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

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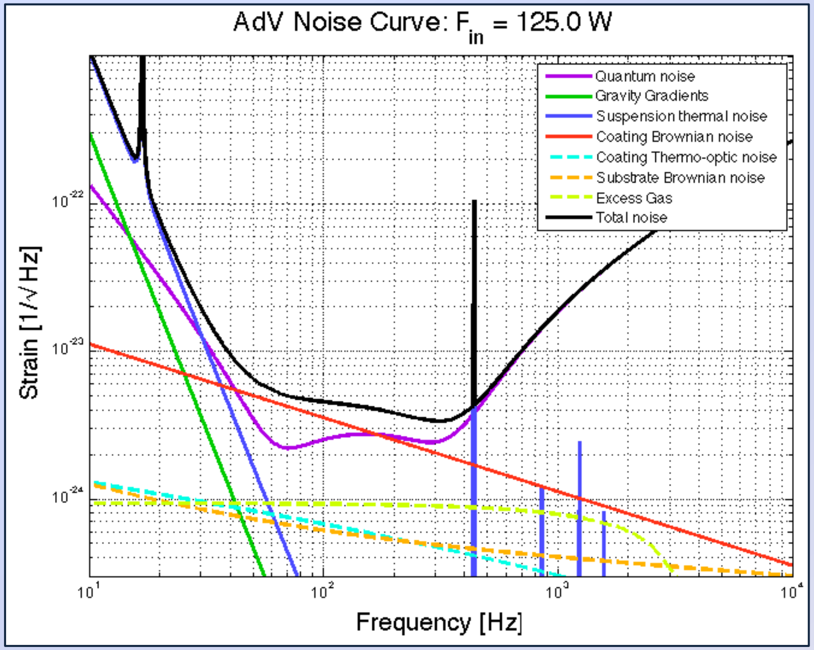
Coating thermal noise

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

- The major thermal noise source is the Ta_2O_5 film
- This thermal noise seems to be a bulk effect
- Double well potential = 2 stable configurations
- Annealing = optical absorption decrease

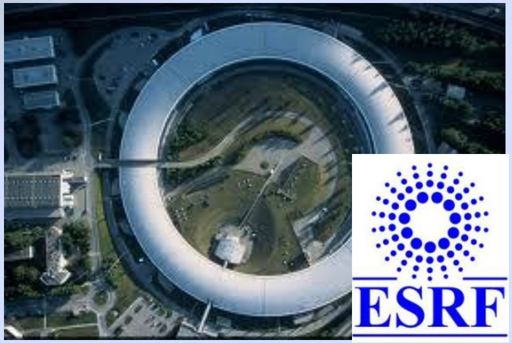


How does the atomic structure of Ta_2O_5 film change with the annealing?

Local atomic structure:

EXAFS
(Extended X-Ray Absorption Fine Structure)

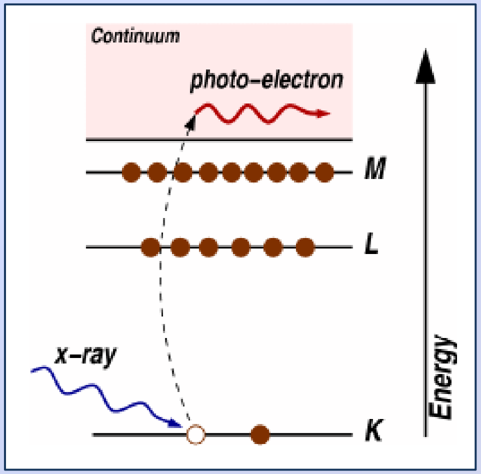
EXAFS

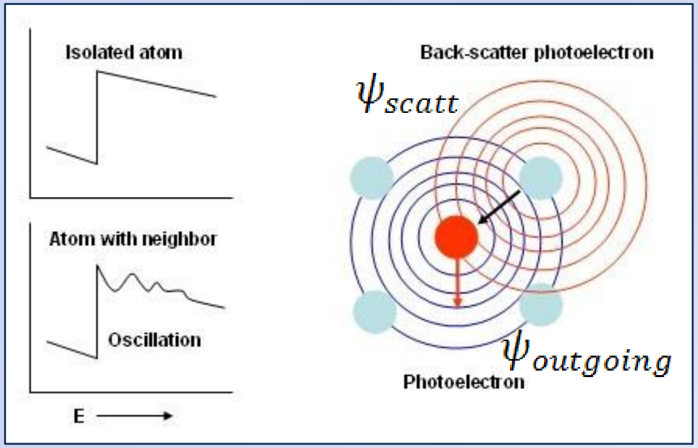


Extended X-Ray Absorption Fine Structure:
local atomic structure.

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

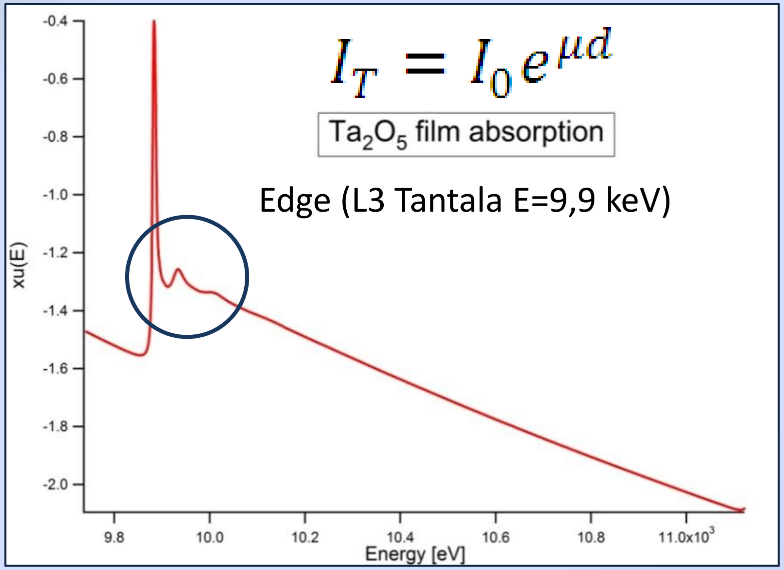
- Very sensitive
- Photo-electric effect
- Absorption coefficient





