CoaCh: recent updates on optical characterization

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CoaCh

CoaCh collaboration involves the following groups:

Firenze/Urbino
Genova
Pisa
Perugia
Padova/Trento

Coordinated by prof. F. Vetrano (Urbino University and INFN Firenze)

Aim:

1) to find the relation between coating mechanical and optical properties
2) to understand how mechanical/optical properties depend on chemistry/ structure/morphology of the coating.

Funded by Italian Ministry of Research and Education (PRINContract 2007T7AC3L)

Results shown @ GWADW 2010

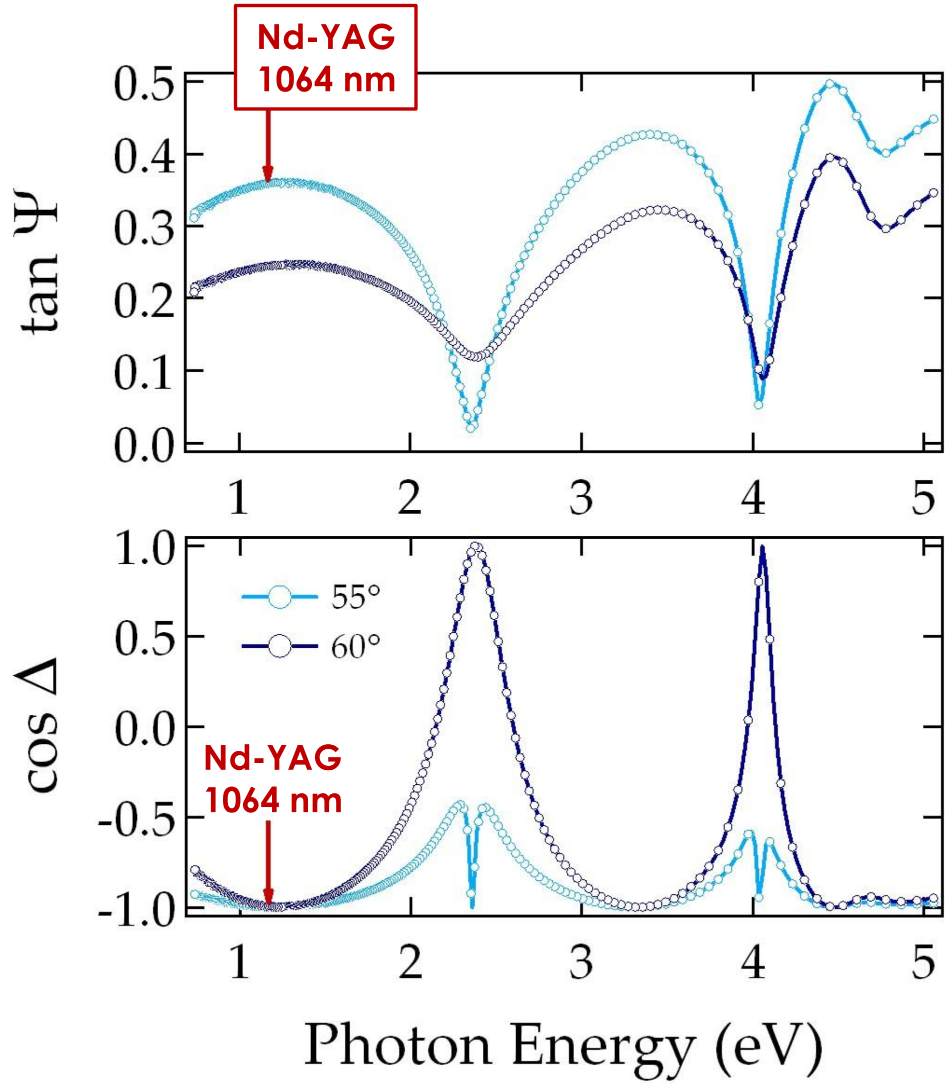
Samples:
Ta_2O_5 (LMA, Lyon) on SiO_2 substrates (Heraeus)
nominal thickness: 131 nm

Spectroscopic Ellipsometry (SE) investigation

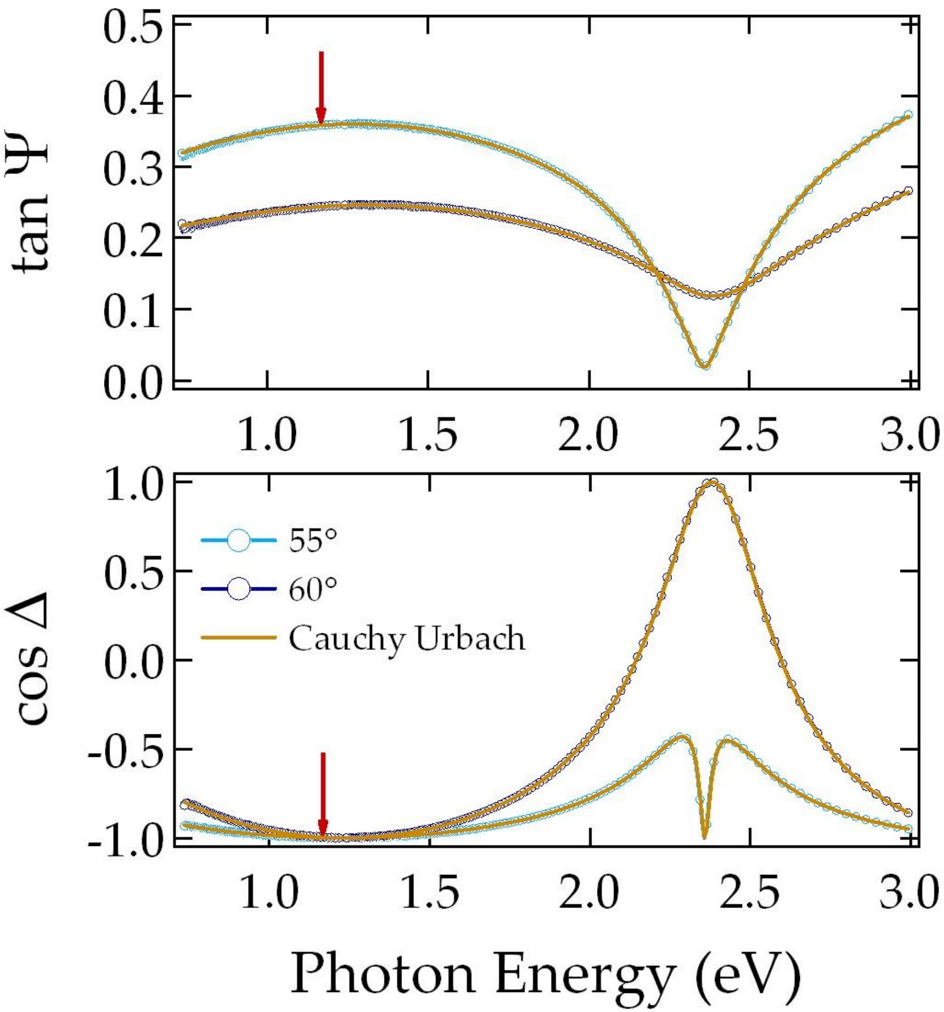
$$\rho = \frac{R_p}{R_s} = \left|\frac{R_p}{R_s}\right| e^{i(\delta_{rp}-\delta_{rs})} = \tan\Psi e^{i\Delta}$$

