Comprehensive PVD simulation: Application to antireflective coatings produced by OAD.

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Introduction

- The initial…

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Nanostructure and Physical Properties Control of Indium Tin Oxide Films Prepared at Room Temperature through Ion Beam Sputtering Deposition at Oblique Angles

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+ all the analyses and modelling performed within this study

- Goal: introduction of porosity in ITO films by OAD IBS to decrease the optical indexes (n, k) and enhance the IR transmission

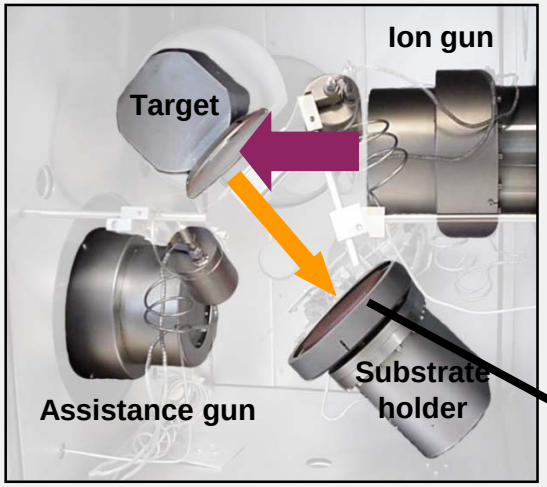
- The question:

→Can we reproduce the optical properties of the films with a comprehensive **process simulation**?

Introduction

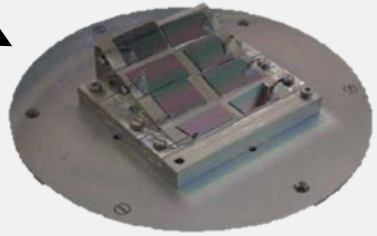
❑ Experimental setup

Ion Beam Sputtering (IBS) deposition technique



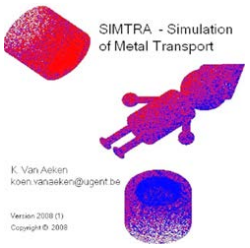
Deposition conditions:

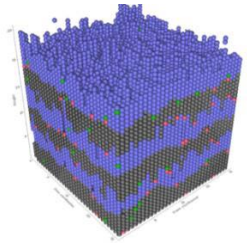
- **Incidents ions: Ar** (or **Xe)** at 1.2 keV
- **Substrate tilt angle:** from 50 to 85º
- **Substrates:** sapphire, silicon
- Target: ITO (In_2O_3/SnO_2 90/10 wt.%)
- Room temperature
- Pressure: $2*10^{-3}$ Pa
- 5 sccm O_2 introduced through assistance gun



❑ Digital process

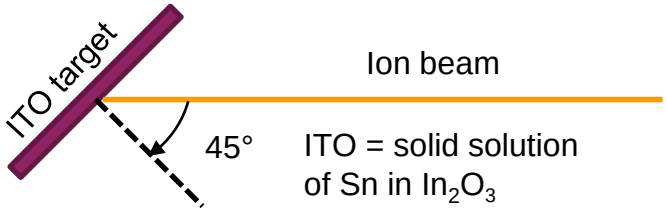
1. Sputtering: SRIM
2. Transport: SIMTRA
3. Growth: NASCAM
4. Optic: NASCAM plug-in