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

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

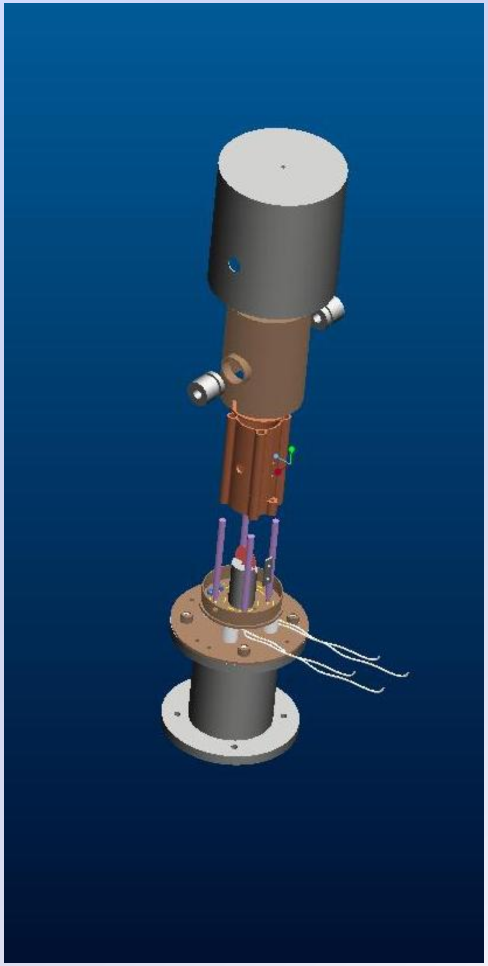
- Peak positions– atomic distances
- Coordination
- Chemical sensitivity

Experimental setup

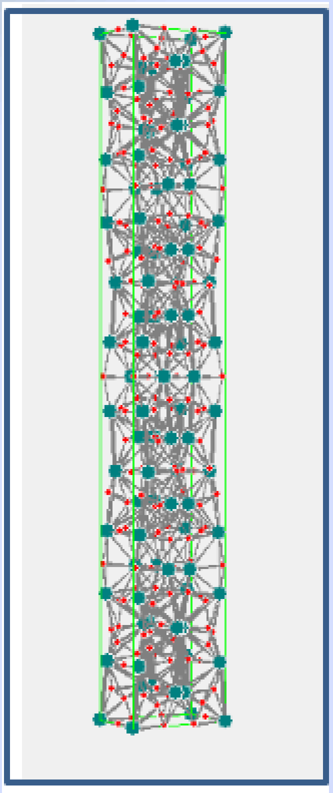
Samples

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	------	------

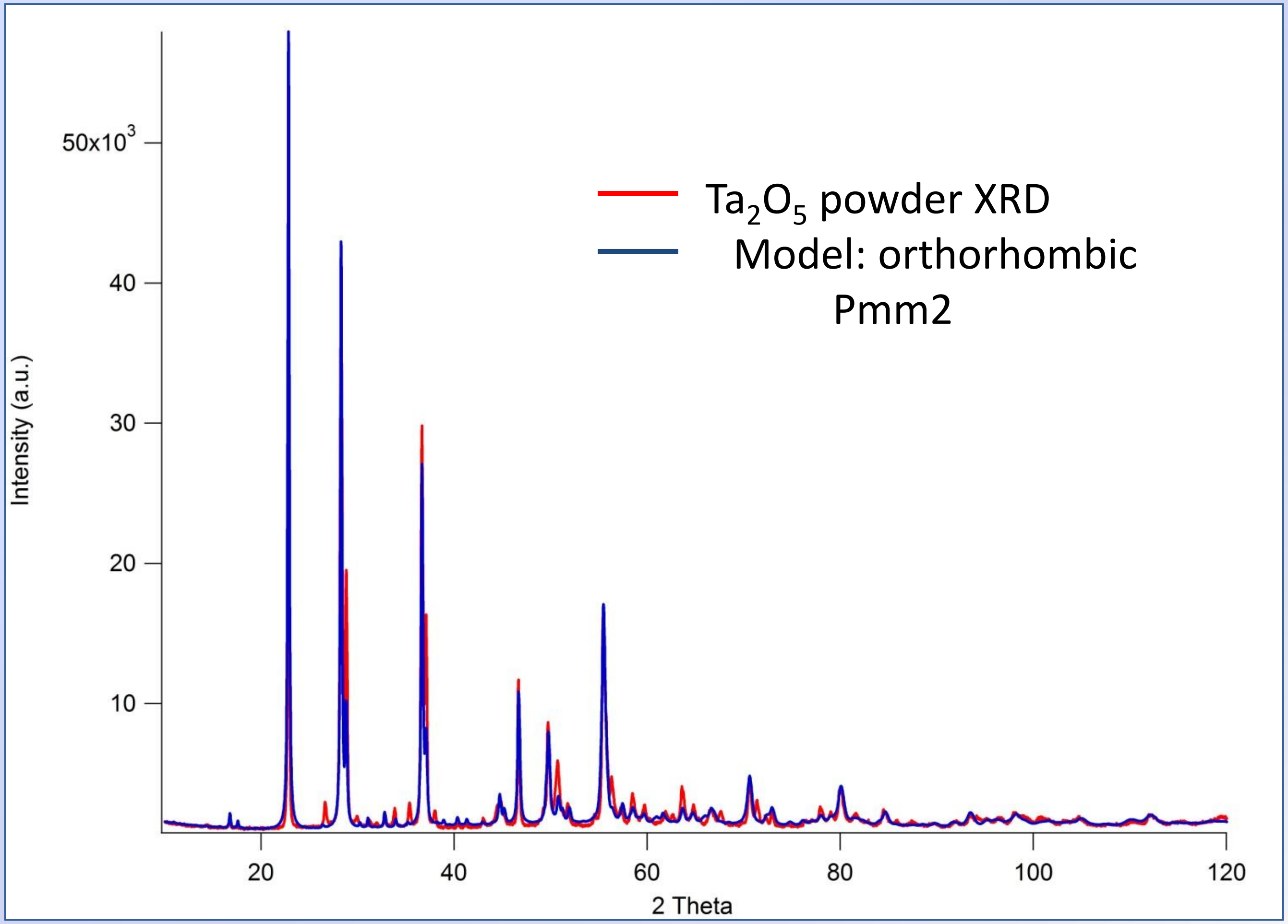


Ta_2O_5 polycristalline powder XRD



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

Ta_2O_5 polycristalline powder (XRD)