$$\Psi = \arctan\frac{|R_p|}{|R_s|}$$

$$\Delta = \delta_{rp} - \delta_{rs}$$



Results shown @ GWADW 2010



Ta_2O_5

Suprasil 311

Cauchy – Urbach model

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

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

Ta_2O_5 thickness ~ 134 nm

Ta_2O_5 n@1064nm ~ 2.057

Ta_2O_5 k@1064nm ~ 8 10^{-4}

MSE = 5.05

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

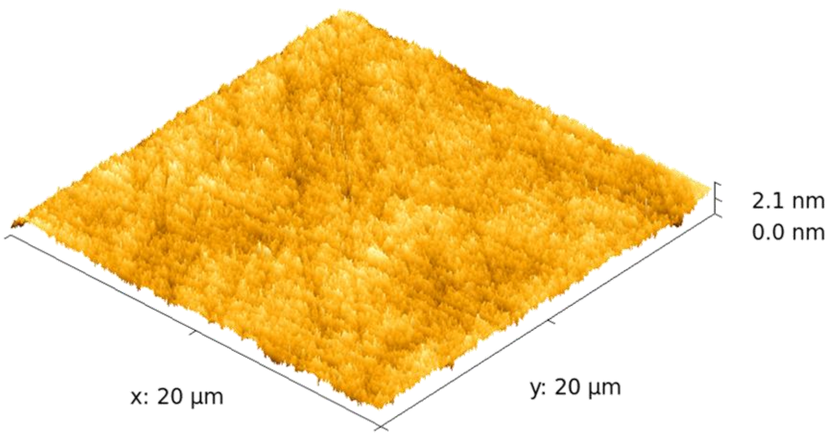
Optical index ~ 2.06

Monolayer absorption ~ 1.2 ppm (i.e. k ≈ 2 10^{-7})

Results shown @ GWADW 2010

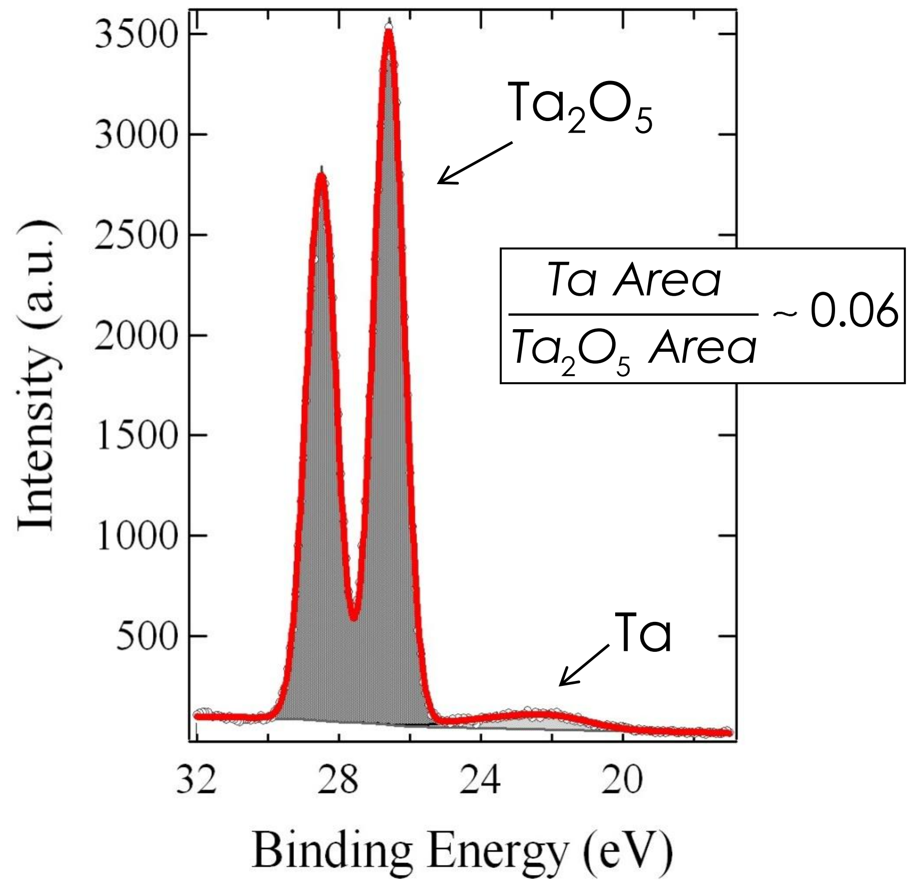
Investigation of the surface layer:

Atomic Force Microscopy (AFM)



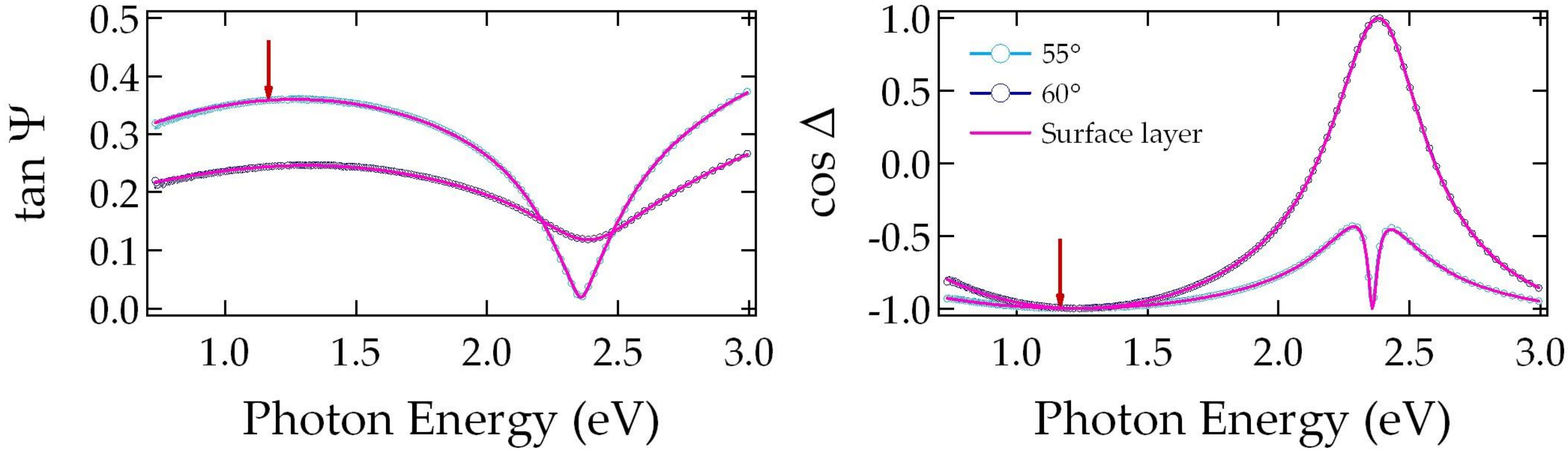
RMS roughness ~ 0.2 nm

X-ray Photoelectron Spectroscopy (XPS)



