

# The interplay between optical properties and structure of coatings for GWD

Spectroscopic Ellipsometry of coatings

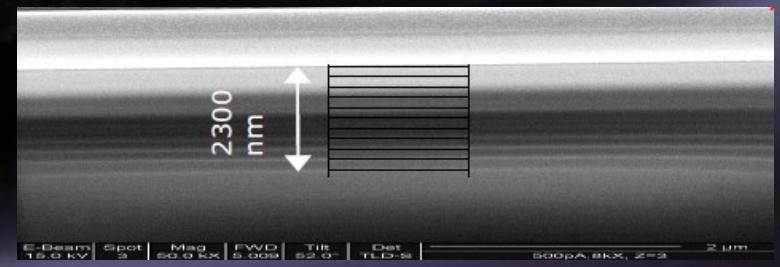
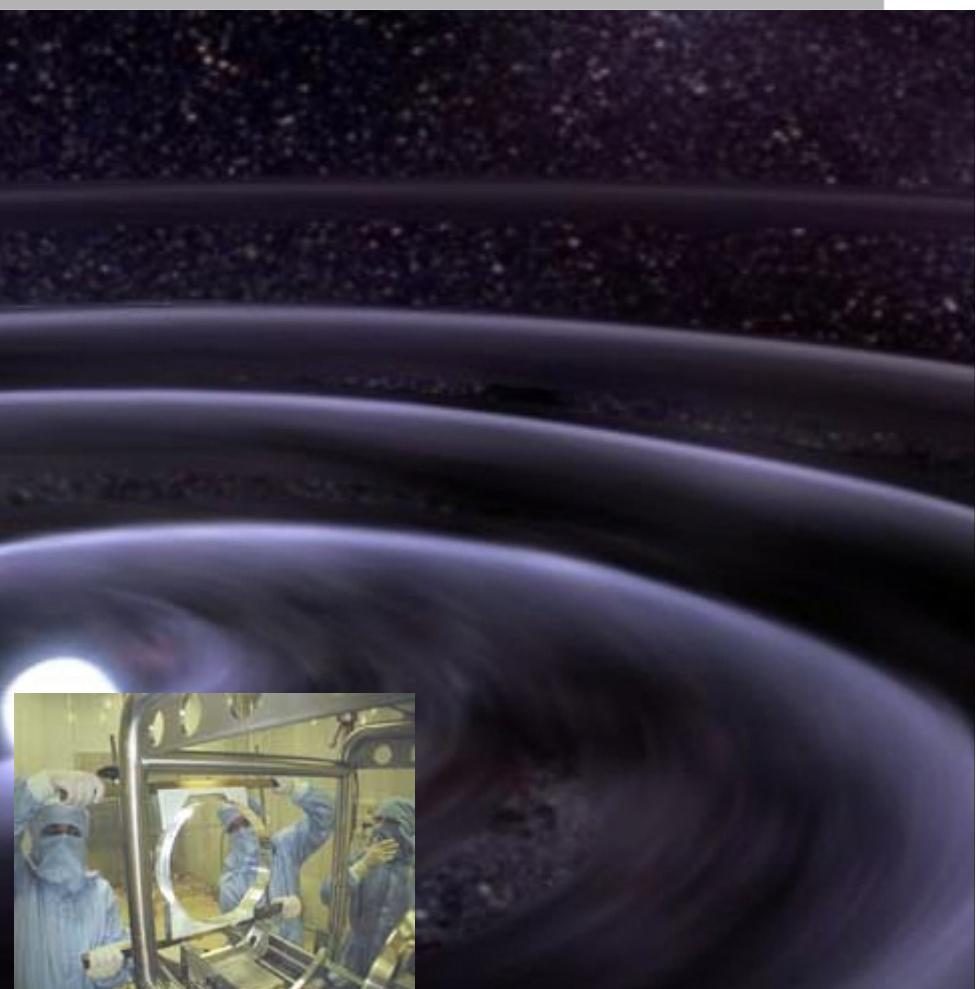
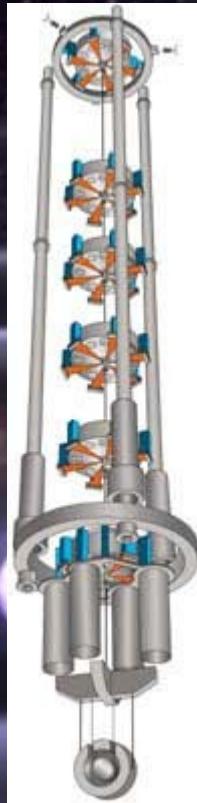
ADCOAT: first results

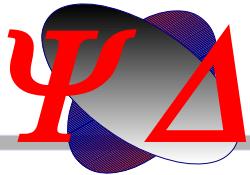
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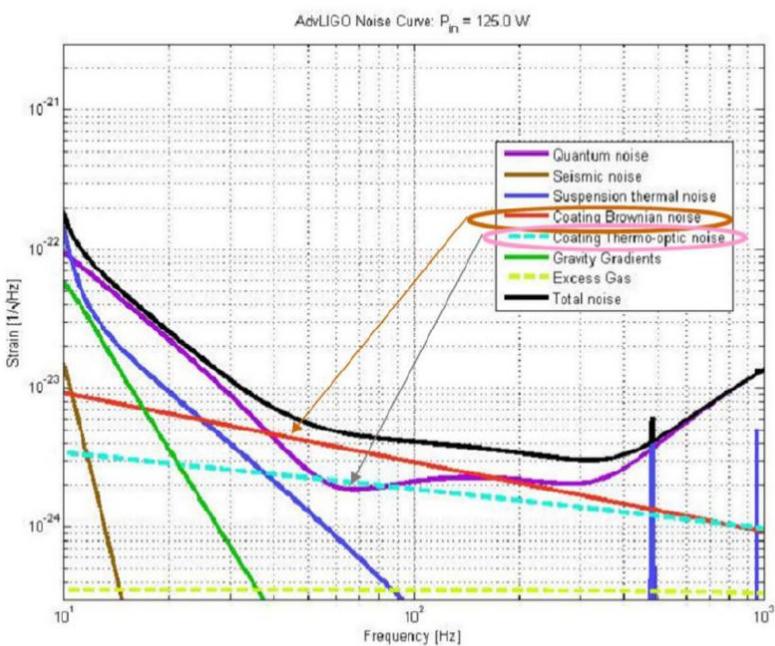


