XRR and GiXRF combined analysis of TCO/metal/TCO structures for photovoltaïc applications

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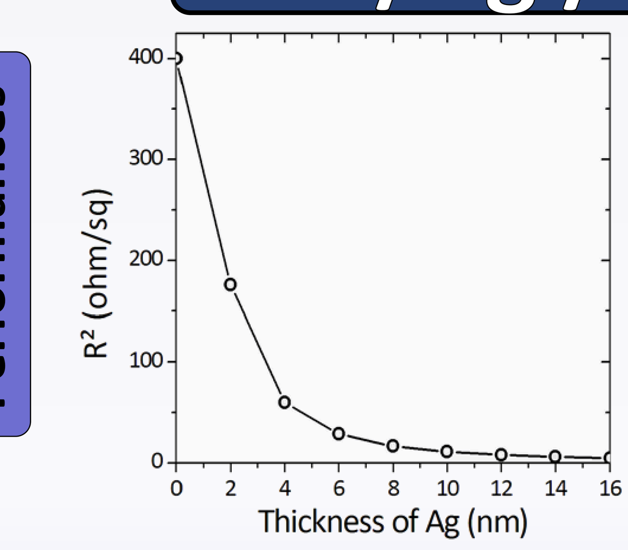
Motivation

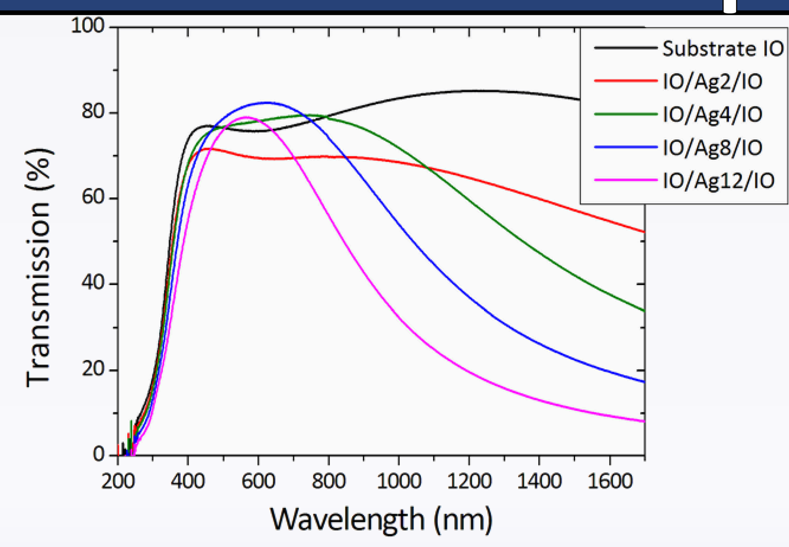
- TCO (transparent conductive oxyde) / metal / TCO structures are essential for a large variety of electronic devices such as flat panel displays, touch screens and thin film solar cells thanks to their optical and electrical characteristics
- The performances of such multilayers depends on the **in-depth chemical and physical properties** of the stack
- We study the composition and density profiling of a In_2O_3/Ag/In_2O_3 multilayer by **XRR & GiXRF combined analysis**

IO /Ag /IO structure for optimal performances

Performances



Resistivity as a function of the target metal thickness



Transmission in the visible spectral range

TCO are commonly used for photovoltaic applications

- Critical parameters :
  - ➡ lower resistivity
  - ➡ superior optical properties

TCO/metal/TCO emerged as an interesting alternative

- Low R^2 and T% possible with a metal thickness of [4;8]nm
- In_2O_3 and Ag are deposited by PVD on 200mm wafers

Samples

In_2O_3 = IO	40nm
Ag	[2 ; 12]nm
In_2O_3 = IO	40nm

Simulate thermal budget + in-depth profile creation
Annealing (200°C ; 1h)

Improvement of the detection sensitivity
CMP (removal of 25nm of IO)

