Transparent conductive oxides: Context? Why?

Long answer

- TCO: large range of applications in optoelectronic devices
  - transparent front-side contact for solar cells
    - ZnO:Al (AZO) : alternative to ITO

Short answer

Multi-scale modelling of TCO coating deposited by reactive magnetron sputtering:
-
application to structured c-Si thin film solar cells

Jérôme Müller, Pavel Moskovkin, Stéphane Lucas, Olivier Deparis, Alexandre Mayer

ASEC2020
10-30/11/2020
online

iCS INNOVATIVE COATING SOLUTIONS

LARN

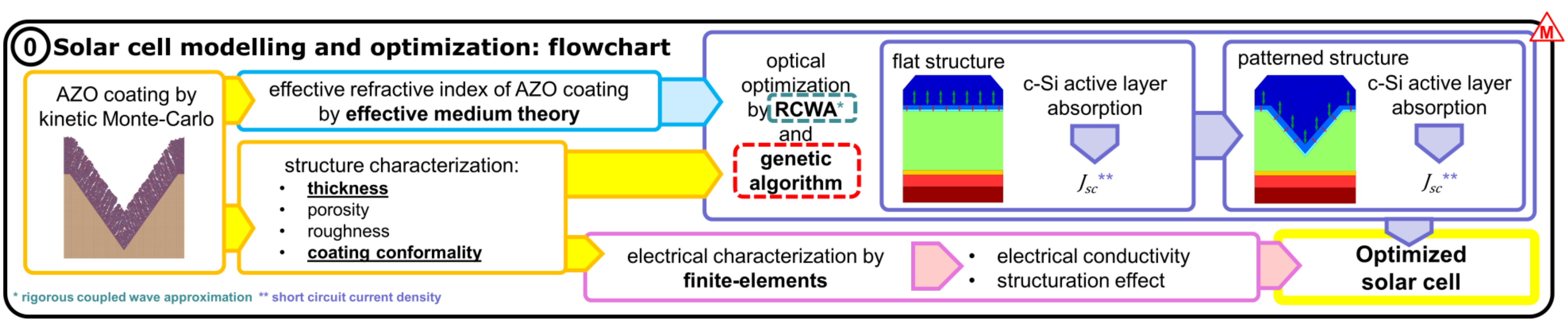
NISM

UNIVERSITÉ DE NAMUR

Poster slices

flowchart

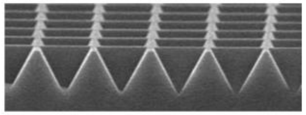
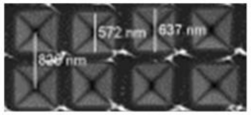
- Goal and flowchart
  - full characterization process of cSi thin film solar cells structured by periodic inverted pyramids (wet etching)
  - thin film characterization by:
    - film growth modelling by kinetic Monte-Carlo
    - effective electrical properties of the AZO coating by finite-elements
    - optical properties of the AZO coating by effective medium theory
  - full optimization of full multi-layered patterned solar cell by
    - genetic algorithm
    - RCWA



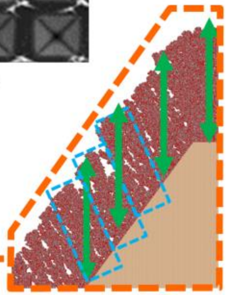
thin film modelling

1 AZO film growth modelling

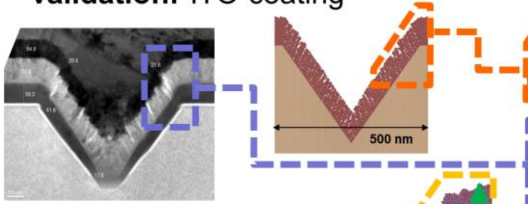
- deposition by reactive sputtering on **inverted pyramids*** (wet etched c-Si)

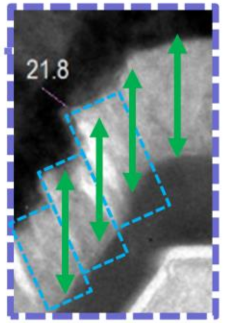



- modelling by **kinetic Monte-Carlo**** (NASCAM software)

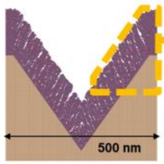


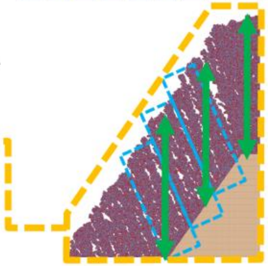
- **validation:** ITO coating





- AZO coating***





- **thickness constant** in the vertical direction
- **higher porosity** in the tilted zone