# A long travel ... from cosmology ... to nanophysics





# The coating affair: issues



- **Very ultra low optical absorptions**  
~ ppm
- **Ultra High Uniformity**  
“bulk” & surface
- **Very ultra low mechanical Losses**  
main source of thermal noise  
@ 100-300 Hz



## $\lambda/4$ Ta<sub>2</sub>O<sub>5</sub>/SiO<sub>2</sub> multilayers

Ta<sub>2</sub>O<sub>5</sub>:Ti still the best option for the high index material in  $\lambda/4$  multilayers

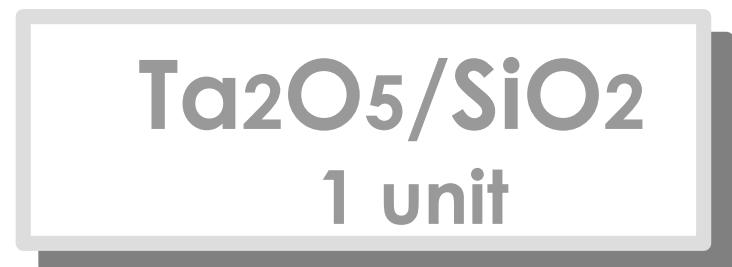
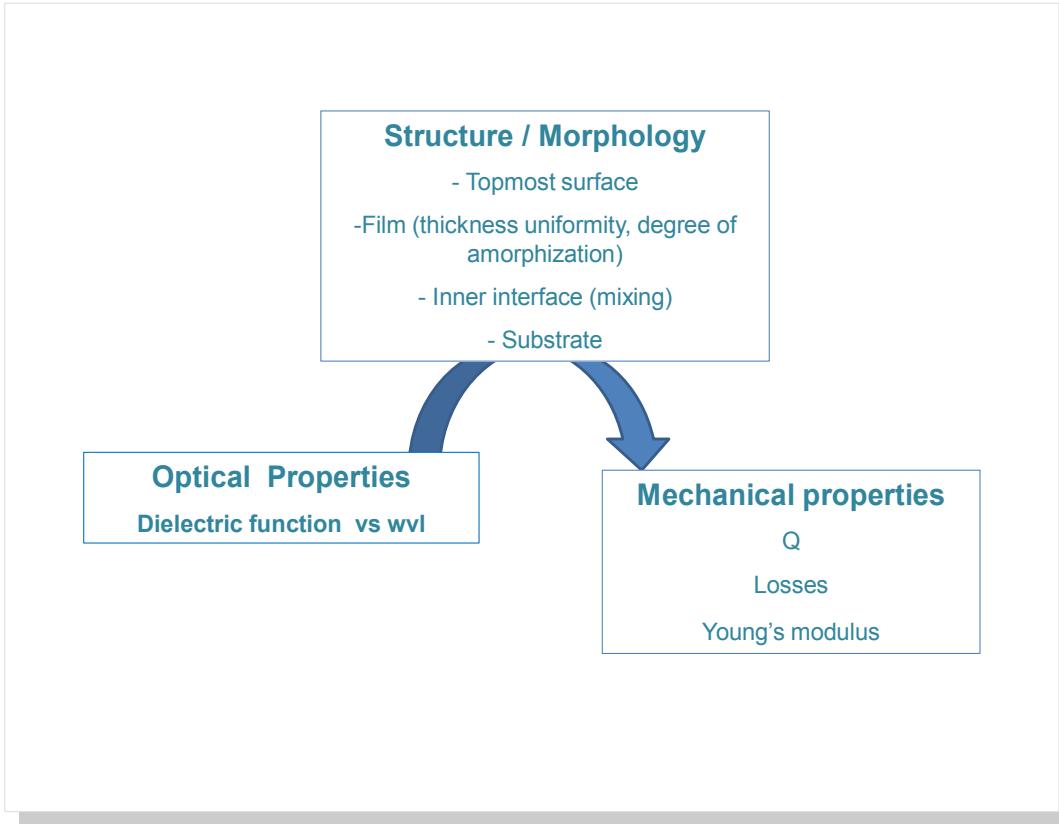
### Mechanical Losses: Main trends (@LMA)

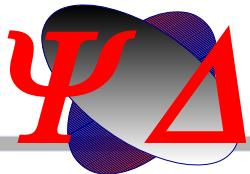
- no significant dependence on thickness of Ta<sub>2</sub>O<sub>5</sub>:Ti sub-unit
- significant increase with the number of interfaces in multilayers
- Losses on multilayers larger than the sum of monolayer losses
- Losses for ALD films comparable to IBS films