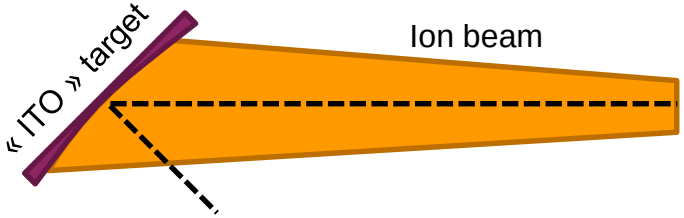




Sputtering

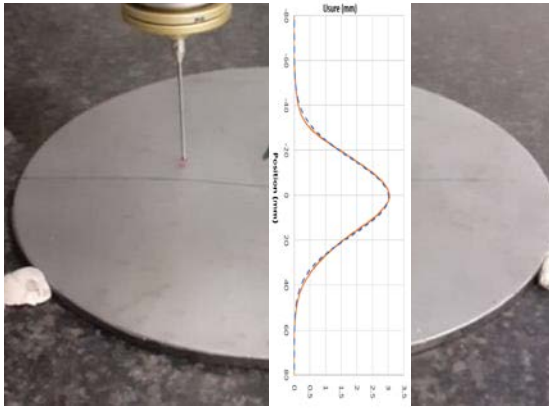
Theoretical setup



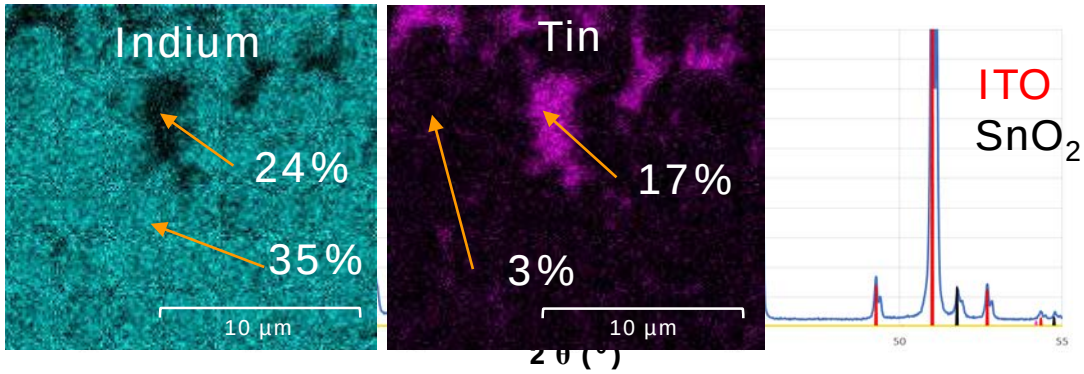


Vs real setup

- Variation of the ion incidence angle:
  - Enlargement of the ion beam: ± 2.3°
  - Wear of the target: max 5°



- Phase composition?
  - XRD
  - EDX



→ 95 % ITO and 5 % $In_4Sn_3O_{12}$ + traces of SnO_2

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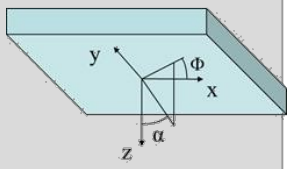
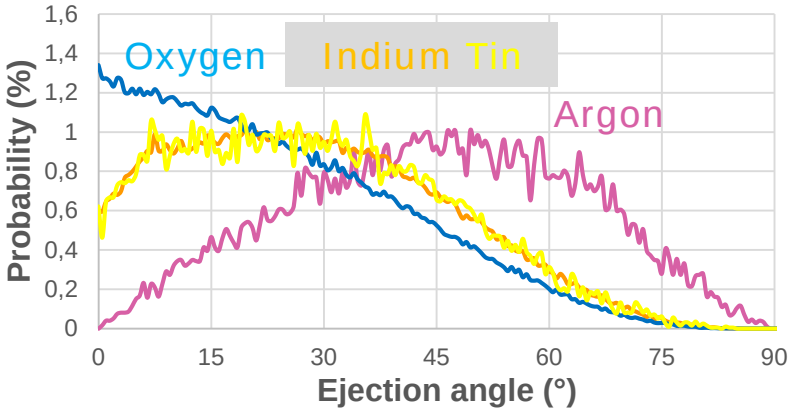
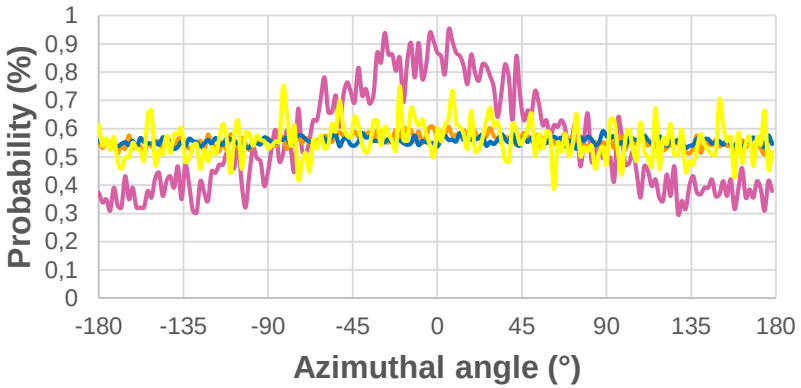
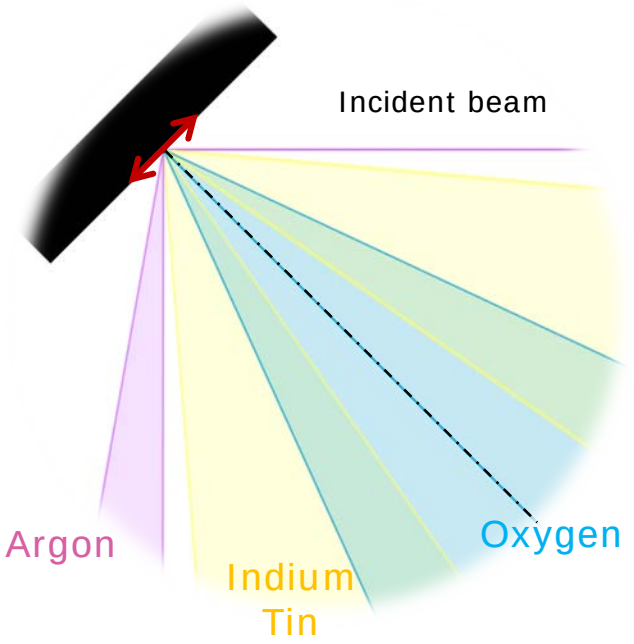