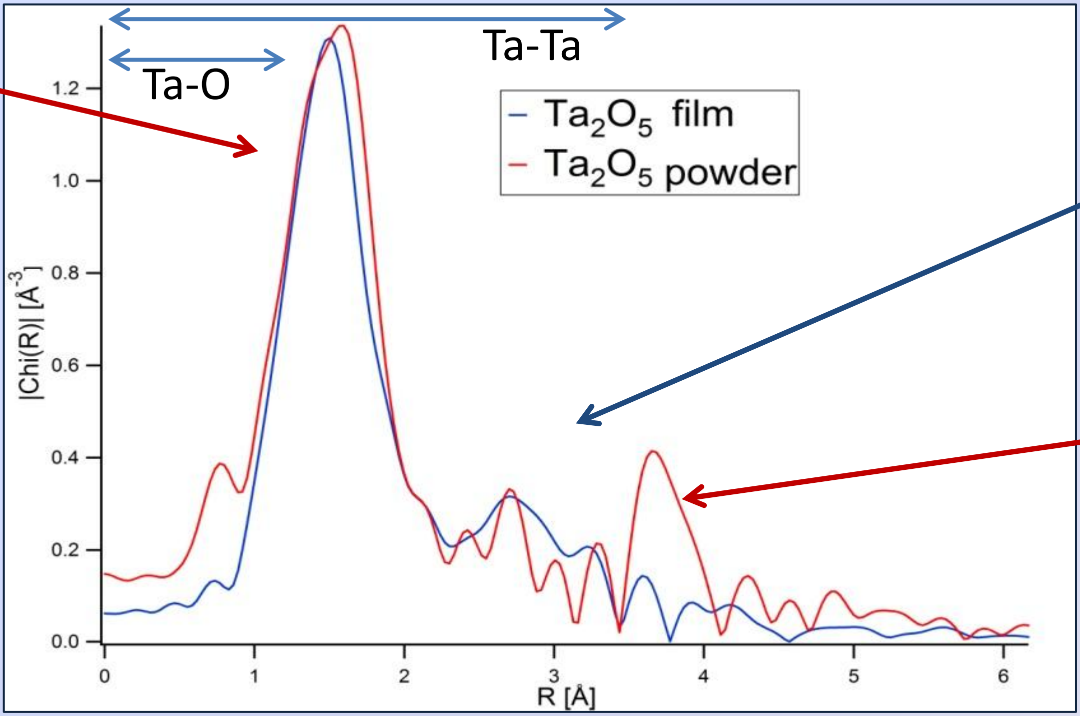


Data analysis

EXAFS

Powder vs. amorphous local structure

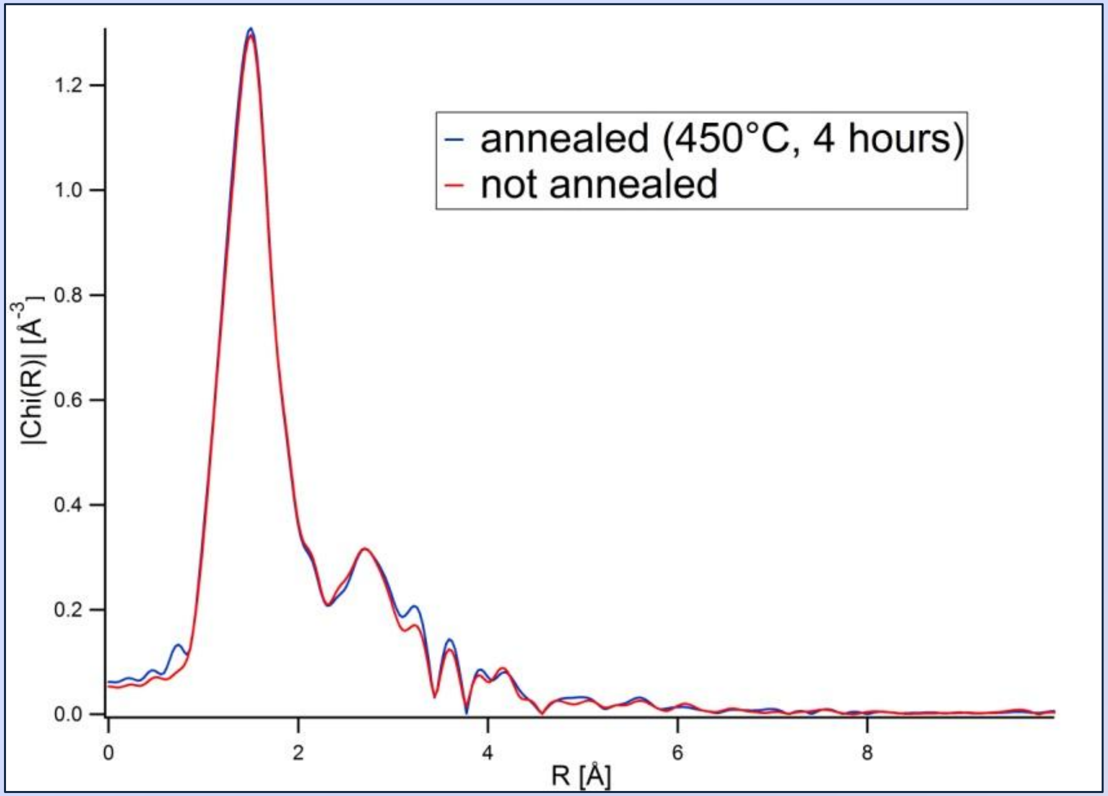
I shell:
Ta-O bond



Amorphous : short range order

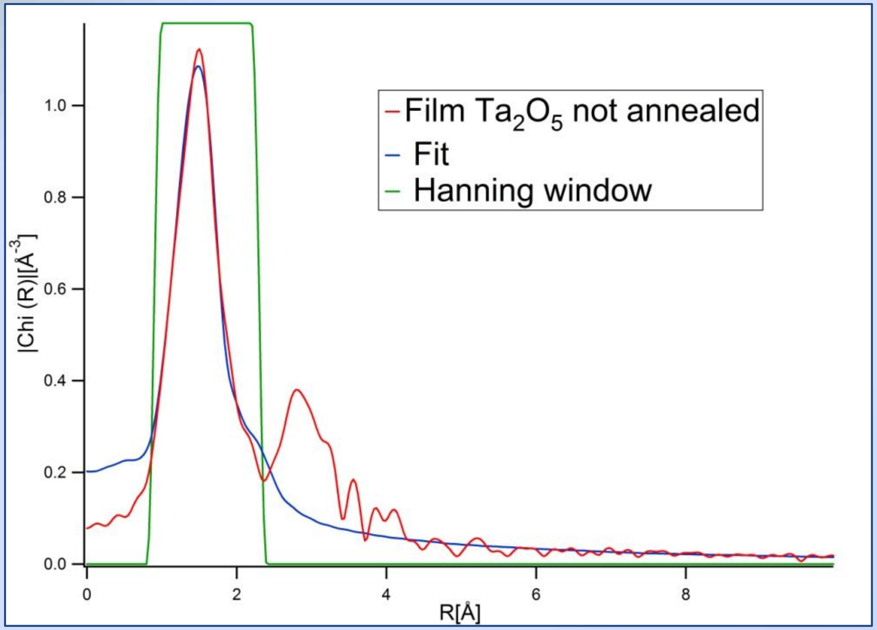
Powder: long range order

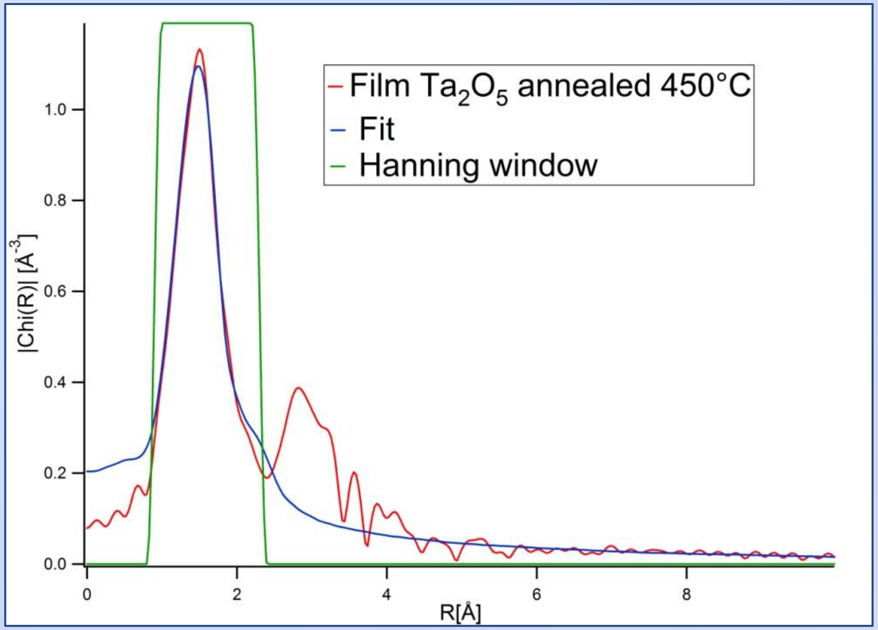