“nano-bugs” at interfaces & film

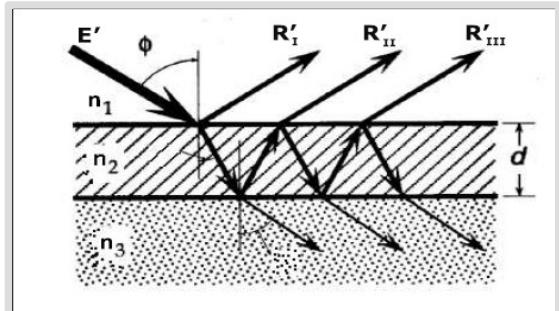
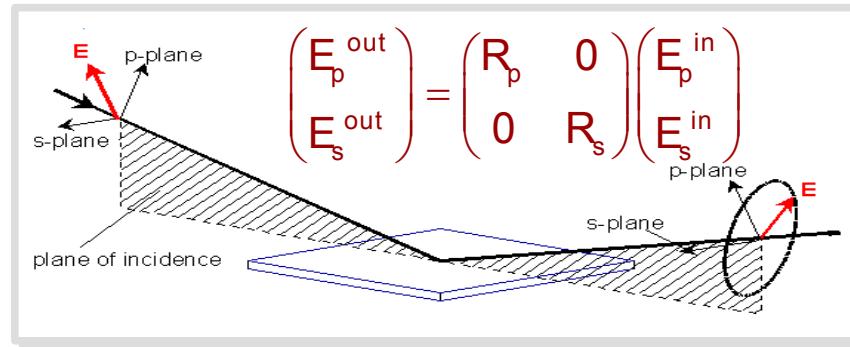


# Spectroscopic Ellipsometry of GWD coatings





# Spectroscopic Ellipsometry (isotropic systems: Fresnel theory)



$$\rho = t g \Psi e^{i\Delta} = \frac{R_p}{R_s} = \frac{r_{0,1}^p + r_{1,2}^p e^{-2i\beta}}{1 + r_{0,1}^p r_{1,2}^p e^{-2i\beta}} \cdot \frac{1 + r_{0,1}^s r_{1,2}^s e^{-2i\beta}}{r_{0,1}^s + r_{1,2}^s e^{-2i\beta}}$$

$$\beta = 2\pi \frac{d}{\lambda} \sqrt{\tilde{N}_1^2 - \tilde{N}_0^2 \sin^2 \phi}$$

$$\rho = \rho(\tilde{N}_0, \tilde{N}_1, \tilde{N}_2, d, \lambda, \phi)$$

**Comparison data/simulations: needs a model of the optical system**  
**If ambient and substrate properties are known with precision**  
**One needs**  
**(n,k) and d of the film**

$$MSE = \frac{1}{2N-M} \sum_{i=1}^N \left[ \left( \frac{\Psi_i^{\text{mod}} - \Psi_i^{\text{exp}}}{\sigma_{\Psi,i}^{\text{exp}}} \right)^2 + \left( \frac{\Delta_i^{\text{mod}} - \Delta_i^{\text{exp}}}{\sigma_{\Delta,i}^{\text{exp}}} \right)^2 \right] = \frac{1}{2N-M} \chi^2$$

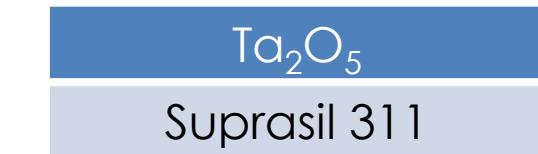
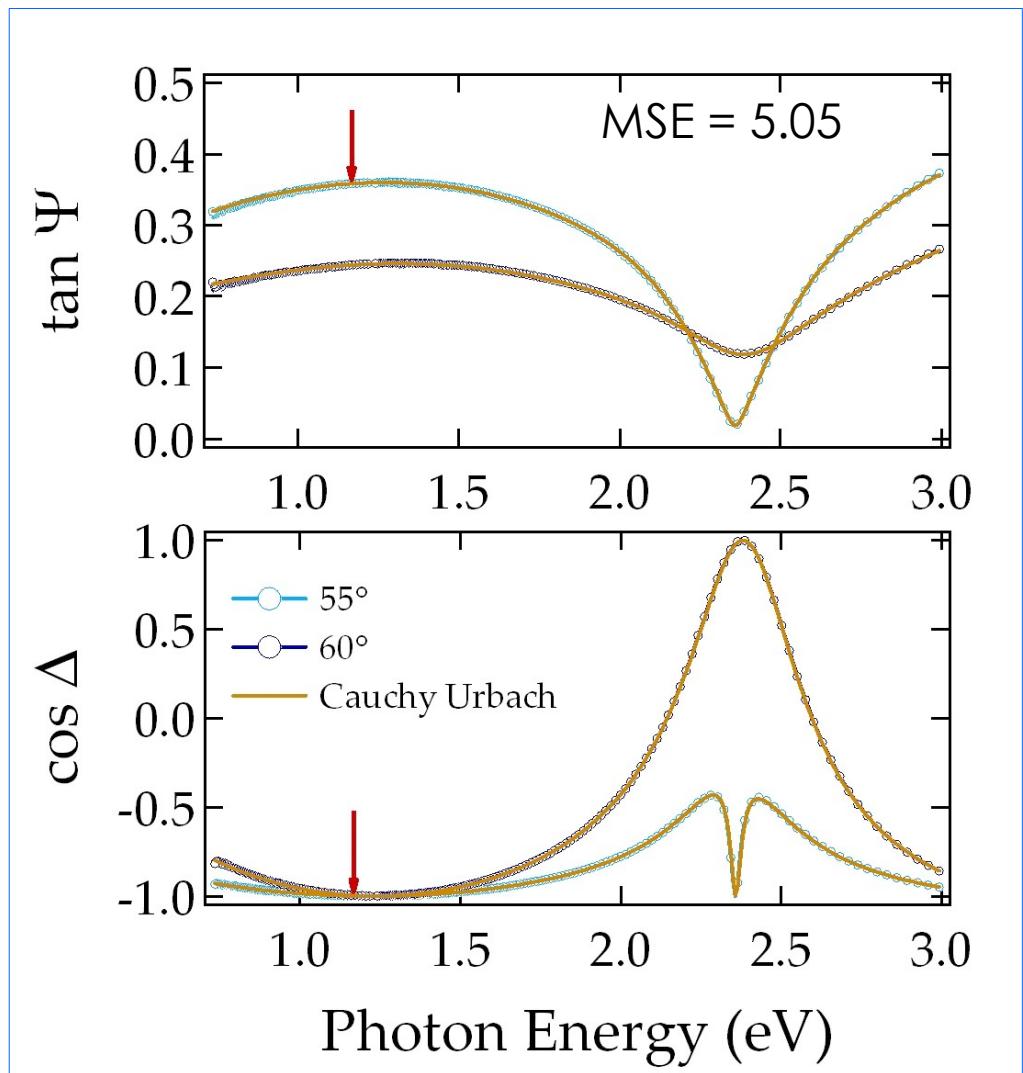