Sputtering

❑ SRIM calculation

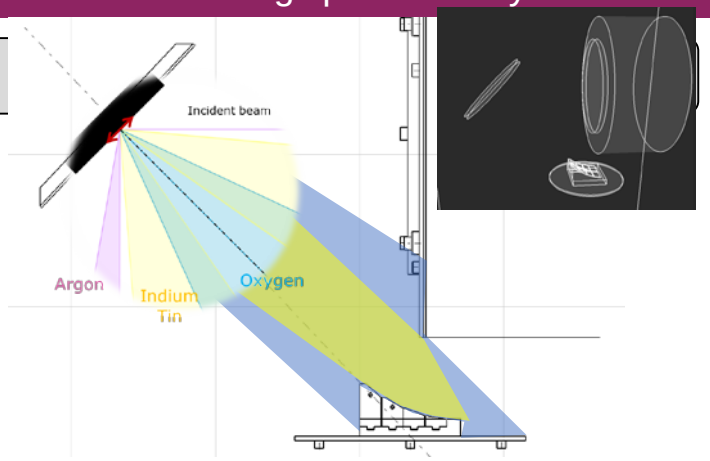






Species	Target composition (%)	Sputtered flow composition (%)	Sputtered flow energy (eV)
Tin	3.62	2.84 (2.91)	27.5
Indium	35.66	35.27(36.20)	23.2
Oxygen	60.72	59.33 (60.89)	16.7
Argon	0	2.56	216.7

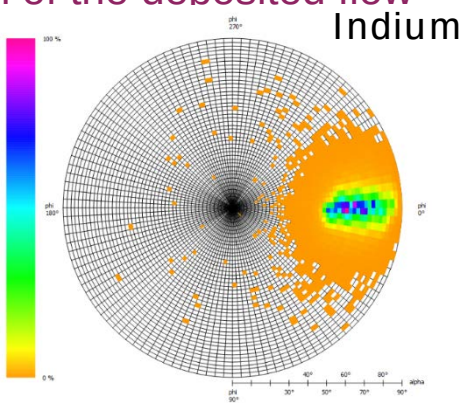
Transport

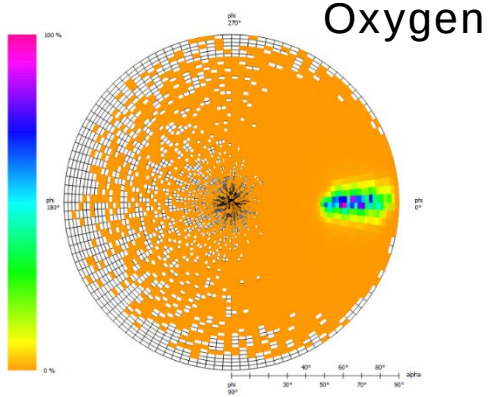


- SIMTRA calculation
  - Low pressure $2*10^{-3}$ Pa
    - → Few collisions
  - Flow filtering
    - → Geometry of the system
    - → Angular distribution of the emitted flow