Results shown @ GWADW 2010

Surface roughness
Ta_2O_5 + Ta
Ta_2O_5 - k@1064nm = 2 10^{-7} (fixed to the LMA value)
Suprasil 311



MSE = 4.99

Ta_2O_5 n@1064nm ~ 2.054

Ta_2O_5 thickness ~ 133 nm

Surface Roughness ~ 0.4 nm

(Ta_2O_5 + Ta) thickness ~ 1 nm

%Ta in(Ta_2O_5 +Ta) ~ 6 %

Results shown @ GWADW 2010

Comments:

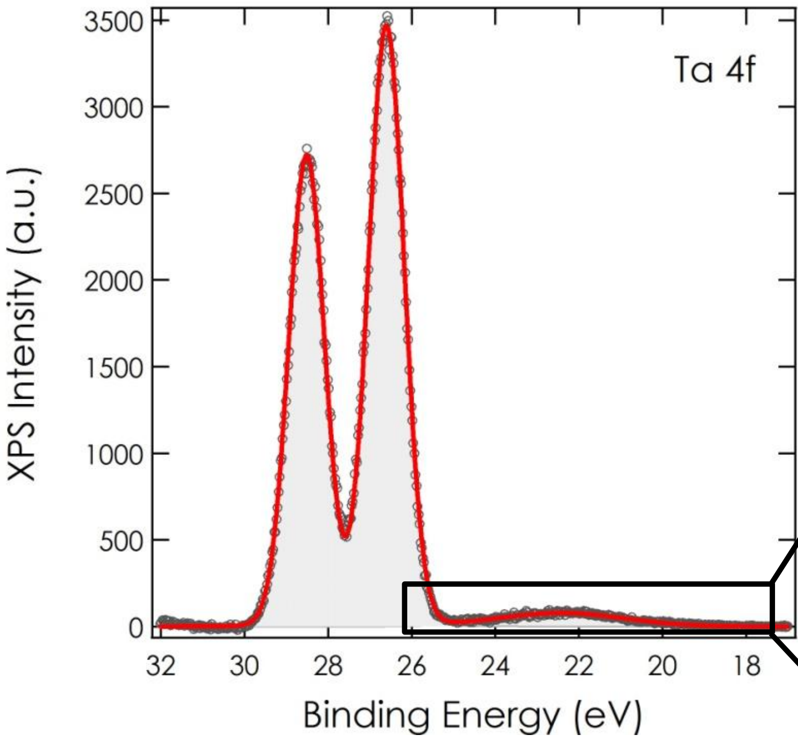
1) The proposed model works on a limited range

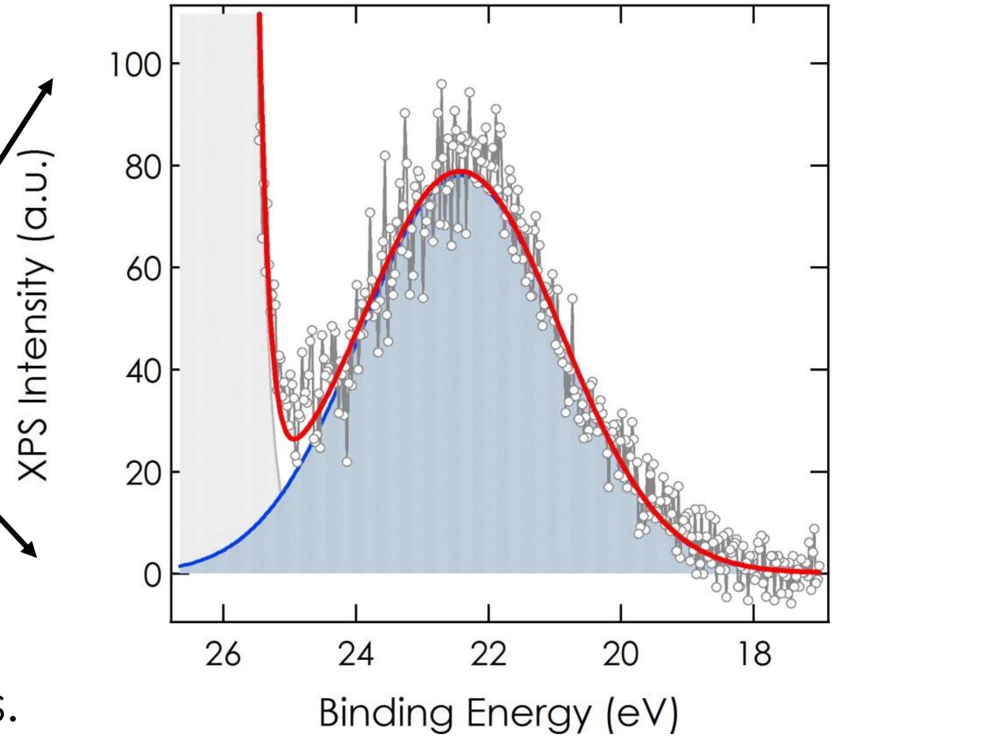
2) It does not count in possible non-idealities at the Suprasil/Tantala interface

3) The metallic Ta fraction seems to be too high

→ We need to improve the interpretation of both the XPS and the SE data

Improving the XPS interpretation

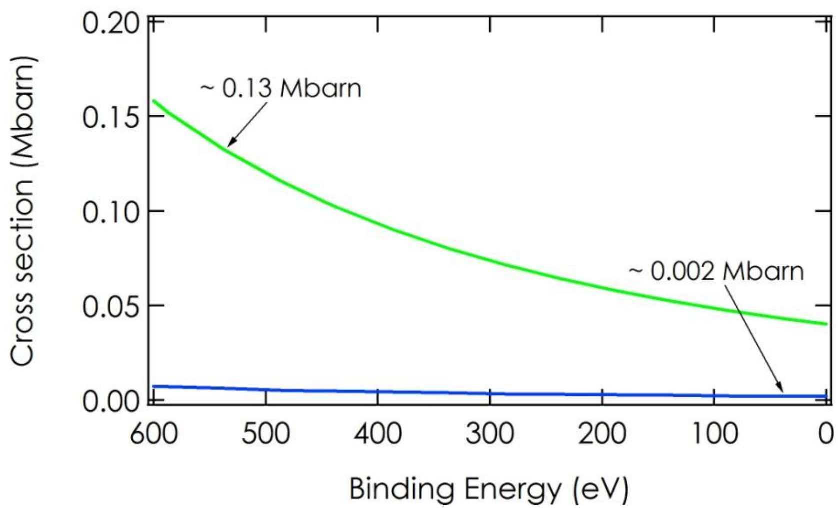




1. High FWHM indicates the presence of more than one chemical species.

2. The BE range (20 ÷ 24) eV is also typical for O 2s photoelectrons of oxides (e.g., TiO_2 @ 22.4 eV, IrO_2 @ 22.0 eV, Cr_2O_3 @ 22.5 eV). [NIST Database]