**Ta<sub>2</sub>O<sub>5</sub> (LMA)**  
nominal thickness: 131 nm



## Transparency region: thickness and n

No surface, no interface...



Cauchy – Urbach model

$$n = A + \frac{B}{\lambda^2} + \frac{C}{\lambda^4}$$

$$k = D \cdot e^{F(h\nu - G)}$$

thickness ~ **134 nm**

n@1064nm = **2.057**

k@1064nm < 10<sup>-3</sup>

R. Flaminio et al.  
Class. Quantum Grav. **27** (2010) 084030

n@1064nm ~ 2.06  
Monolayer absorption ~ 1.2 ppm (i.e. k ≈ 2 10<sup>-7</sup>)



# Extending the wavelength range over the gap 0.75-5 eV (245-1700 nm)

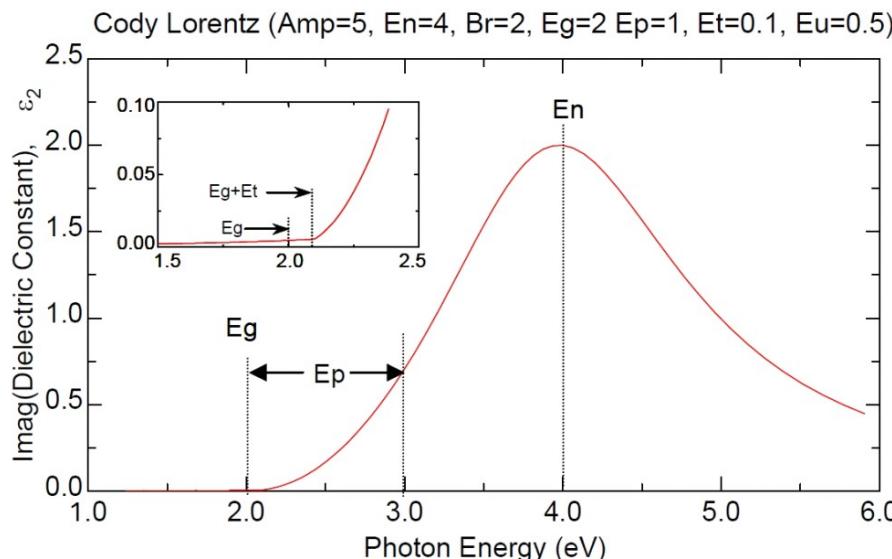
## Including defects

Amorphous oxides: Cody-Lorentz model + Urbach tail

[A. S. Ferlauto et al., Journal of Applied Physics 92 (2002)]

$$\epsilon_2(E) = \begin{cases} \left(\frac{E_1}{E}\right) e^{\left[\frac{(E-E_g-E_t)}{E_u}\right]} & 0 < E \leq (E_g + E_t) \\ \frac{(E-E_g)^2}{(E-E_g)^2 + E_p^2} \frac{AE_0\Gamma E}{[(E^2 - E_0^2)^2 + \Gamma^2 E^2]} & E > (E_g + E_t) \end{cases}$$