Species	Target composition (%)	Sputtered flow composition (%)	Deposited flow composition (%)	Sputtered flow energy (eV)	Deposited flow energy (eV)
Tin	3.62	2.84 (2.91)	1.62 (1.63)	27.5	13.01
Indium	35.66	35.27(36.20)	19.65(19.70)	23.2	11.57
Oxygen	60.72	59.33 (60.89)	78.48 (78.67)	16.7	11.65
Argon	0	2.56	0.24	216.7	167.12

- Angular distribution of the deposited flow





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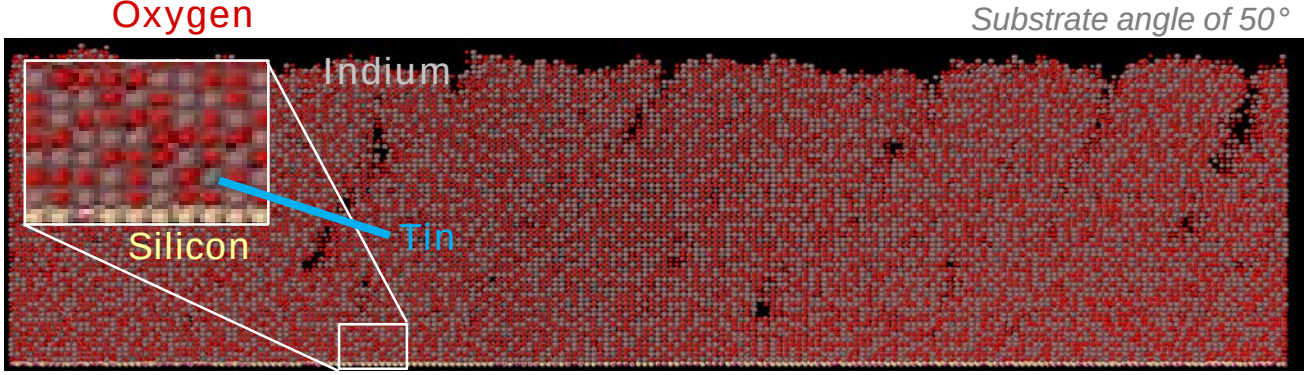
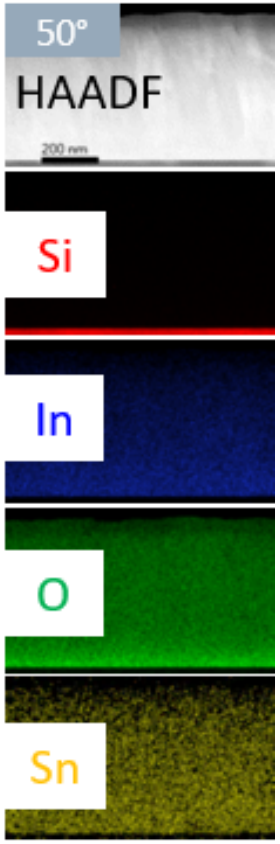
Growth

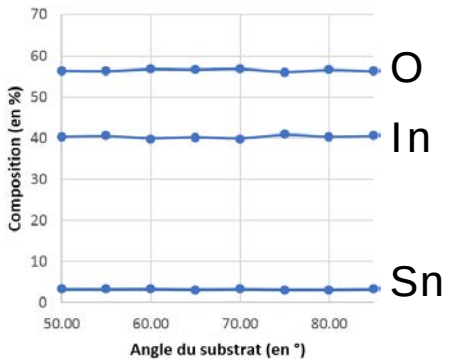
❑ NASCAM (4.7.X) calculation in reactive mode: stoichiometry of 1.5 (3O / 2Me)