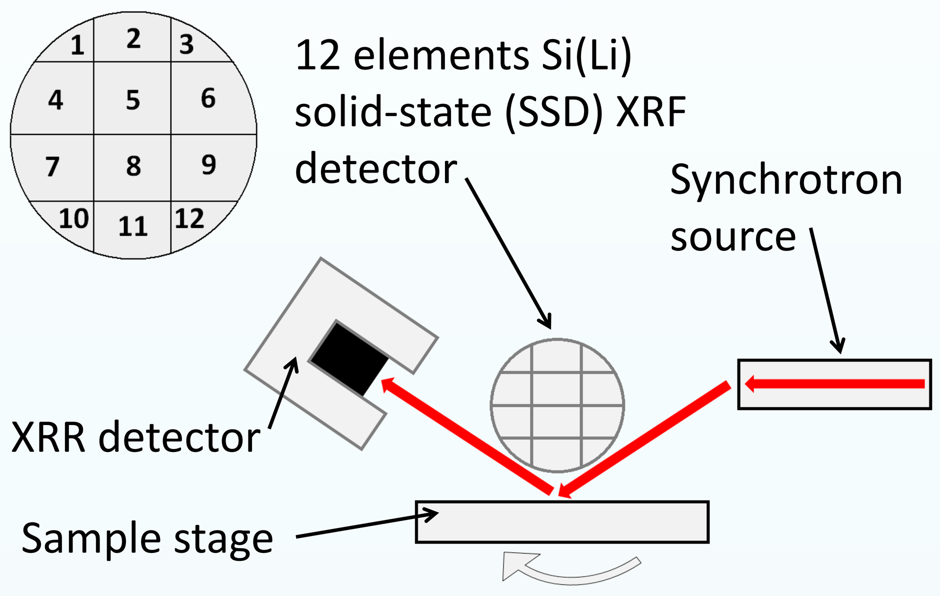
Sample preparation

- Choice of Ag because of its low resistivity
- Multiplication of the samples via different experimental steps (Annealing + CMP)

Experiments

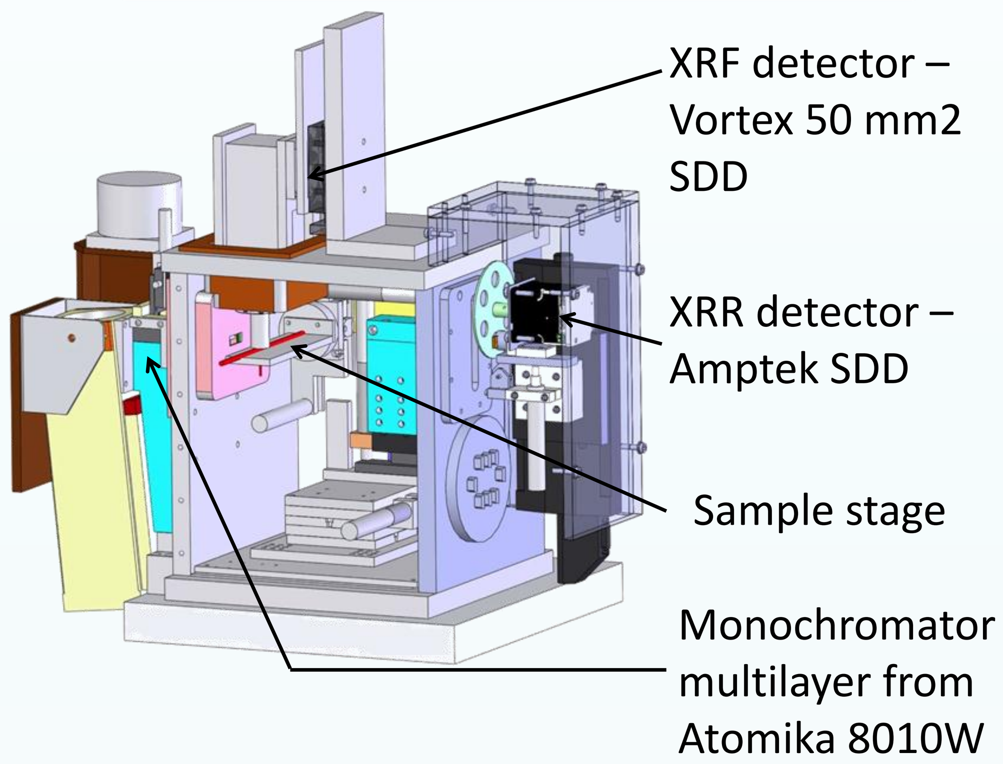
2 setups at different X-Ray energies ➡ 2 instrumental functions to define and calibrate