EXAFS: amorphous films



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

EXAFS: analysis



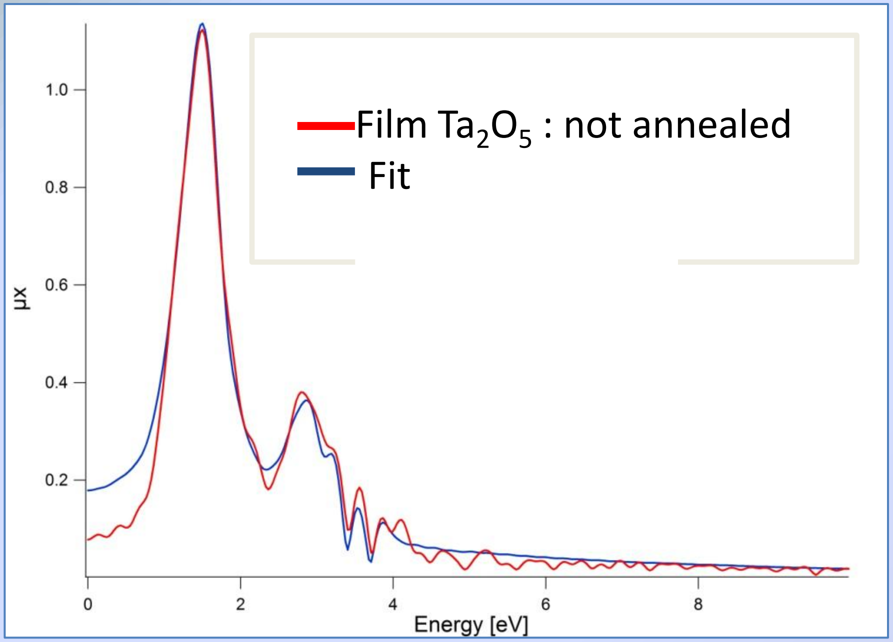


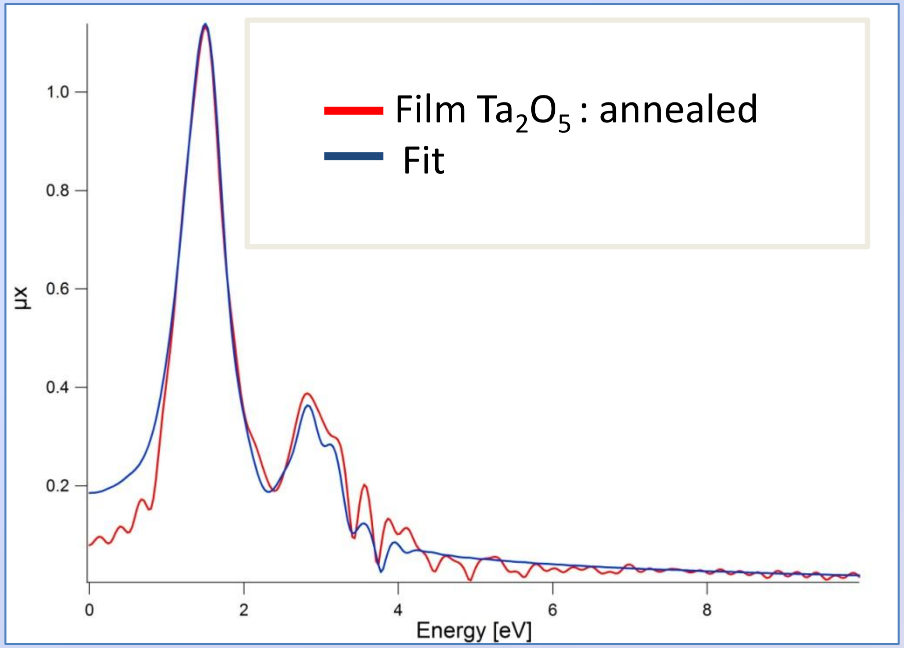
Analysis :
first coordination shell

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
σ^2 [Å^2]	0,0078±0,0003	0,0082±0,0003