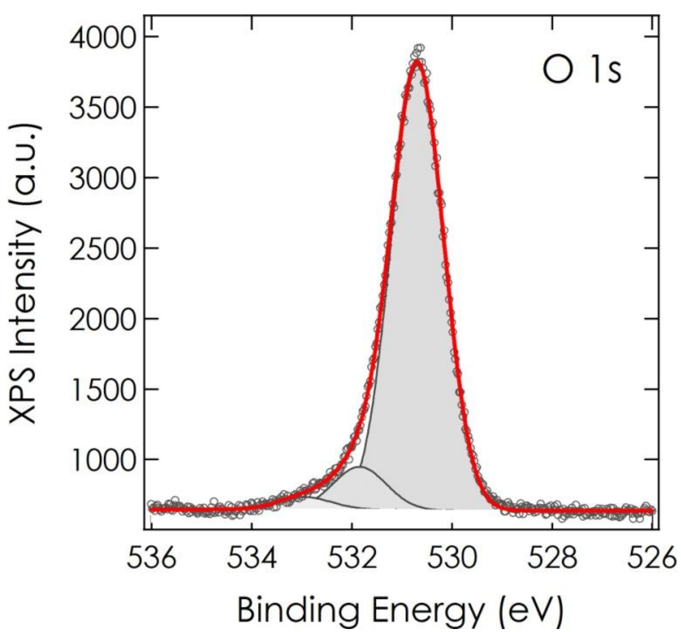
Improving the XPS interpretation



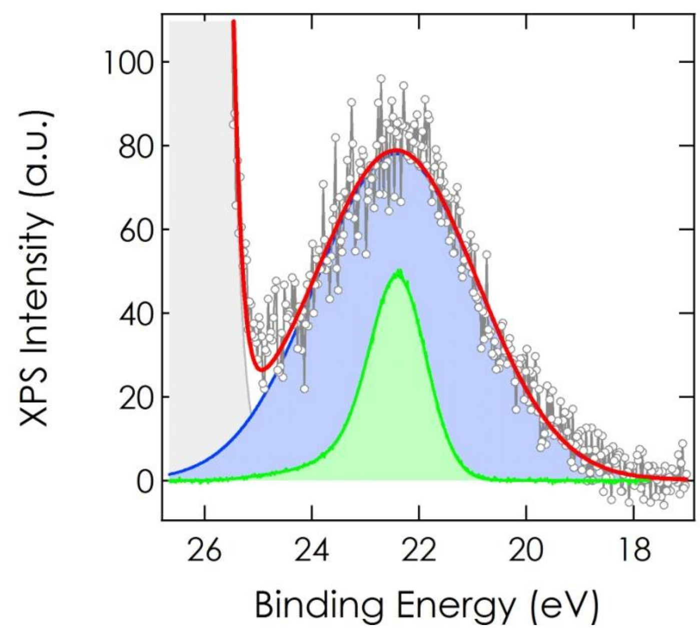
O1s vs. O2s cross-sections

http://ulisse.elettra.trieste.it/services/elements/WebElements.html

25 – 30% of the peak is due to O 2s photoelectrons.



Scaled & shifted



Improving the SE interpretation

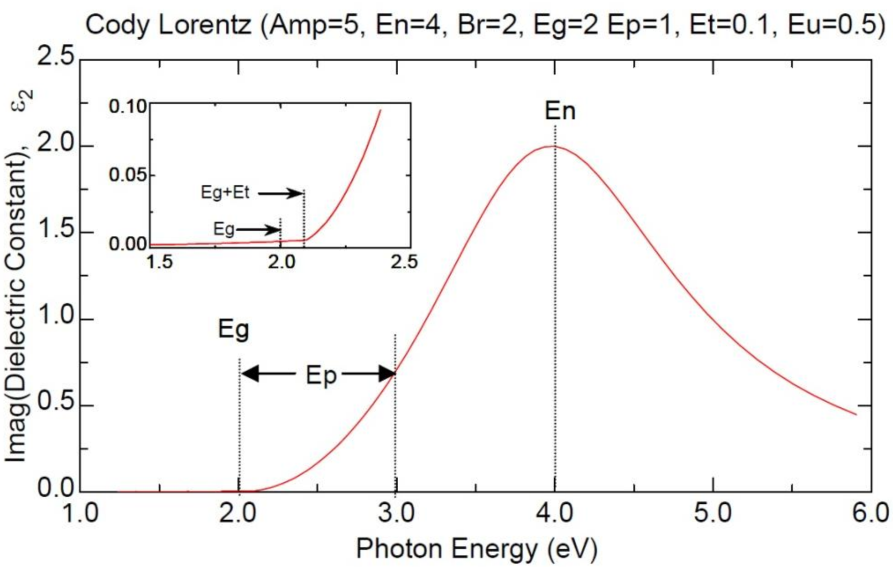
1. Extend the analysis to the whole energy range: 0.75 – 5 eV

Amorphous oxides: Cody-Lorentz model + Urbach tail

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

$$\varepsilon_2(E) = \begin{cases} \left(\dfrac{E_1}{E}\right) e^{\left[\frac{(E-E_g-E_t)}{E_U}\right]} & 0 < E \le (E_g + E_t) \\ \dfrac{(E-E_g)^2}{(E-E_g)^2+E_p^2} \dfrac{AE_0\Gamma E}{[(E^2-E_0^2)^2+\Gamma^2E^2]} & E > (E_g+E_t) \end{cases}$$

$$\varepsilon_1(E) = \varepsilon_1(\infty) + \frac{2}{\pi} P \int_{E_g}^{\infty} \frac{\xi \varepsilon_2 \ \xi}{\xi^2 - E^2} d\xi$$