ESRF – Gilda line



- Synchrotron source
  - below In-Kα edge at 26400 eV
  - above In-Kα edge at 28800 eV
- Theta-2 theta goniometer
- Vacuum (< 1 mbar)

Vienna University of Technology

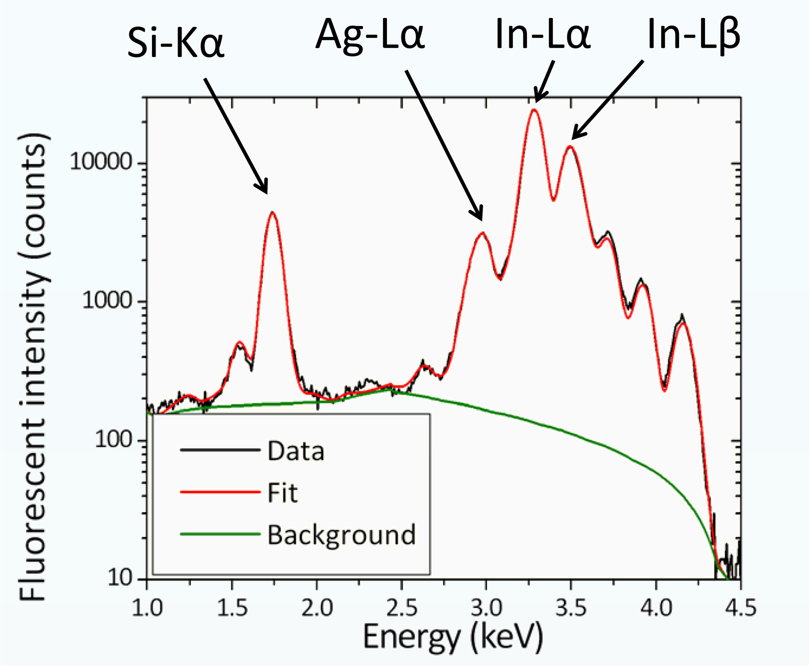


- Cu tube (8050 eV)
- Theta-2 theta goniometer
- Vacuum (< 1 mbar)

XRF acquisitions at Cu-Kα1

Correlation between Ag and In Lα lines

- Pre-treatment via PyMCA allow appropriate deconvolution
- Experiment above In-Kα edge ➡ clear separation of Ag and In-K contributions

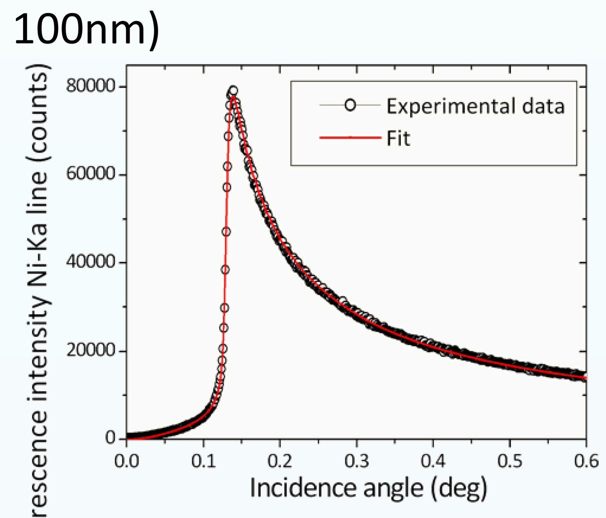


Fluorescence spectrum and fit of IO/Ag6/IO at 8keV

Instrumental function

Multi experimental setups approach

- Metrology of the complete experimental setup not adapted
- Use of well-known reference samples (Ni 100nm)