EXAFS: analysis





Analysis :

•Structure: orthorhombic Pmm2

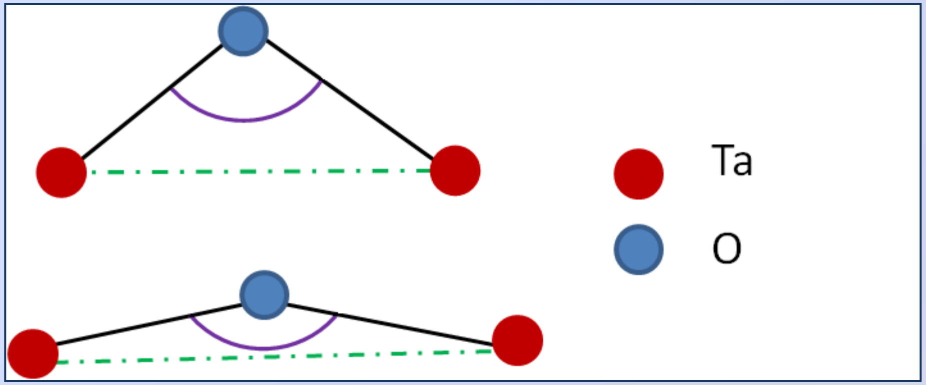
Significant differences in the Ta-Ta distance.

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

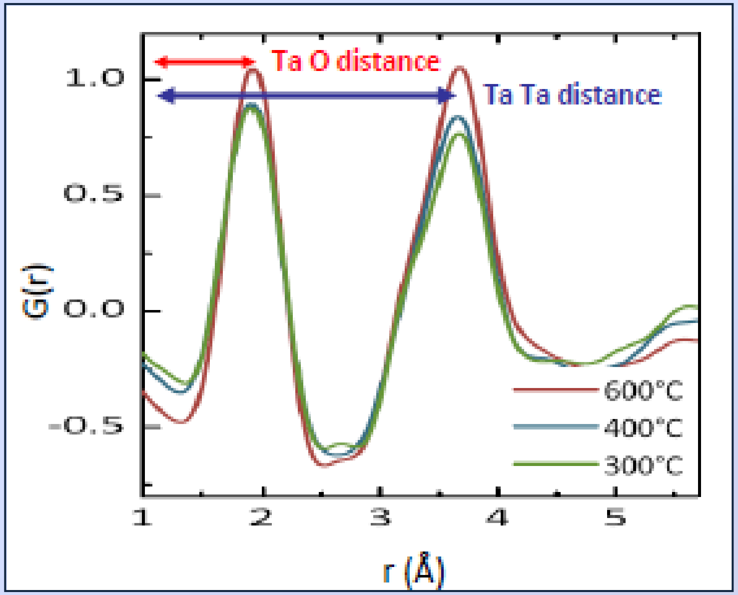
EXAFS: analysis

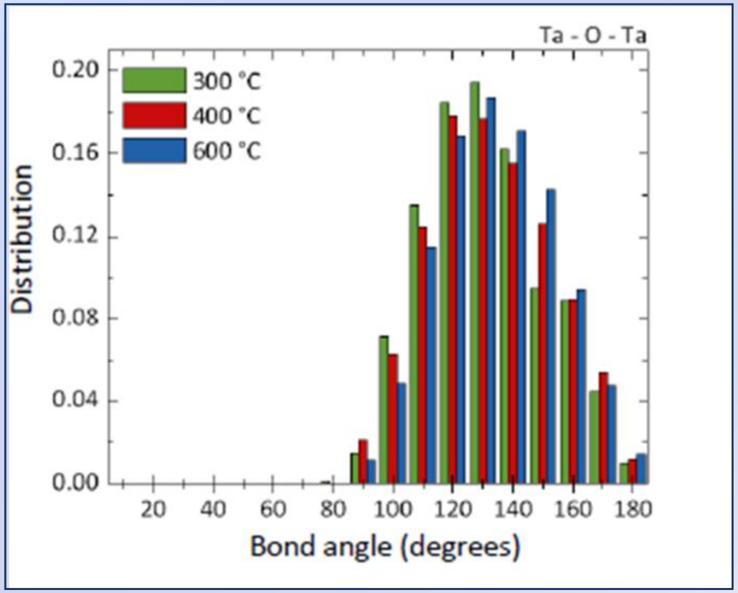
•Change in the bond-angle (Ta-O-Ta)

•Double well potential = 2 stable configurations of bond-angles



Martin et al. (2011):