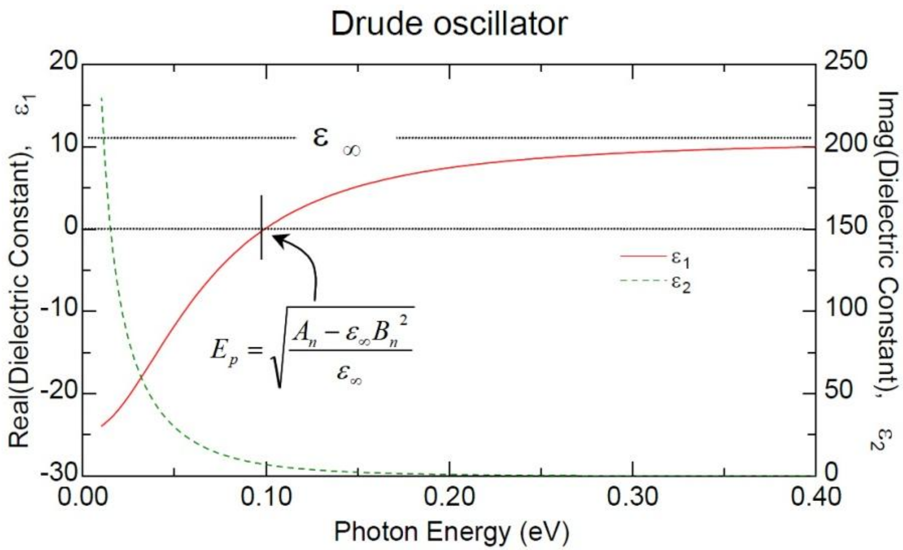


Improving the SE interpretation

2. Include in the model the optical absorption due to defect-related free carriers in the lowest energy range

Free carriers: Drude oscillator

$$\varepsilon(E) = \varepsilon_\infty - \frac{A}{E^2 + iBE}$$

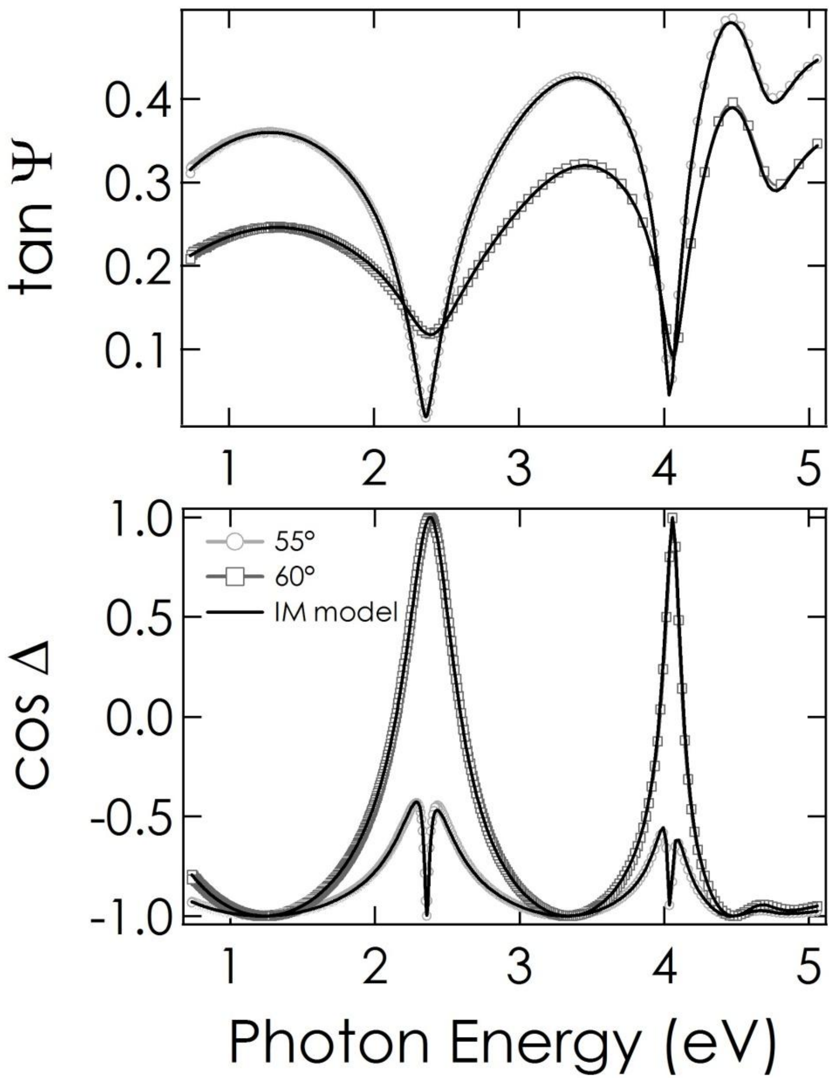


3. Include in the model the presence of an interface layer

Interface:
- Intermix (50:50)of SiO_2 and Ta_2O_5 (IM model)
- Low density Ta_2O_5 layer, i.e. voids (GV model)