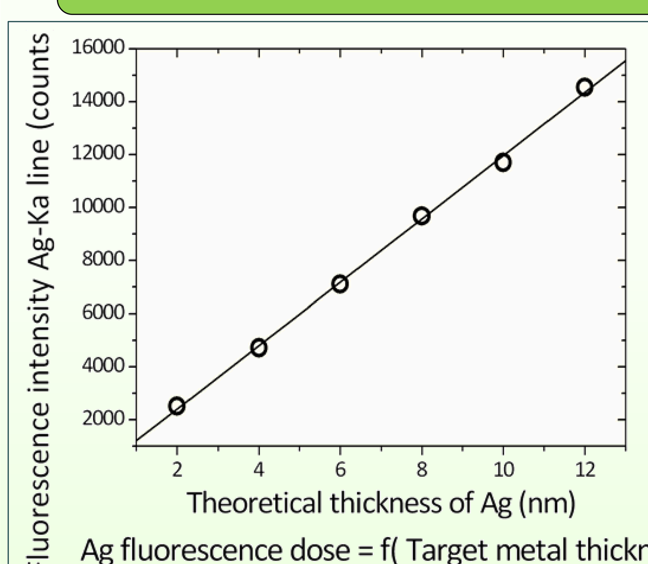


GiXRF fit of a reference sample at 26.4keV

- Beam divergence
- XRR and XRF detectors area
- Size of the irradiated area

Results

Fluorescence dose comparison & XRR modeling



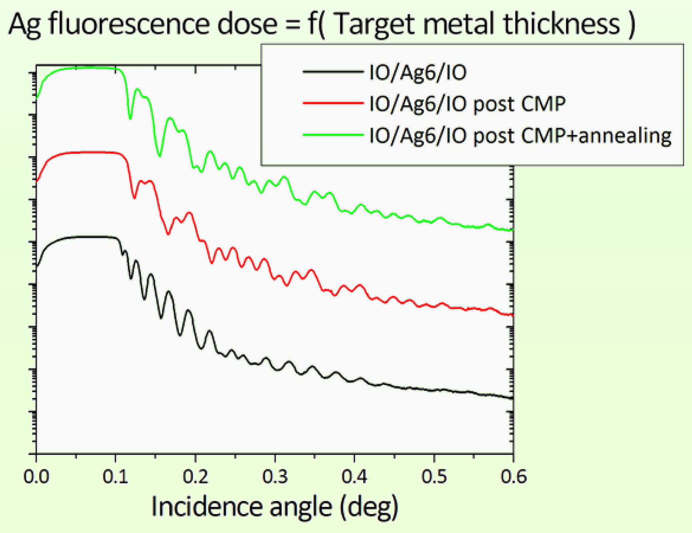
Ag fluorescence dose = f(Target metal thickness)

Fluorescence dose at 3θc

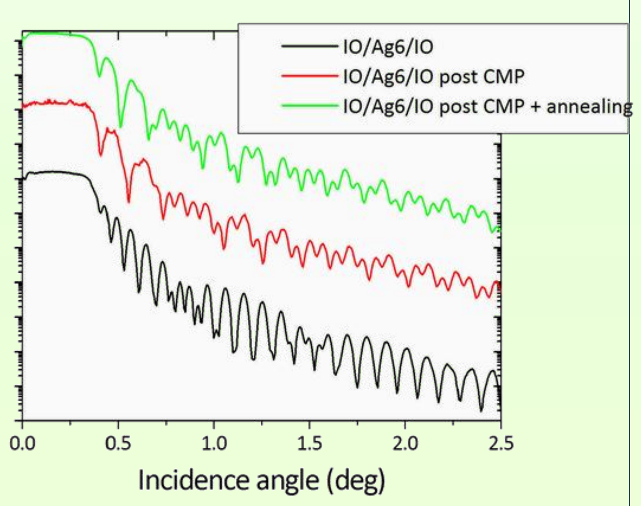
- Thickness of the metal layer

XRR modeling results from a simple sample model (e.g 3 layers)