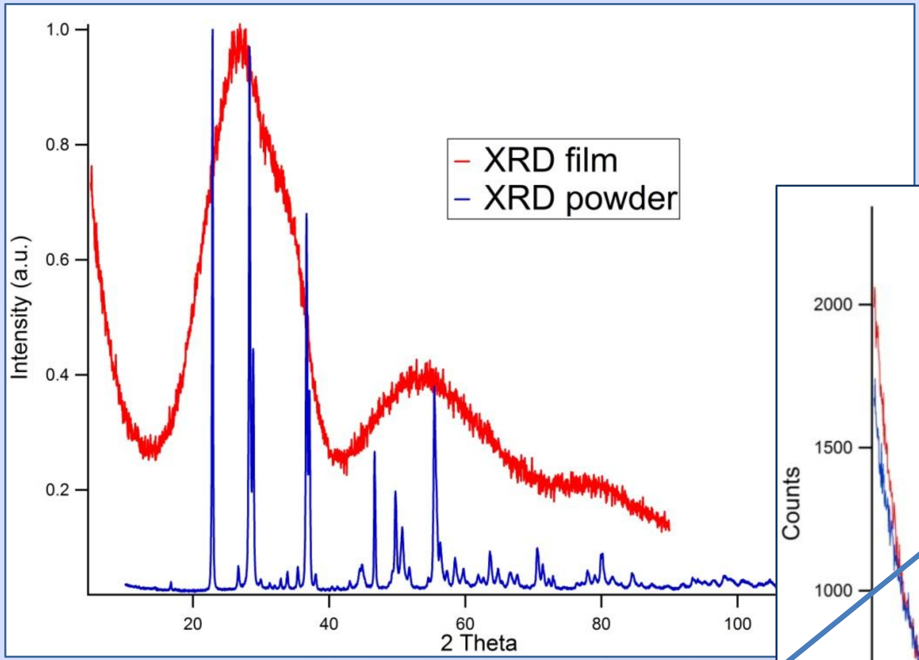


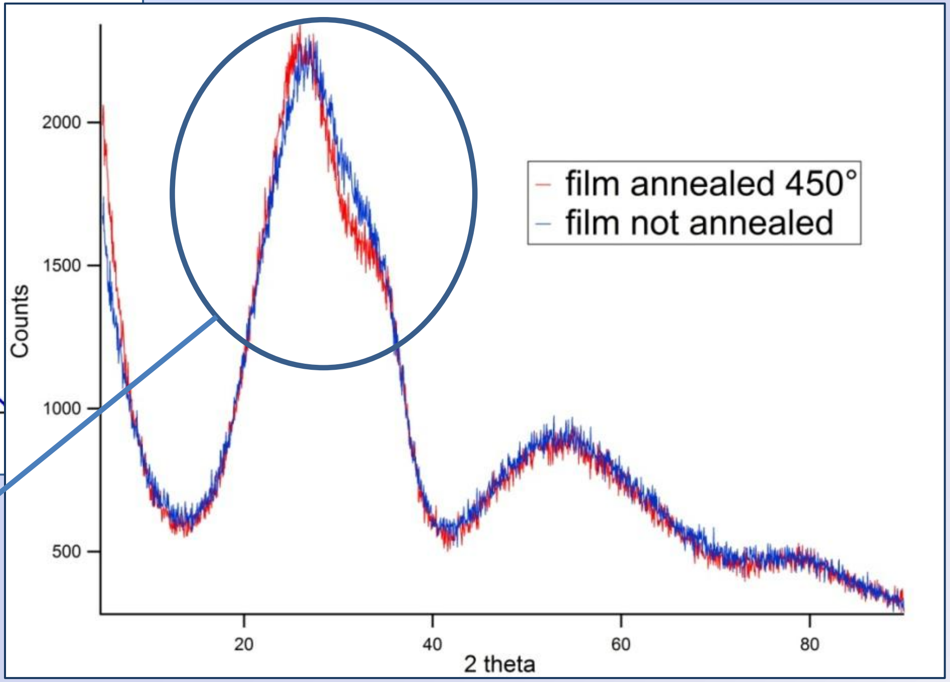


X-Ray Diffraction and Ellipsometry

XRD: amorphous samples

<u>X-Ray Diffraction</u>:
atomic structure of the material .





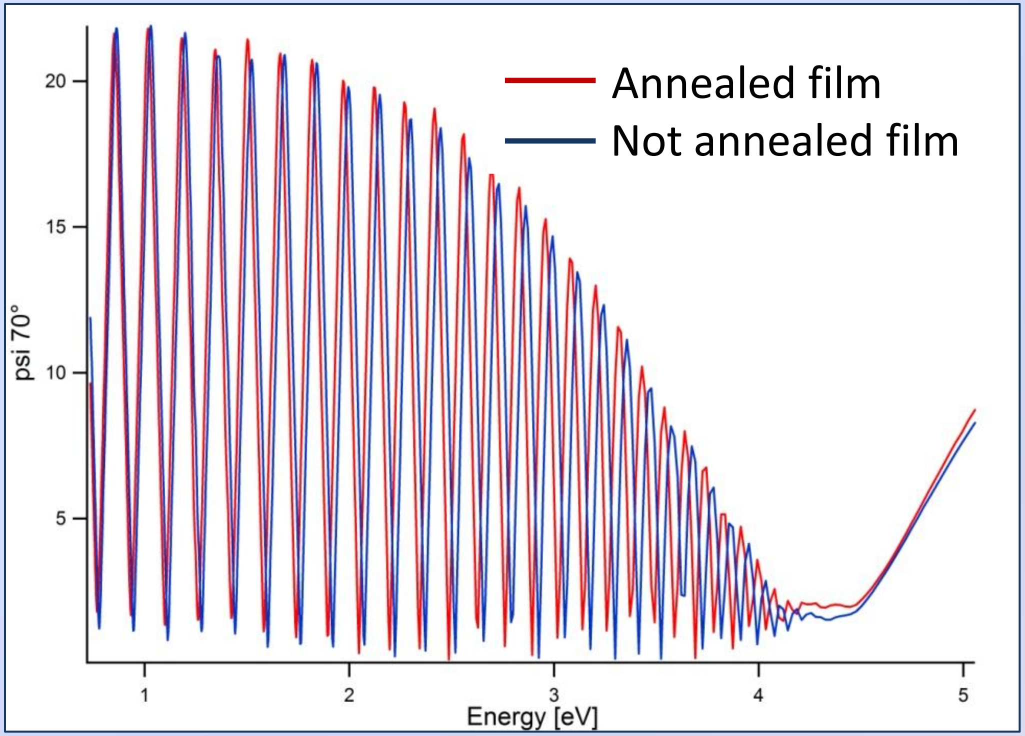
The diffraction pattern of the annealed sample is sharper than the not annealed one

More detailed structure = more ordered structure

Ellipsometry

<u>Ellipsometry</u>:
Optical properties and surface sensitivity.