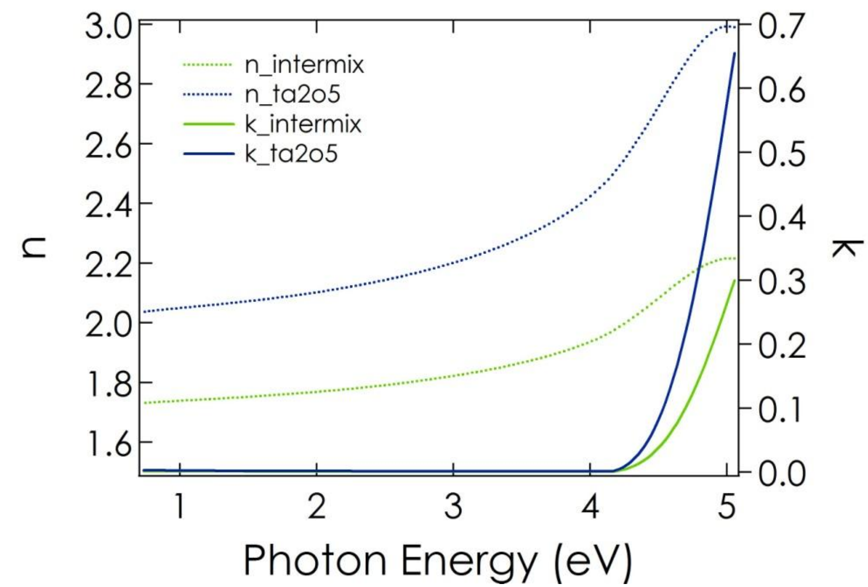
Improving the SE interpretation

Intermix



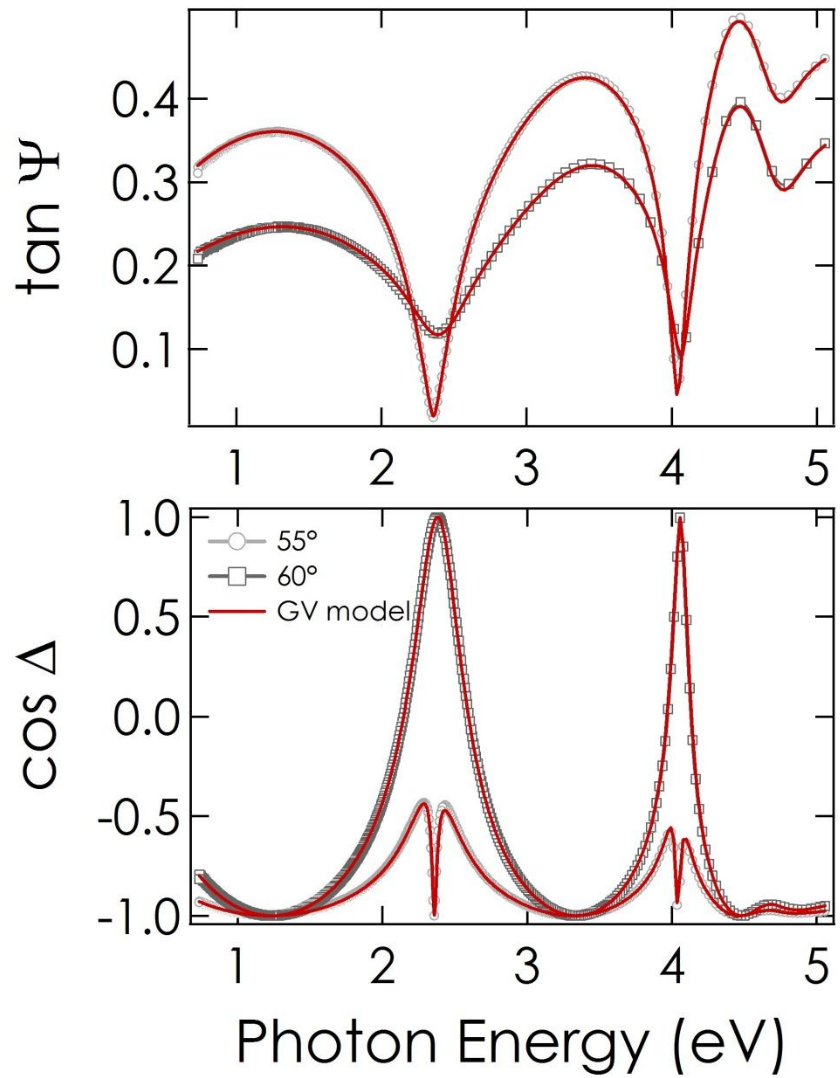
Surface roughness ~ 0.3 nm
Ta_2O_5 ~ 131 nm
Intermix 50:50 ~ 6 nm
Suprasil 311

MSE = 10.15



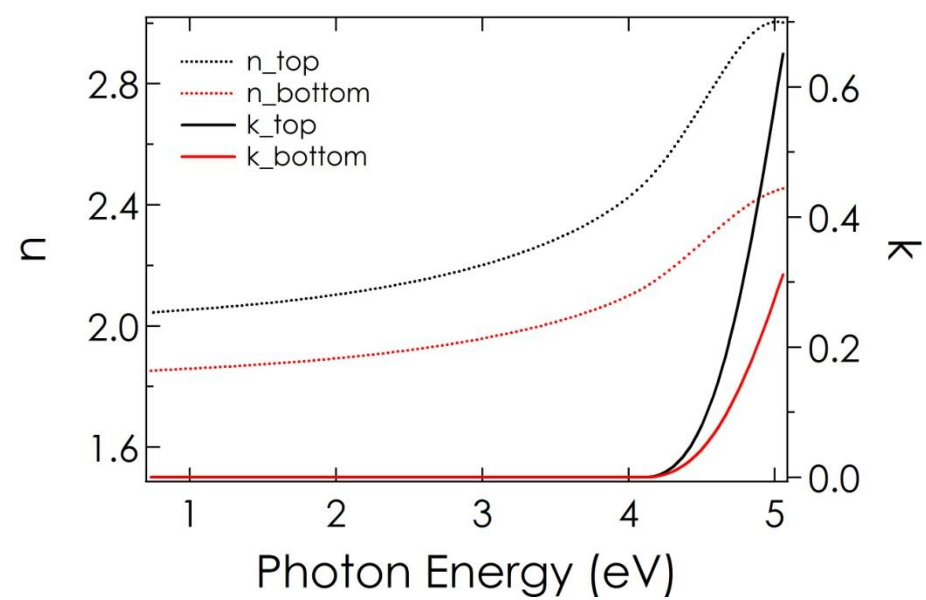
Improving the SE interpretation

Voids



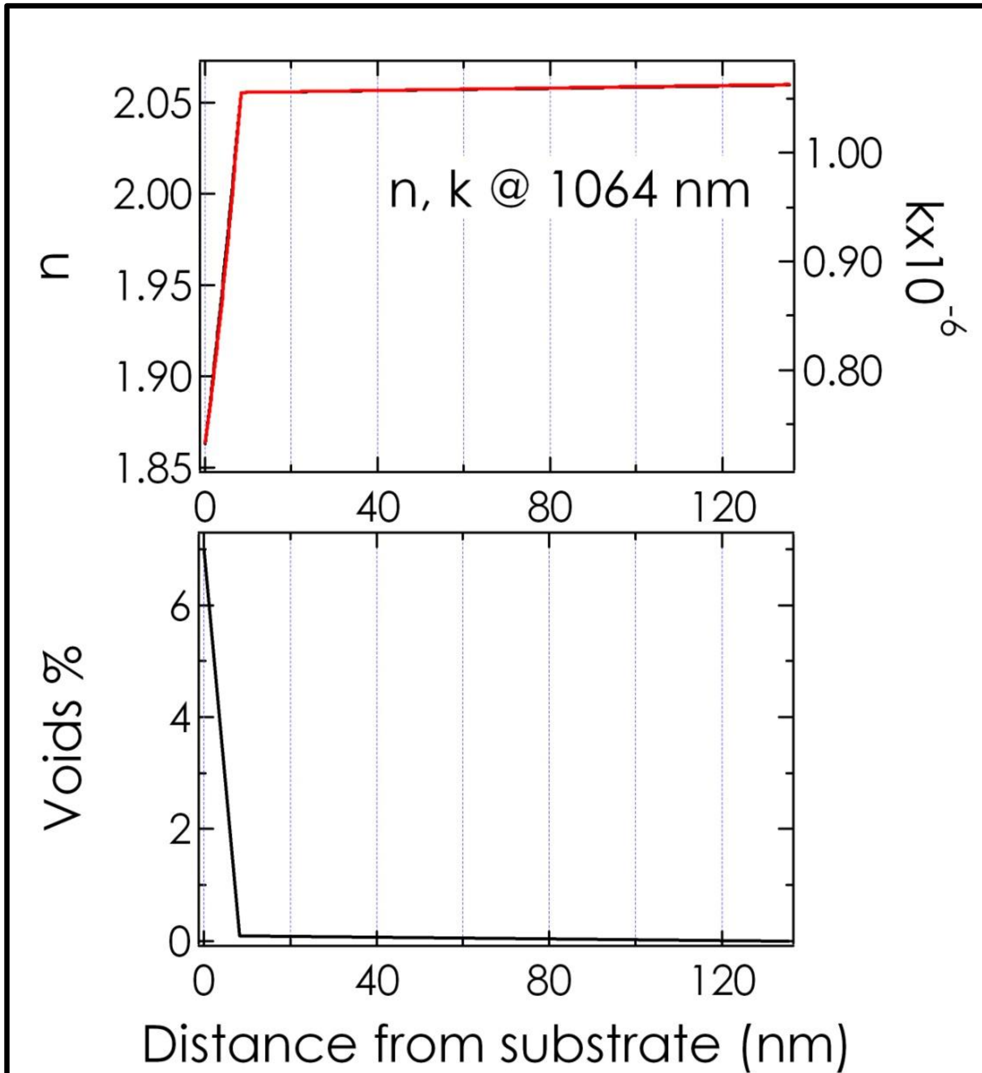
Surface roughness ~ 0.4 nm
Ta_2O_5 ~ 136 nm (density increasing with thickness)
Suprasil 311