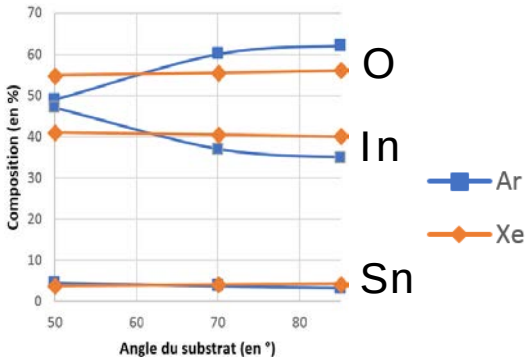




❑ Composition

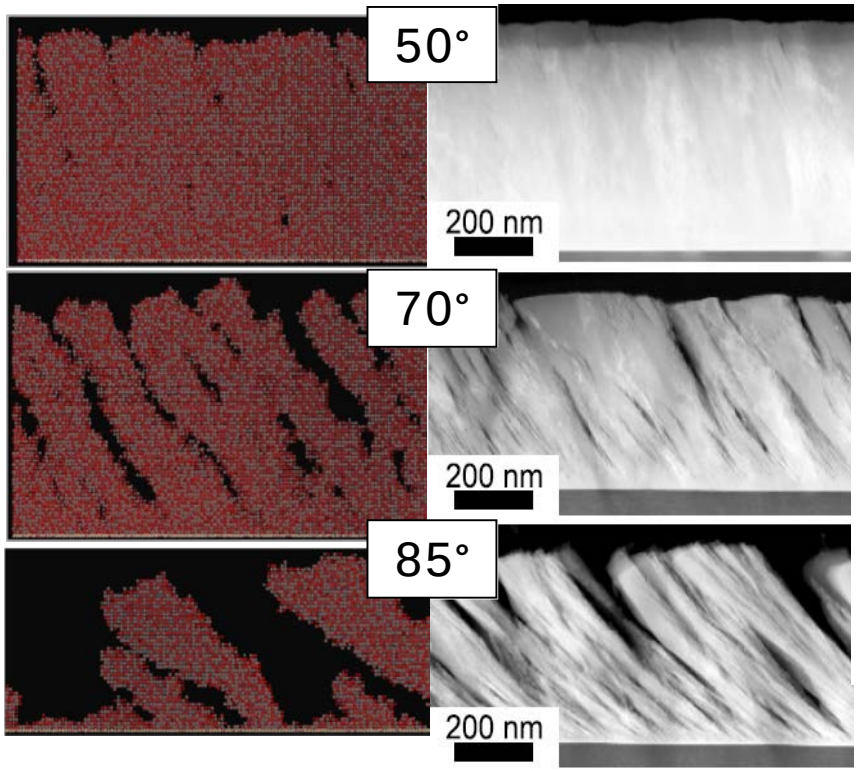
Species	Target composition (%)	Sputtered flow composition (%)	Deposited flow composition (%)	Film composition (%)
Tin	3.62	2.84 (2.91)	1.62 (1.63)	3.33
Indium	35.66	35.27(36.20)	19.65(19.70)	40.35
Oxygen	60.72	59.33 (60.89)	78.48 (78.67)	56.31
Argon	0	2.56	0.24	0.01