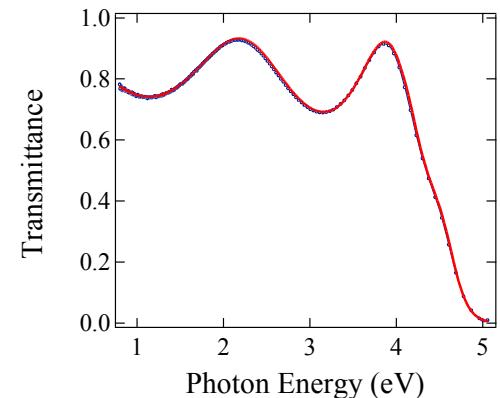
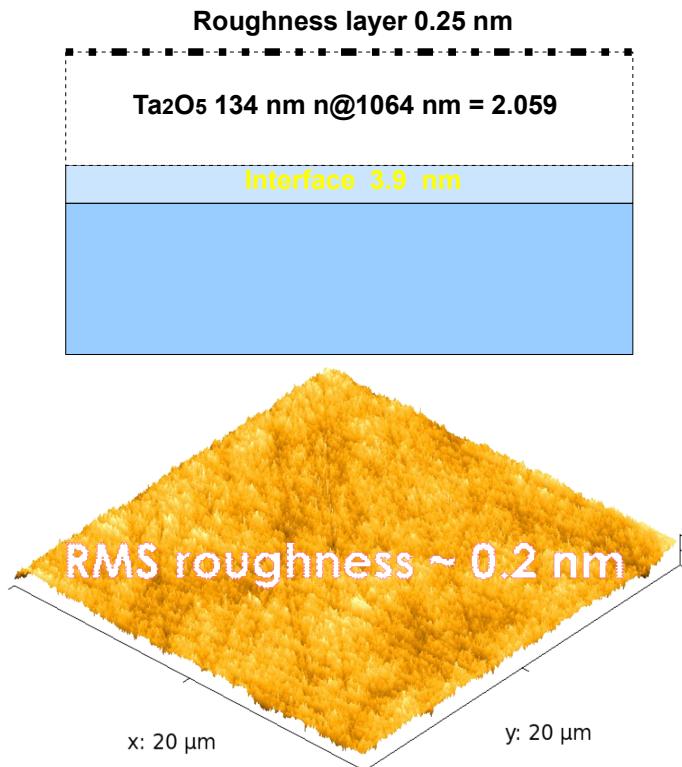
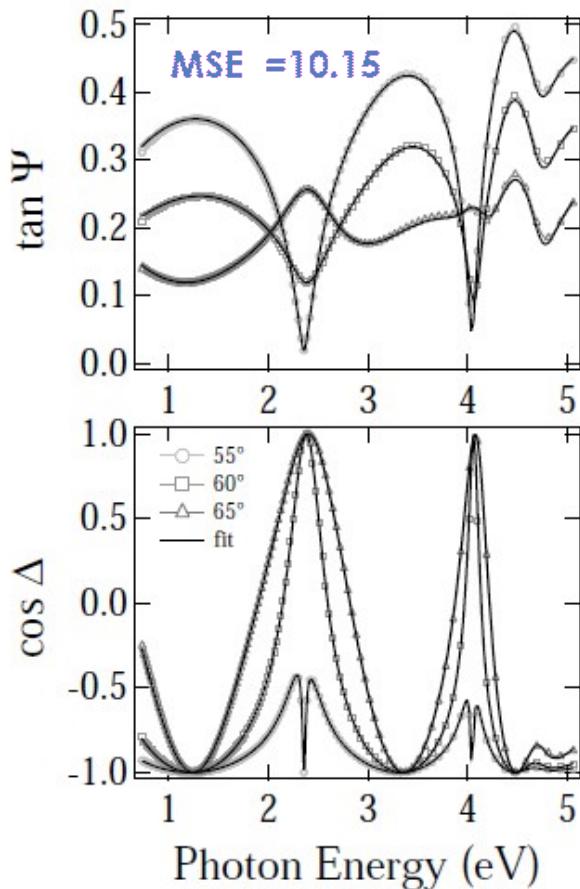
$$\epsilon_1(E) = \epsilon_1(\infty) + \frac{2}{\pi} P \int_{E_g}^{\infty} \frac{\xi \epsilon_2(\xi)}{\xi^2 - E^2} d\xi$$





## Including non-uniformity

The “simplest model” : Roughness layer + transition layer



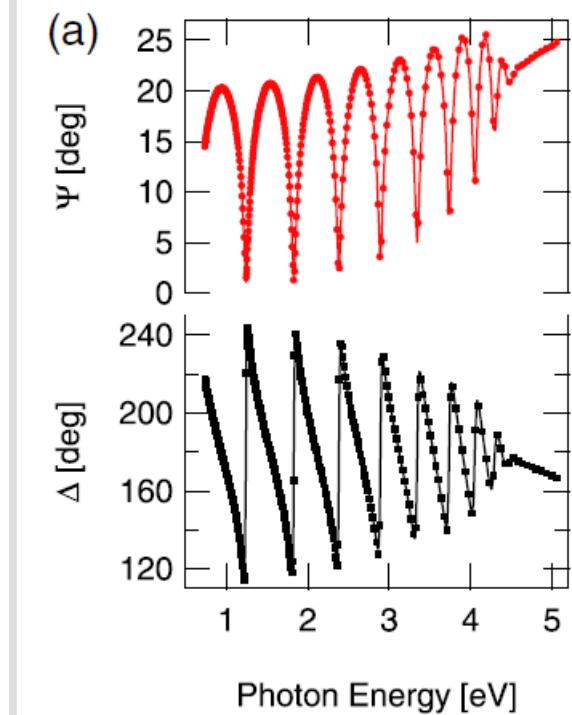
...Non-ideal interface....



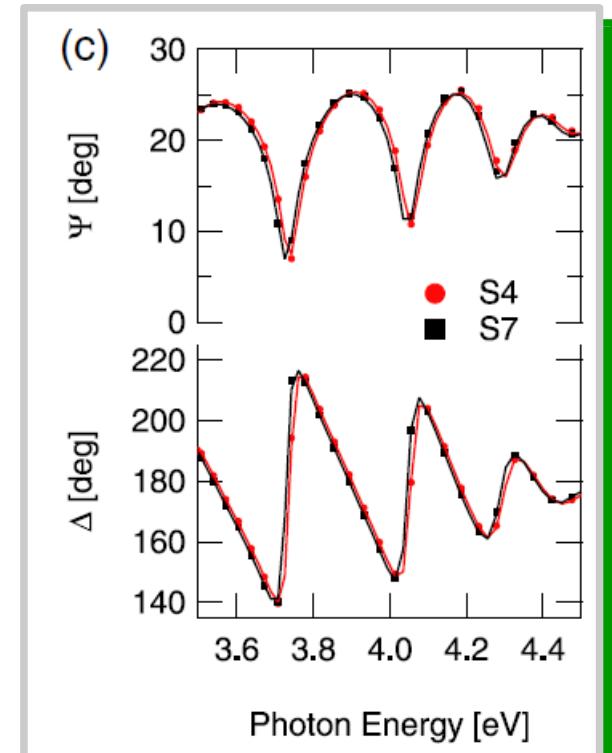
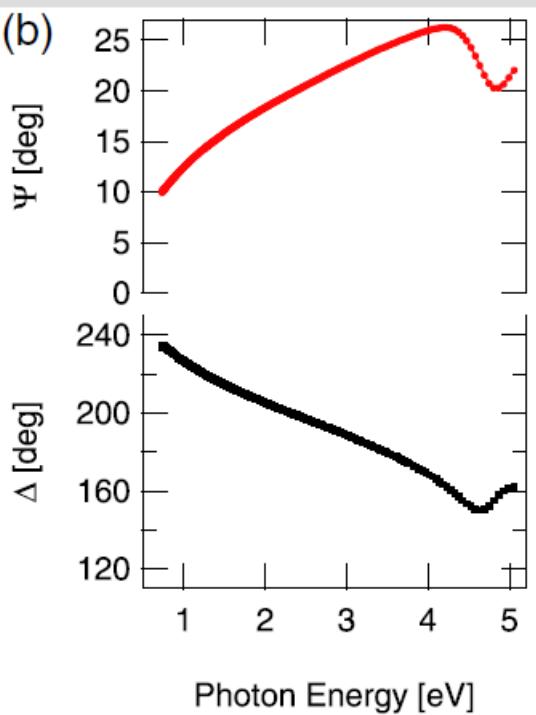
# Spectroscopic Ellipsometry + PCI@1064nm