MSE = 8.96



Improving the SE interpretation

Voids



Surface roughness ~ 0.4 nm

Ta_2O_5 ~ 136 nm
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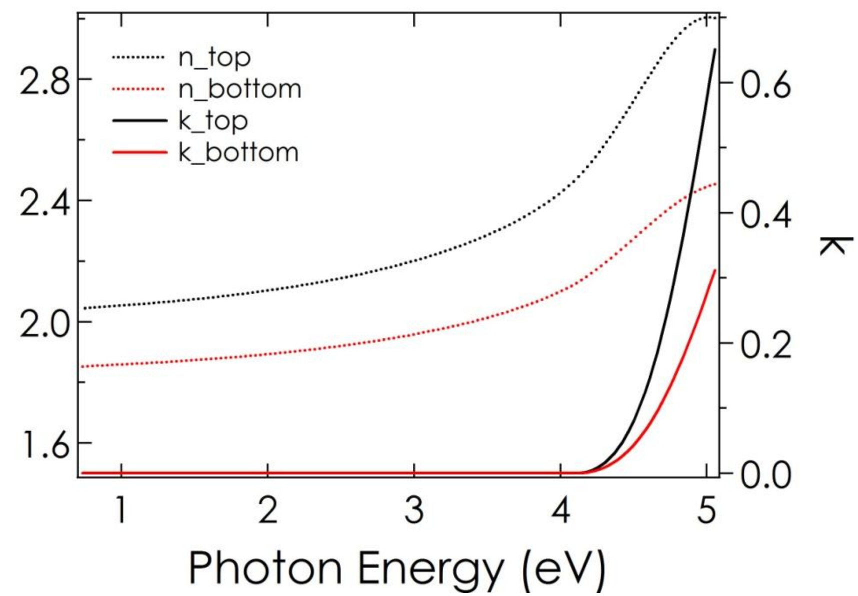
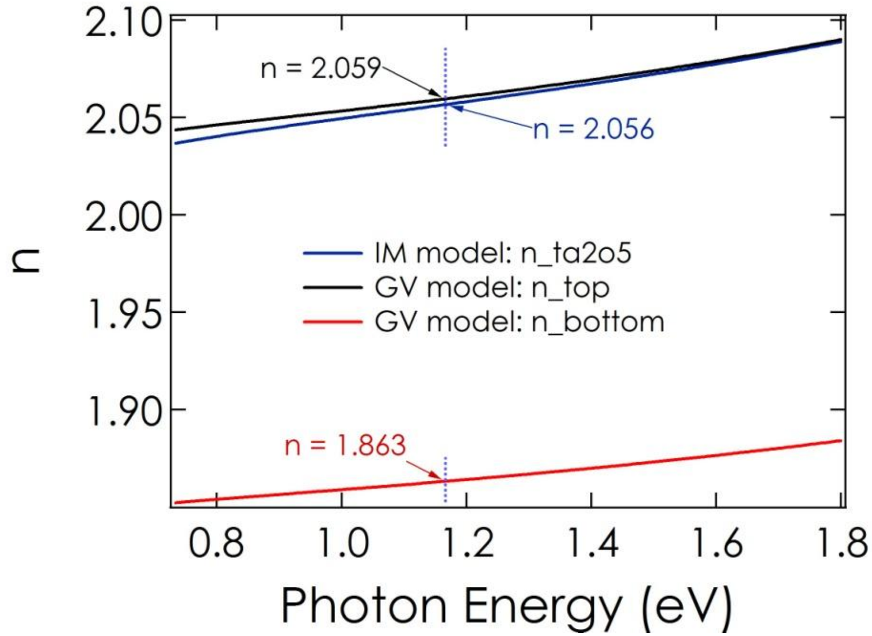
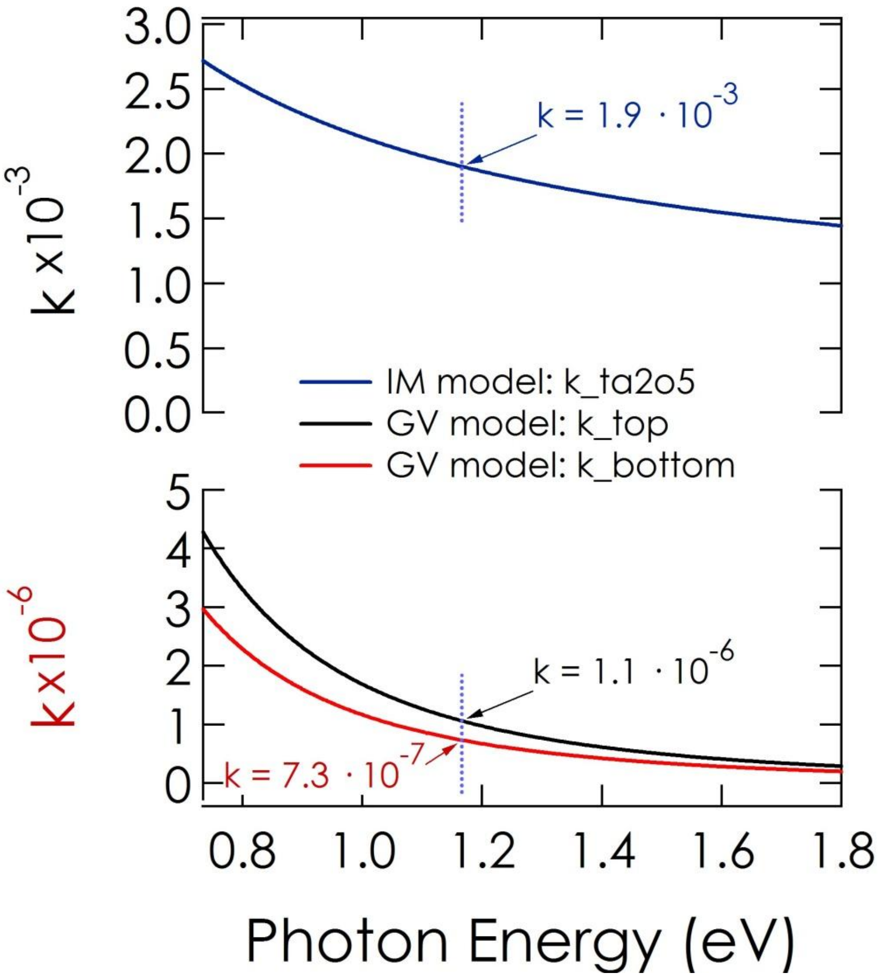
MSE = 8.96