- Thickness of the layers
- Density of the layers



XRR results of IO/Ag/IO samples at 26400 eV



XRR results of IO/Ag/IO samples at 8050 eV

Better dynamics on measurements at 8keV -> Used for modeling

Creation of a simple model stacking

In_2O_3 = IO	40nm
Ag	6nm
In_2O_3 = IO	40nm

Iterative process

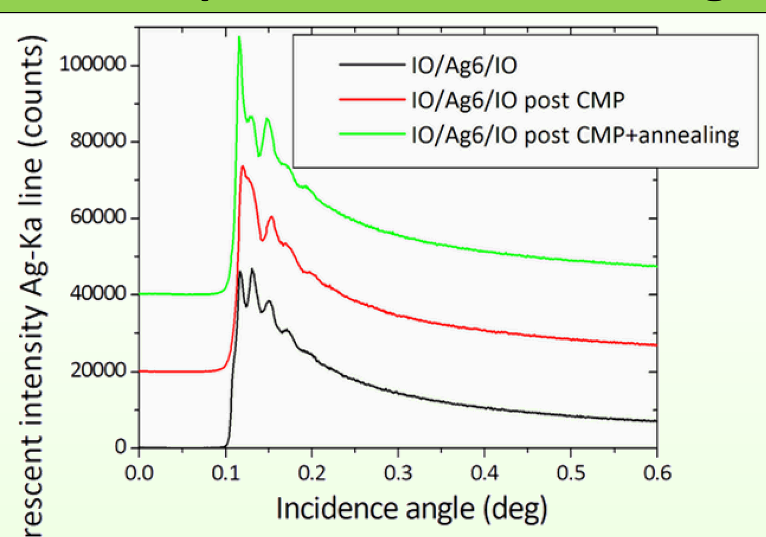
In_2O_3 = IO	16nm
	3.3nm
Ag	5.3nm
	1.6nm
In_2O_3 = IO	40nm

Results for IO/Ag6/IO post CMP+annealing

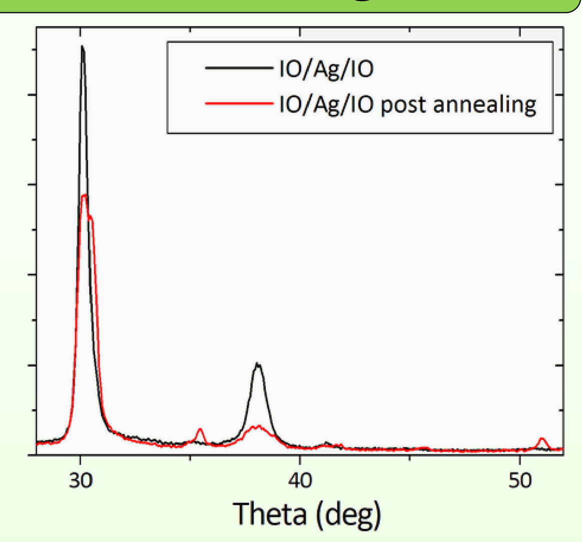
Refinement of the model sample

- Highlight of an intermediate layer due to the annealing
- Possibility to detect an in-depth chemical profile of the multi-layer

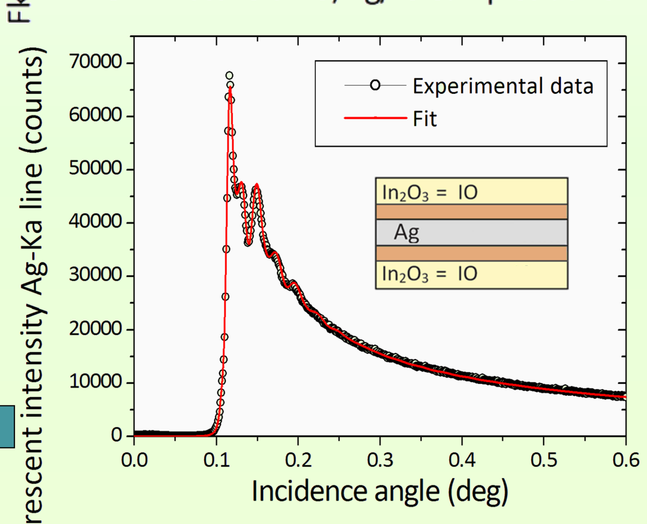
Complete fluorescence angular scan modeling



GiXRF scans of IO/Ag/IO samples at 26.4keV



XRD theta-2 theta of IO/Ag/IO samples



GiXRF fit of IO/Ag6/IO post CMP+annealing

Impact of annealing

- Modification of grain size and phase orientation (XRD)
- Complex in-depth distribution of Ag (GiXRF)
- Need for a new complex model (interdiffusion of Ag through In_2O_3)

Perspectives

- Simultaneous (not iterative) XRR & GiXRF combined analysis based on MAUD (L. Lutterotti) and guifitlayer (D. Ingerle) software
- Complementary data (EXAFS & XRD) will feed the combined analysis
- Evaluation of this improved combined analysis for accurate characterization of in-depth dependent properties of stacks for photovoltaic, flat panel displays and touch screens applications

Bibliography

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