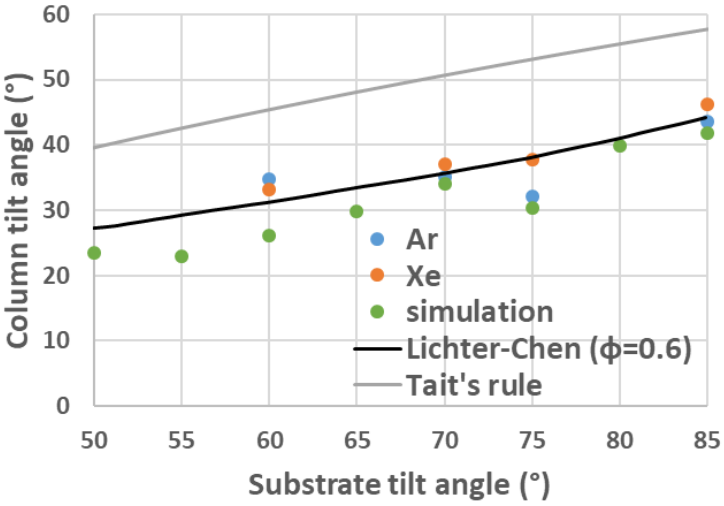


Growth

- Cross sections



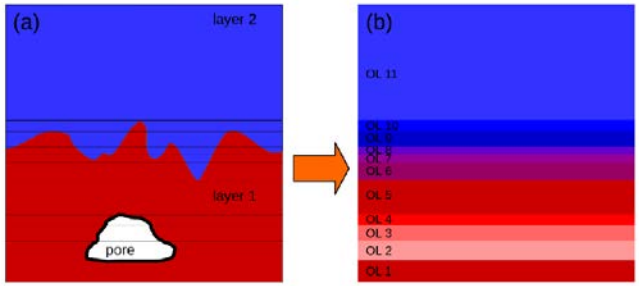
- Column tilt angle



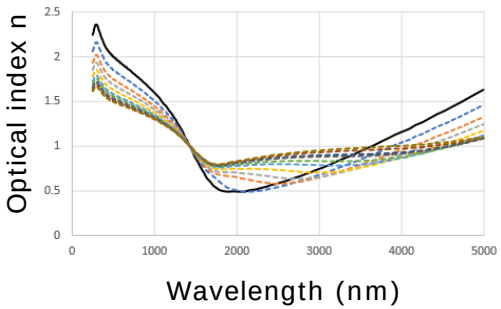
- Good reproduction of the composition, the morphologies and the column tilt angle.
- What about the optical properties?

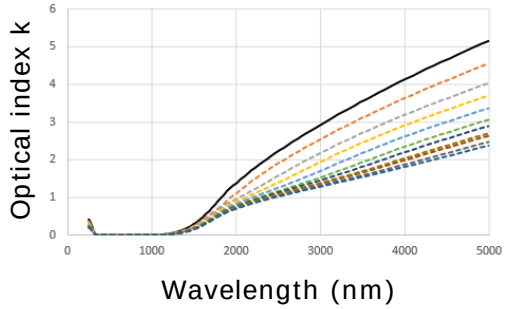
Optic

- NASCAM (7.7.x) Plugin : “Optics”



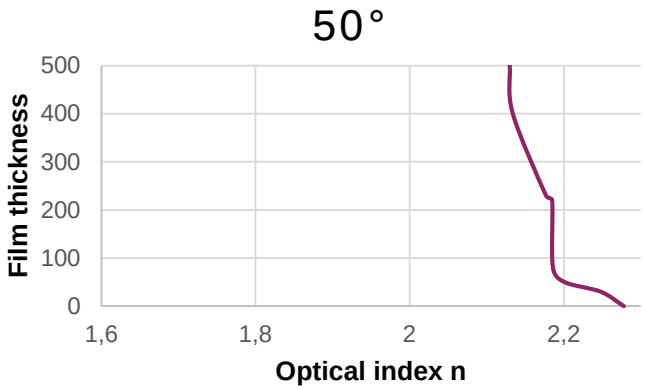
→ Convert the film morphology into a multilayer with optical indexes related to the porosity.