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



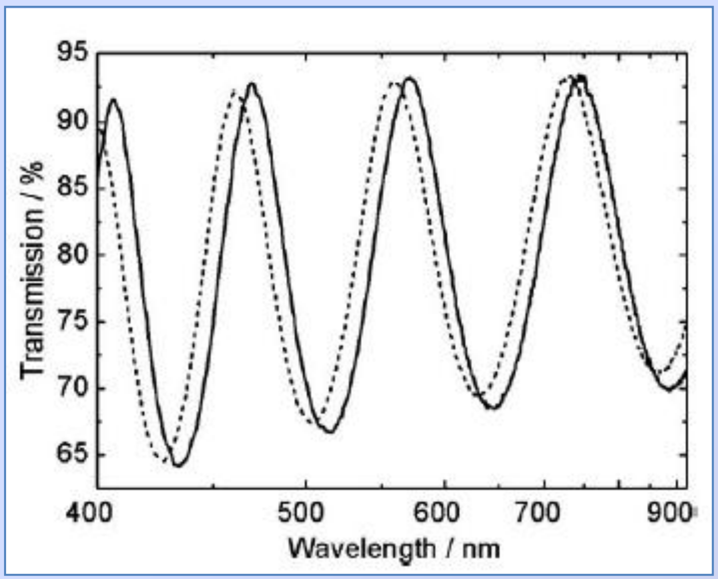
Evident spectra energy shift.

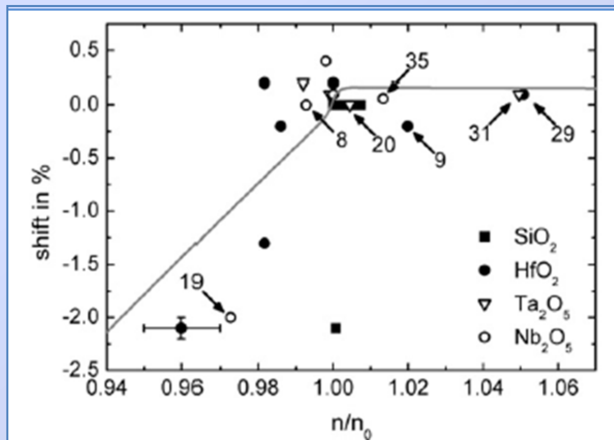
Ellipsometry

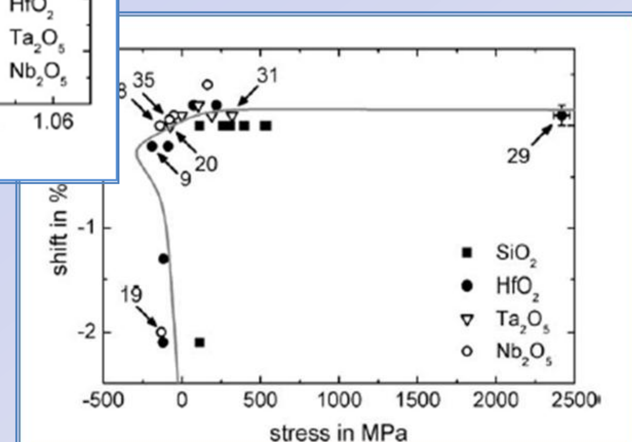
Energy shift:

- 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 .

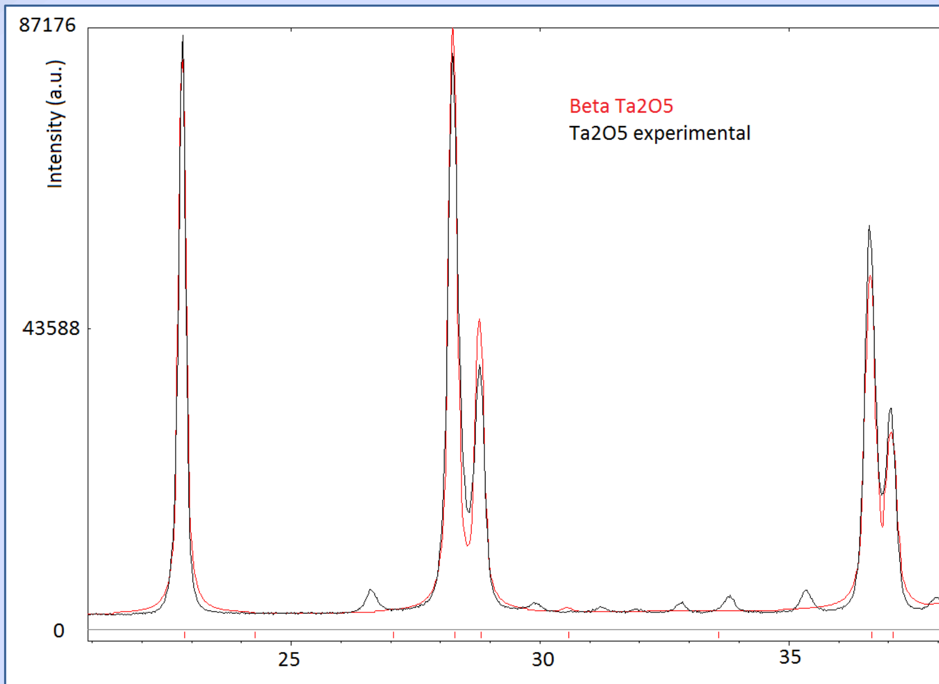
- The annealing produces a change in the Ta-Ta distance
  Testing the bond angle model ⇒ double well potential:
  2 configurations = 2 bond-angle configurations

