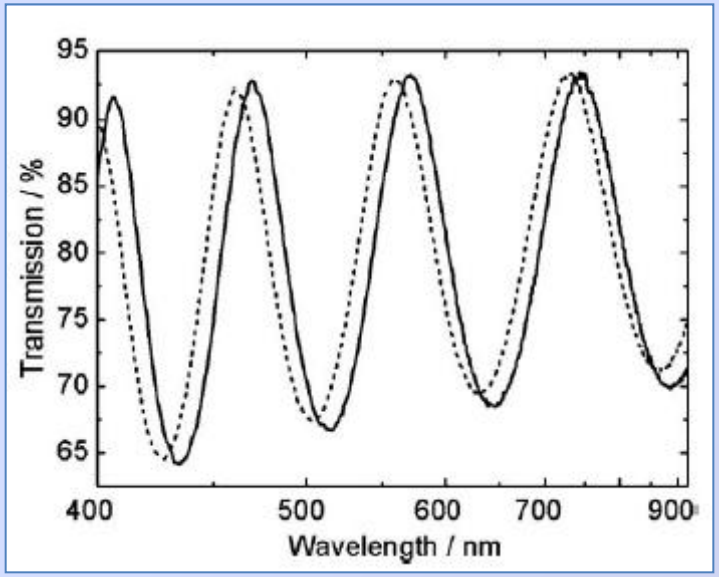

Evident spectra energy shift.

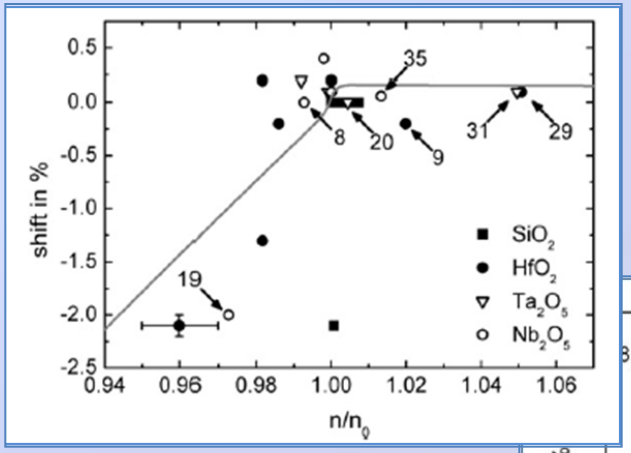
# Ellipsometry

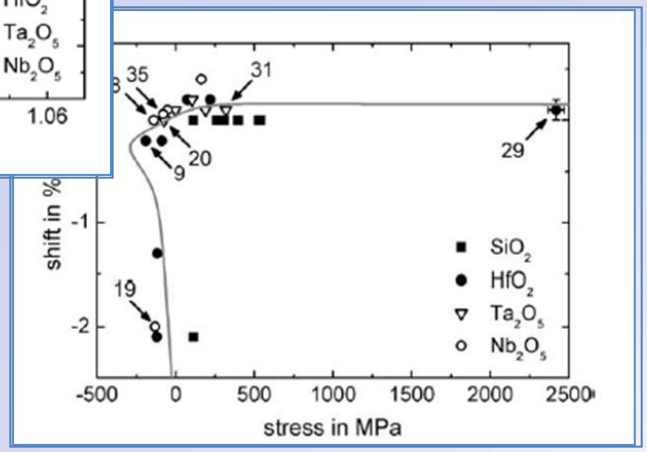
Energy shift:

- the refraction index changes with temperature
- mechanical stress release
- thickness change

Stenzel et al. (2009)




- surface changes

# Conclusions
# and future developments

# Conclusions

- EXAFS → the annealing process seems to change the Ta-Ta distance

- XRD → differences in the diffraction spectra.

- Ellipsometry → differences in the optical properties .

- The annealing produces a change in the Ta-Ta distance
  Testing the bond angle model

- A possible Ellipsometric interpretation leads to Mechanical losses as surface effect. From bulk to surface?