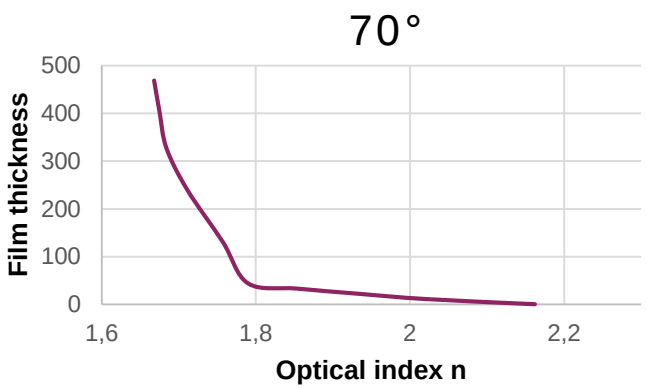




0 %
Porosity
50 %

- Variation of the film optical indexes with the depth





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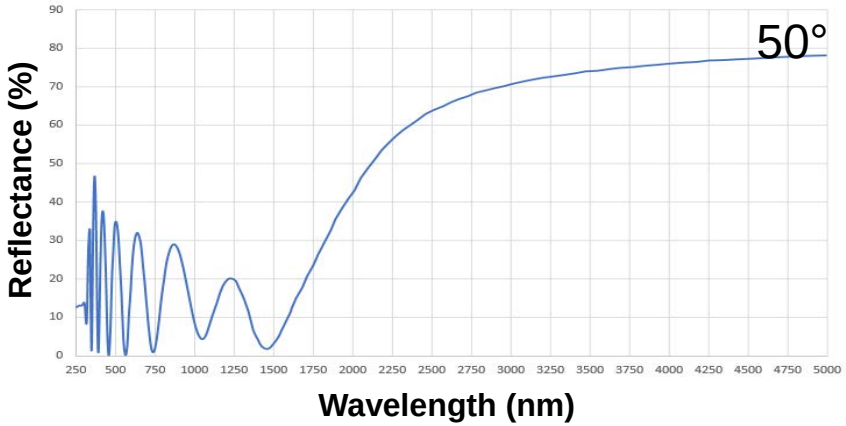
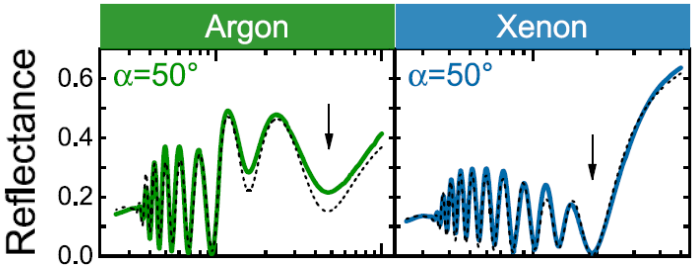
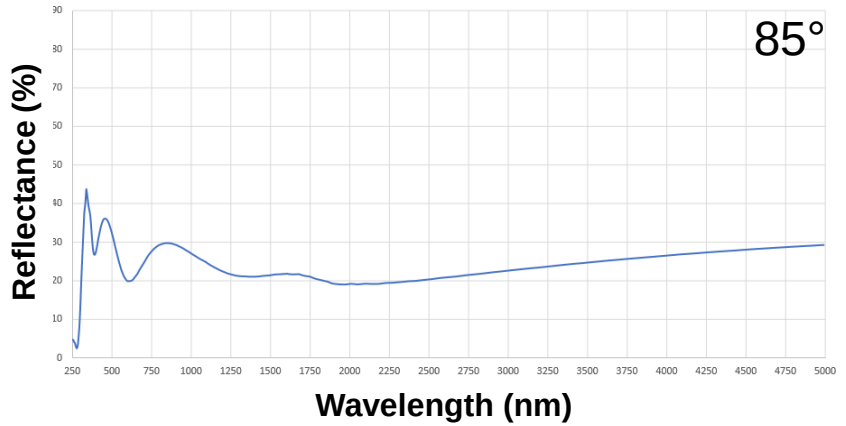
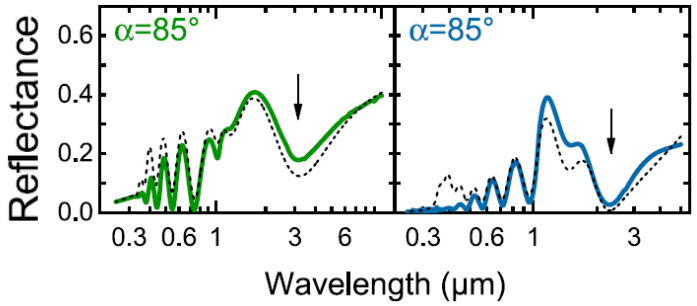
Optic

- Reflectance









- Good results for the visible range. More deviations in the IR range.
- Globally excellent results taken into account the simplification used in the simulations!

Conclusion

- Oblique angle deposition of ITO by ion beam sputtering was reproduced digitally.

  It requires a good knowledge of:
  - The system geometry (size and relative position of the components in the vacuum chamber)
  - The deposition conditions (pressure, temperature, energy of the ion beam, etc.)
  - The target specifications (elemental and phases composition, racetrack)

- SRIM, SIMTRA, NASCAM were used for the three steps of the process. For each step, millions of particles are used as input to ensure enough particles in the output for the statistical treatments (around few hundred of thousands).
  - Digital films morphologies, composition, thicknesses correctly reproduce the experimental ones.

- Optical properties of the digital films are calculated from the NASCAM plugin “Optics”
  - The principle of the variation of the optical indexes with the depth in the films (and function of the substrate tilt angle) is found
  - The reflectance curves gives positive results but can be improved

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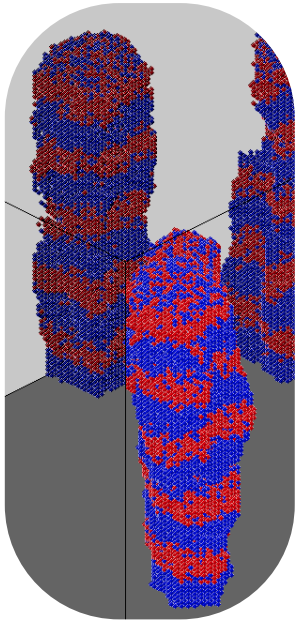
Thank you for your attention.



Have you got some questions?