(Ta<sub>2</sub>O<sub>5</sub>/SiO<sub>2</sub>- CSIRO)

Anghinolfi et al., JPhysD 46 (2013) 455301



Two sets of samples  
annealing temperature up  
to 600 °C



	Id	$T_{\text{ann}}$ °C	CL ( $E_g$ )	TL ( $E_g$ )	TP (CL,TL,Psemi)	Thickness (nm)	Abs. @ 1064 nm(ppm)
40 nm	S1	n/a	4.15	4.13	$4.20 \pm 0.1$	38.2	0.9
	S2	450	4.18	4.17	$4.24 \pm 0.1$	38.9	3.2
500 nm	S3	550	4.16	4.16	$4.24 \pm 0.1$	39.1	2.9
	S4	300	4.13	4.13	$4.19 \pm 0.1$	514.6	1.1
	S5	400	4.13	4.13	$4.19 \pm 0.1$	515.6	1.4
	S6	500	4.13	4.13	$4.19 \pm 0.1$	517.6	2.1
	S7	600	4.15	4.13	$4.19 \pm 0.1$	519.9	1.9



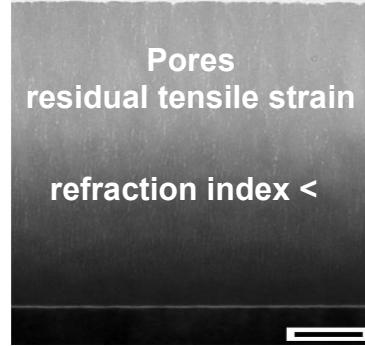
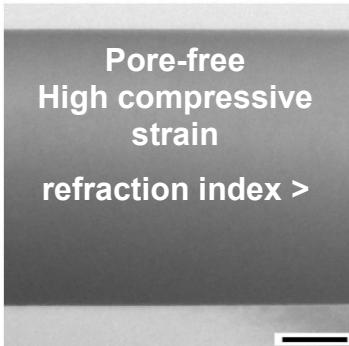
# Ta<sub>2</sub>O<sub>5</sub>/Void Graded EMA (Maxwell-Garnett)



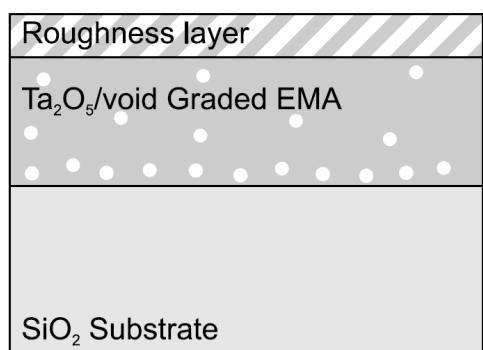
The correlation between mechanical stress, thermal shift and refractive index in HfO<sub>2</sub>, Nb<sub>2</sub>O<sub>5</sub>, Ta<sub>2</sub>O<sub>5</sub> and SiO<sub>2</sub> layers and its relation to the layer porosity

O. Stenzel<sup>a,\*</sup>, S. Wilbrandt<sup>a</sup>, N. Kaiser<sup>a</sup>, M. Vinnichenko<sup>b</sup>, F. Munnik<sup>b</sup>, A. Koltsch<sup>b</sup>, A. Chuvilin<sup>c</sup>, U. Kaiser<sup>c</sup>, J. Ebert<sup>d</sup>, S. Jakobs<sup>d</sup>, A. Kales<sup>d</sup>, S. Wüthrich<sup>d</sup>, O. Treichel<sup>d</sup>, B. Wunderlich<sup>d</sup>, M. Bitzer<sup>d</sup>, M. Grössl<sup>d</sup>

**"pores are helpful to obtain a reasonable balance between optical and mechanical layer properties"**



Cfr. O. Stenzel JPhysD2009



Nano-voids  
size<< $\lambda$   
(not at scale)

No intermixing

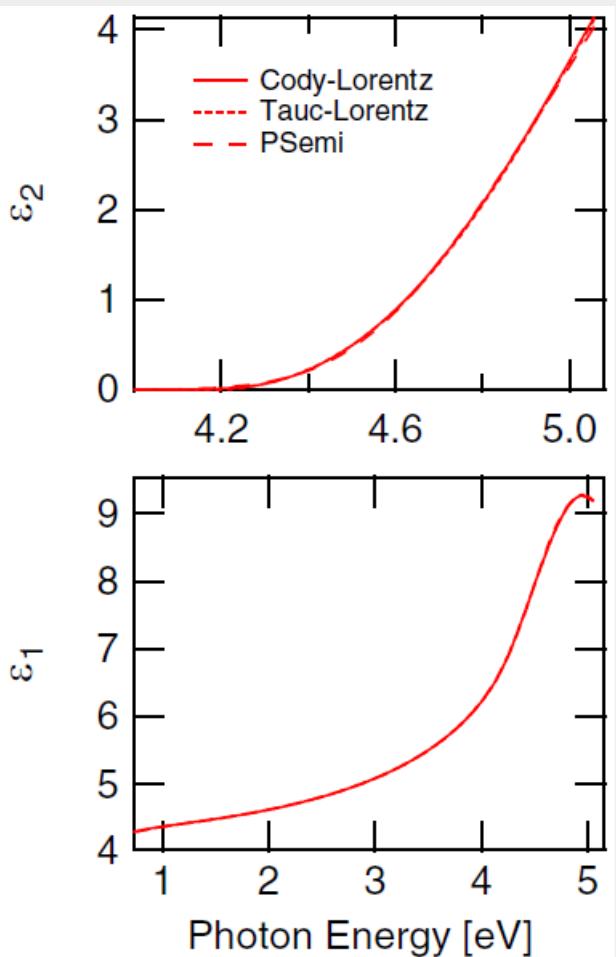
Three models for absorption edge of amorphous semiconductors