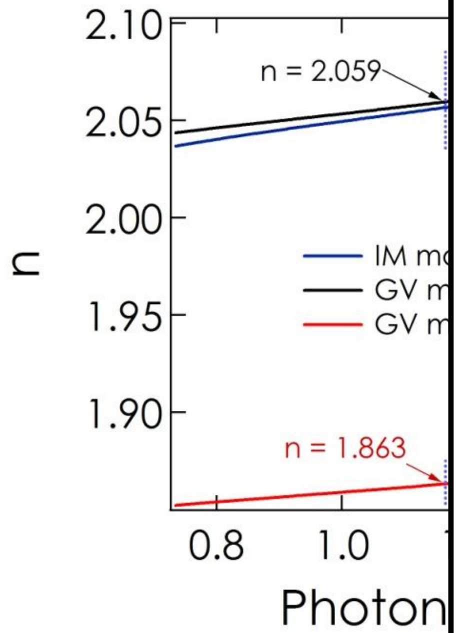
Discussion

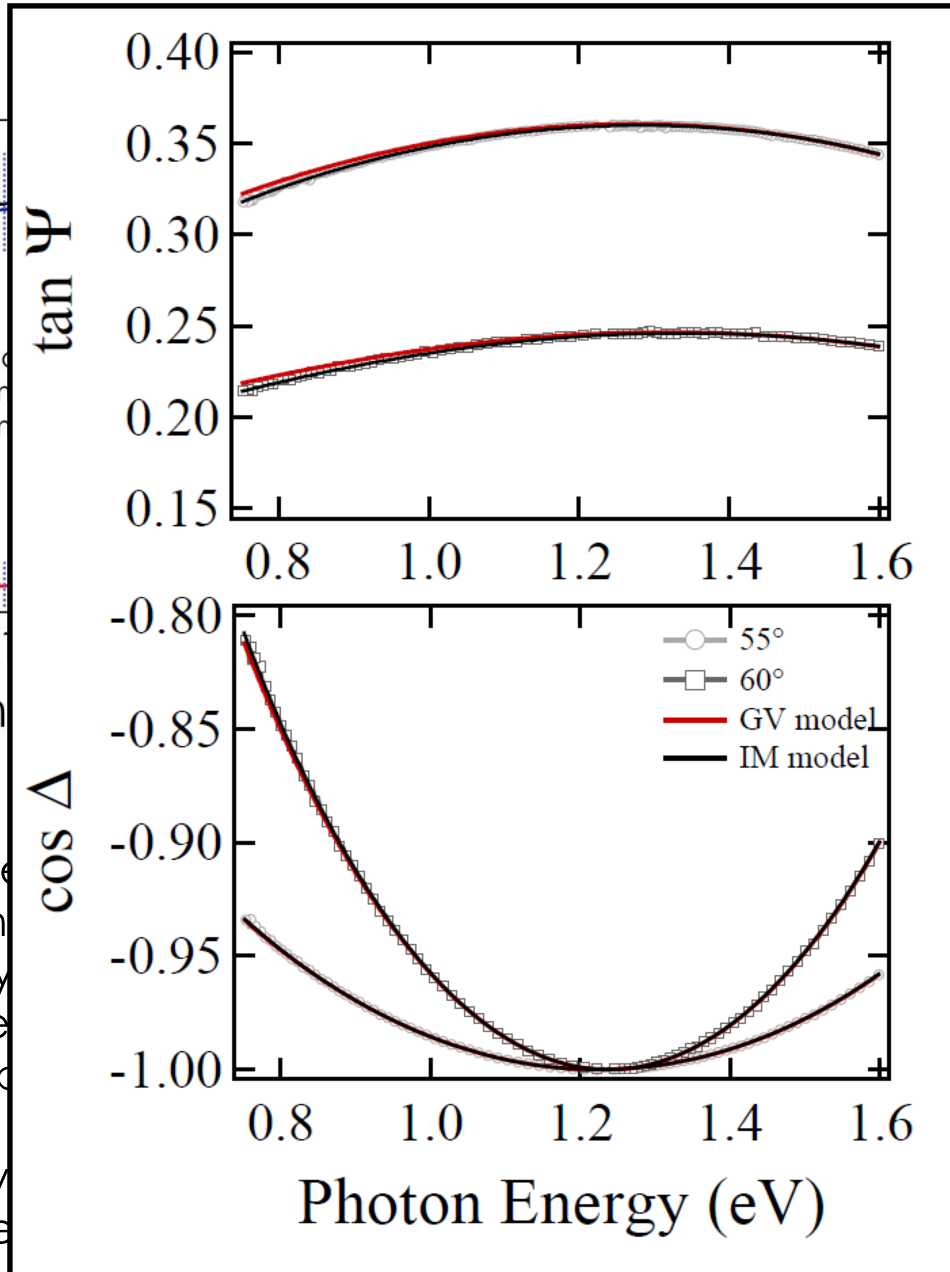


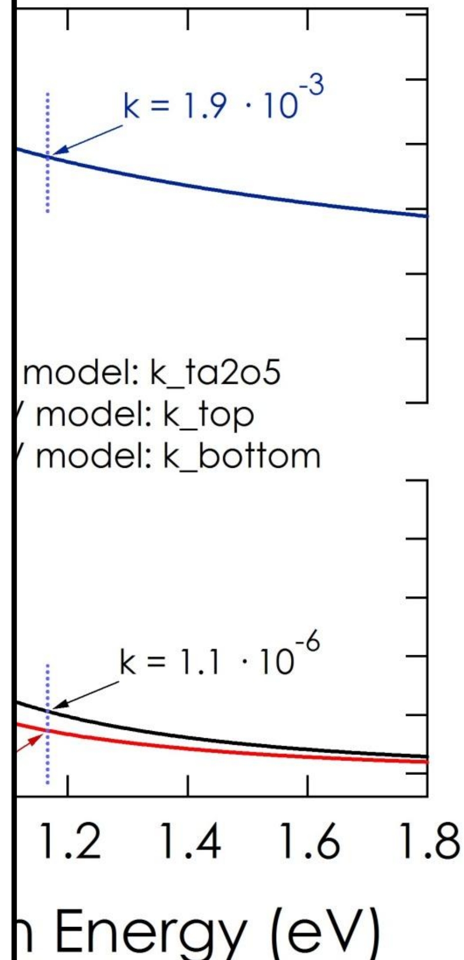


The value of n seems to be substantially model-independent: its value is determined with an uncertainty of a few parts per mil and it is in excellent agreement with the value $n_{LMA} \approx 2.06$, obtained by LMA.
The uncertainty on the value of k is really large as it is strongly affected by the choice of the optical model.

Discussion







The value of n see
model-independen
with an uncertainty
and it is in excelle
value $n_{LMA} \approx 2.06$, ob
The uncertainty on
large as it is strongly
of the optical mode

Conclusions

1) The metallic Ta fraction is appreciably lower than 6%. The low BE peak in the XPS spectrum is likely due to O2s photoelectrons (~ 30%) and to non-stoichiometric Ta_2O_5 species, including also metallic Ta.

2) SE data analysis shows that intermixing effects at the interface, voids, and defect-related free carriers in the bulk of the film improve the interpretation of the optical response of the Ta_2O_5 layer.

3) Further XPS and SE investigations will be useful to improve the model and reduce the uncertainty on k, such for example measurements on samples of reduced thickness, to gain direct information on the interface layer. A TEM analysis of the Ta_2O_5 layer could add useful information about the interface morphology.

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