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

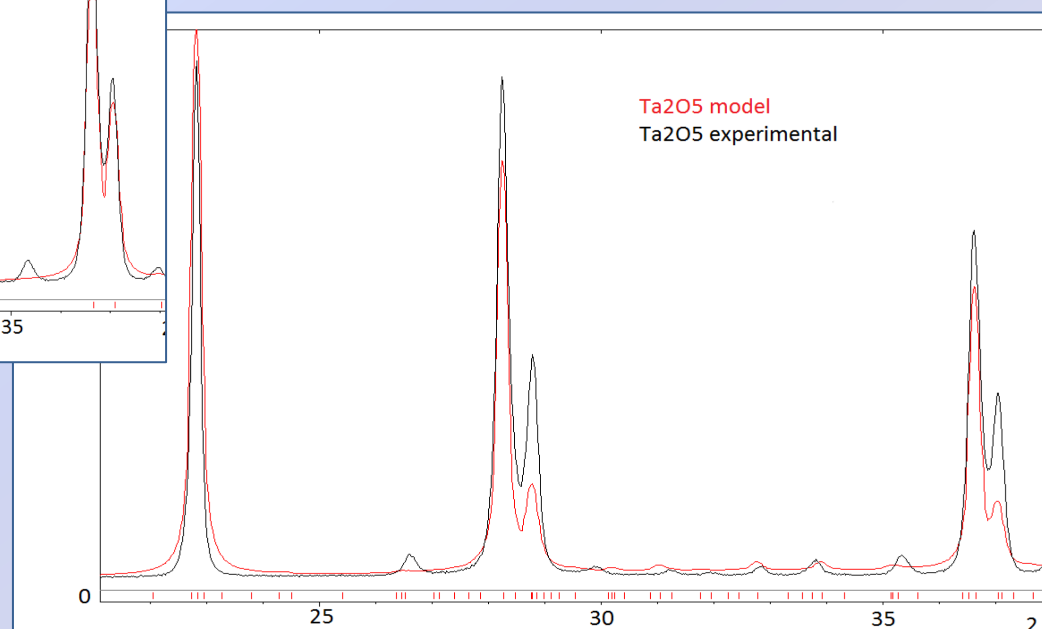
Ta_2O_5 polycristalline powder XRD

Principal peaks [20-40]°

β-phase



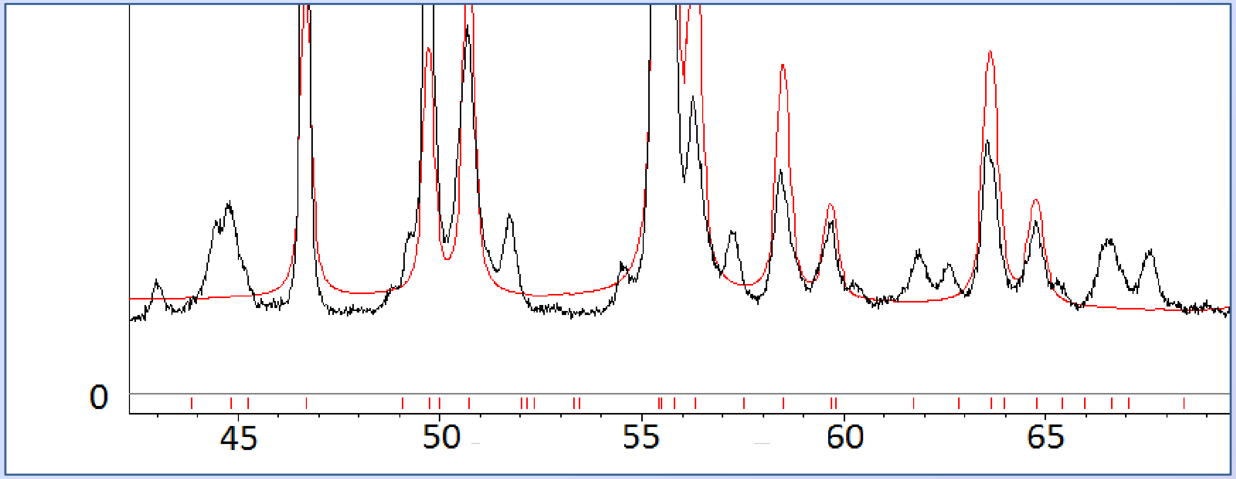
Orthorhombic Pmm2



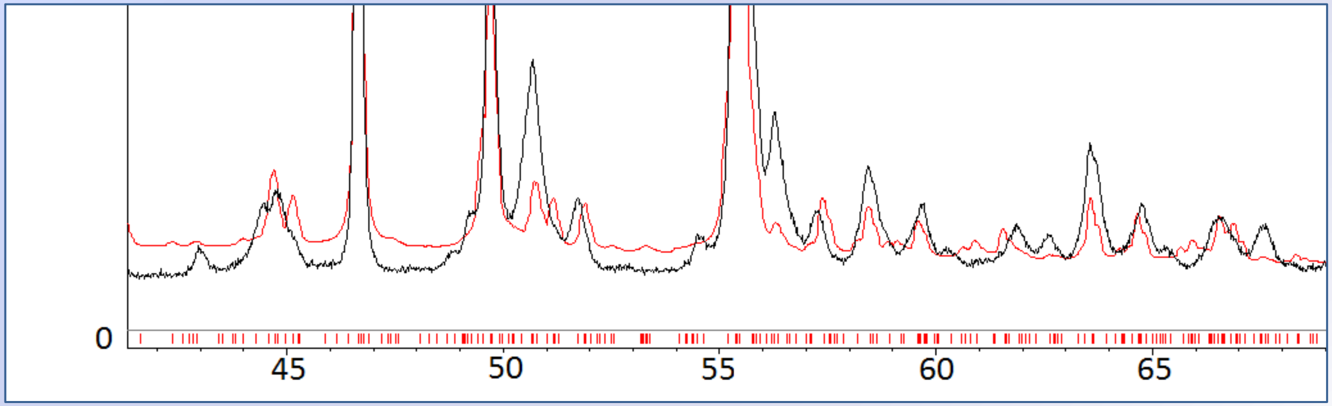
Ta_2O_5 polycristalline powder XRD

Secondary peaks

β-phase



Orthorhombic Pmm2



(1) D.R.M. Crooks et al, *Class.Q.Gravity*, 21, 1059 (2004); K.Numata et al.,*Phys.Rev.Letters*, 91,260602 (2003);S.Penn et al, *Class.Q.Gravity*, 20,2917 (2003); D.R.M. Crooks et al, *Class.Q.Gravity*, 23, 4953 (2006); G.Harry et al, *Class.Q.Gravity*, 24, 405 (2007)
(2) R. Flaminio, D. Forest, J. Franc, M. Galimberti, B. Lagrange, C. Michel, N. Morgado, L. Pinard, B. Sassolas, E. Saracco, R. Bonnand, J. Degallaix, *Coating R&D for future GW detectors,* 2011

(3) Powder of Ta_2O_5 : Aldrich , crystallite size < 5 µm, 99.99% metal basis

- β-phase
- Orthorhombic Pccm
- a=6,226 Å
- b=3,682 Å
- c=7,806 Å