Anghinolfi et al., JPhysD 2013

	Id.	T <sub>ann</sub> (°C)	CL (E <sub>g</sub> )	TL (E <sub>g</sub> )	TP (CL,TL,Psemi)	Thickness (nm)	Abs. @ 1064 nm(ppm)
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# Ta<sub>2</sub>O<sub>5</sub>/SiO<sub>2</sub>- CSIRO



- Best fit independent from the model
- 6-7% of porosity
- empty, spherical nano-pores
- quasi-uniform distribution across the film.

increasing  $T_{ann}$ -

	Id.	$T_{ann}$ (°C)	CI ( $E_g$ )	TL ( $E_g$ )	TP (CI, TL, Psemi)	Thickness (nm)	Abs @ 1064 nm(ppm)
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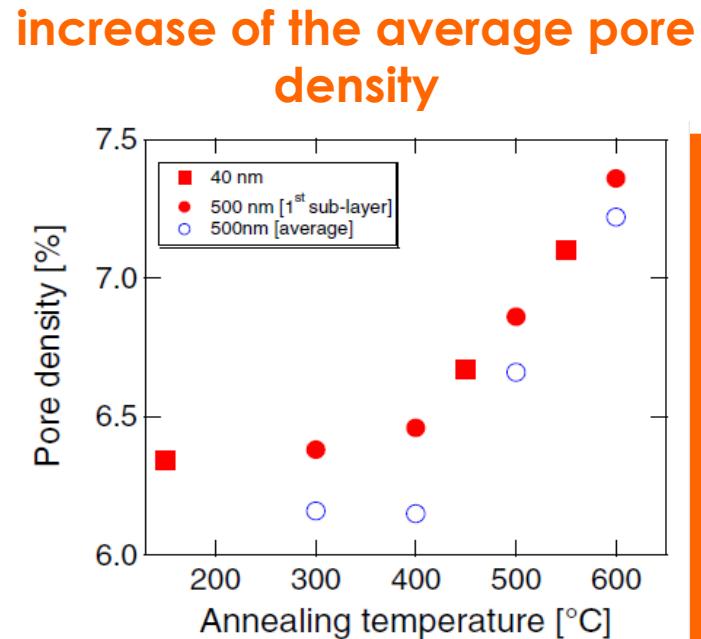
Tiny blue-shift of  $E_g$

- slight increase (1-2%) of thickness

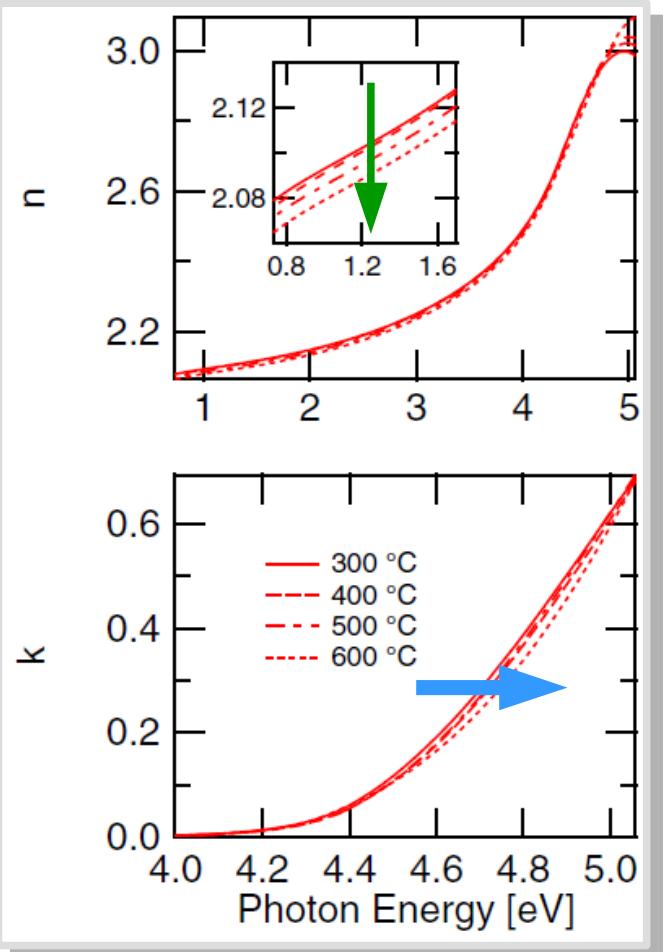
increase of NIR absorption losses (PCI at 1064 nm).



# Ta<sub>2</sub>O<sub>5</sub>/SiO<sub>2</sub>- CSIRO: increasing T<sub>ann</sub>



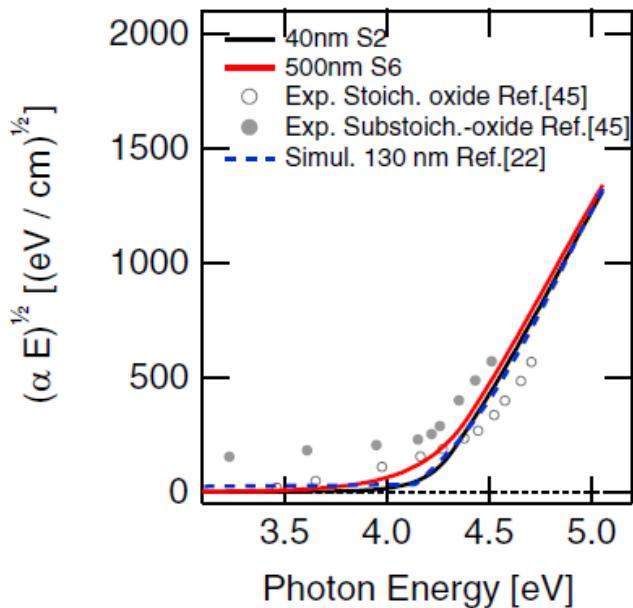
small reduction of n



slight blue-shift of Eg (+ evident on the 40 nm thick coating)  
Improved stoichiometry  
Onset of (nano)-crystallization (to be checked e.g. With Raman)



# Ta<sub>2</sub>O<sub>5</sub>/SiO<sub>2</sub>- CSIRO: increasing T<sub>ann</sub>



Optical properties vs. Tann testify micro-structural modifications → (nano-pores model)

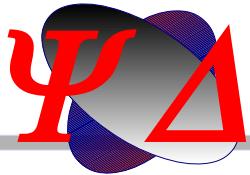
pores may play a crucial role in the release of compressive strain induced by the densification @ deposition

pores (especially open ones) tend to reduce the effective refractive index of the coating. The relatively modest effects on n are consistent with a main population of closed pores

the increase in d<sub>Ta2O5</sub> and in the average pore density with increasing T<sub>ann</sub>, coupled to the reduction of n can be associated with the expansion of nano-cavities

## future

- extending the range in the UV → 190 nm
  - scatterometry (in-plane)
- couple SE with high ex-situ sensitivity structural probes (Raman, XRD) and with TEM
  - study SiO<sub>2</sub>/Ta<sub>2</sub>O<sub>5</sub>/SiO<sub>2</sub> system vs annealing
    - real time SE to monitor slow annealing



# Moving ahead (glassy-oxide paradigm)



- “Debugging” Ta<sub>2</sub>O<sub>5</sub>:Ti
  - better control of annealing process (T, t)
  - unambiguous “decoding” of trends
  - How and why “dopants” work?
- Searching for “the best” glassy oxide mixture
  - “failed” sofar
- Optimizing the design
  - e.g. fine tuning of thickness of bilayer units  
[Villar et al., PRD 81 (2010) 122001]
- Testing new materials and multilayers
  - e.g for low T operation (silica doped Hafnia)
  - **nanolayered composites** (Titania::Silica and Hafnia::Silica)

- modelling  
**(Effective Medium Theory)**
  - mechanical losses  
[Villar et al., LIGO- G1100 976]
  - optical properties  
[Anghinolfi et al. JphysD, 2013]
- Testing
  - extensive trial-and-error



# ADCOAT People



*Innocenzo M. Pinto (PI, AdCOAT Coordinator)  
Vincenzo Galdi, Vincenzo Pierro, Maria Principe,  
Dario Castellano, Silvio Savoia*



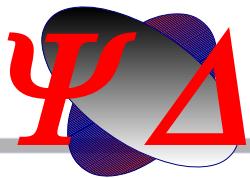
*Maurizio Canepa (PI), Corrado Boragno, Francesco Buatier de Mongaot, Mauro Giovannini,  
Lorenzo Mattera, Gianluca Gemme, Martina Neri*



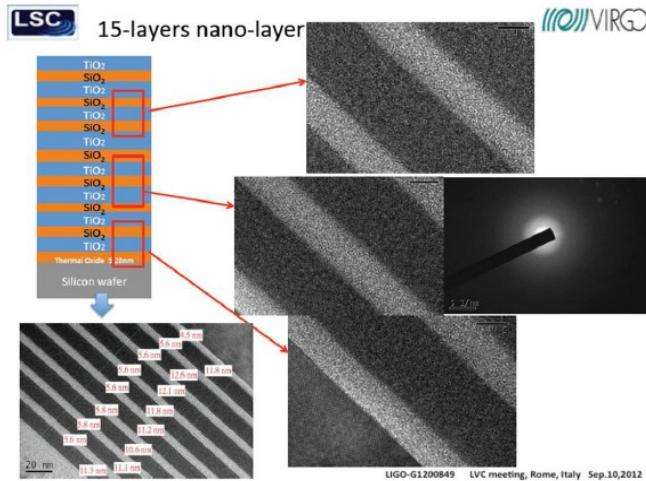
*Helios Vocca (PI), Marzia Colombini, Luca  
Gammaitoni, Fabio Marchesoni, Maurizio  
Mattarelli, Igor Neri*



*Alessio Rocchi (PI), Elisabetta Cesarini, Eugenio  
Coccia, Viviana Fafone, Yuri Minenkov*



# ADCOAT Nanolayer composites Prototypes



Full details in S. Chao et al., LIGO-G1200849

As deposited

$$d_{(\text{TiO}_2)} = 27.30 (\pm 0.05) \text{ vs. } 27.1 \text{ nominal}$$

$$n_{\text{TiO}_2} @ 1064\text{nm} = 2.32$$

$$d_{(\text{SiO}_2)} = 20.15 (\pm 0.05) \text{ vs. } 19.9 \text{ nominal}$$

$$n_{\text{SiO}_2} @ 1064\text{nm} = 1.48$$

Work in progress ... 19 units  
M. Magnozzi, M. Neri, I. Solano, S. Uttiya