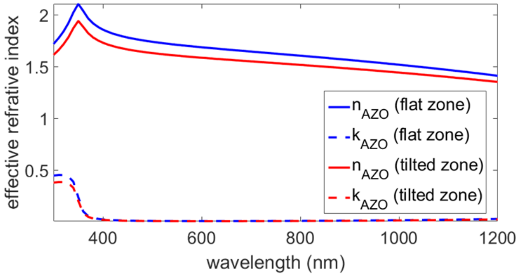
* V. Depauw and al., *Nanophotonics for ultra-thin crystalline silicon photovoltaics: when photons meet electrons*, Proceedings of EU PVSEC, p. 1461 - 1469 (2014).
** R. Tonneau and al., *TiOx deposited by magnetron sputtering: a joint modelling and experimental study*, Journal of Physics D: Applied Physic. 51 (2018) 195202 (17pp).
*** Neng-Fu Shih and al., "Properties and Analysis of Transparency Conducting AZO Films by Using DC Power and RF Power Simultaneous Magnetron Sputtering," Advances in Materials Science and Engineering, vol. 2013, Article ID 401392, 6 pages, 2013.

AZO effective refractive index

3 AZO effective refractive index

- effective medium theory based on Maxwell-Garnett method:

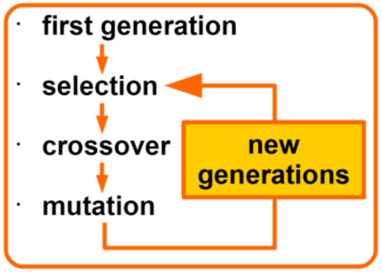
$$\frac{\epsilon_{eff} - \epsilon_h}{\epsilon_{eff} + y\epsilon_h} = \sum_{i=1}^{n-1} f_i \frac{\epsilon_i - \epsilon_h}{\epsilon_i + y\epsilon_h}$$



optimization numerical tools

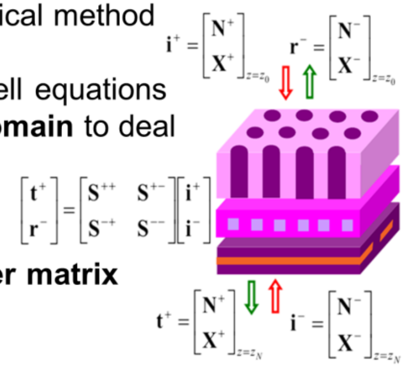
Tool Genetic Algorithm*

- **optimization** algorithm inspired by the natural selection process
- powerful tool for optimization of a **large number of parameters** (≥3)



Tool Rigorous Coupled Wave Approx.*

- semi-analytic optical method
- solves the Maxwell equations in the **Fourier domain** to deal with **periodic structures**
- based on **transfer matrix** computation
- possible to have access to the electric field maps and then to the **local absorption**



* J. Müller and al., *A fair comparison between ultrathin crystalline-silicon solar cells with either periodic or correlated disorder inverted pyramid textures*, Opt Express 2015 Jun 1;23(11):A657-70.

Optimization process

4 Optical optimization

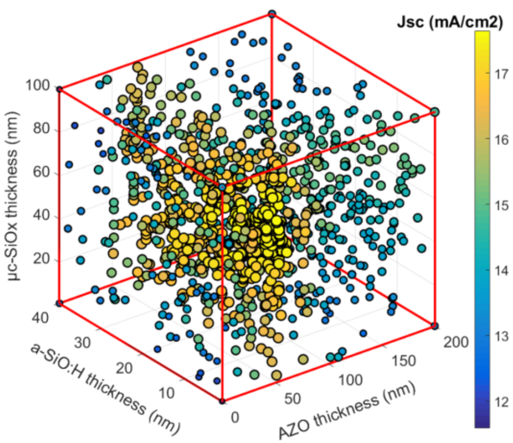
- computation for absorbance spectrum in the active layer (A_{cSi})
- computation of the **short circuit current**:

$$J_{sc} = \frac{e}{h\,c}\int_{300\text{nm}}^{1200\text{nm}} \lambda\, S(\lambda)\, A_{cSi}(\lambda)\, \partial\lambda \,^{*}$$

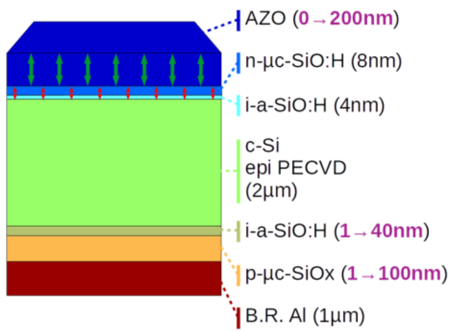
- optimization by **genetic algorithm**

* with e the electron charge, h the Planck constant, c the light speed, λ the wavelength, S the reference solar spectral irradiance, A_{cSi} the absorption in the cSi layer computed by RCWA.

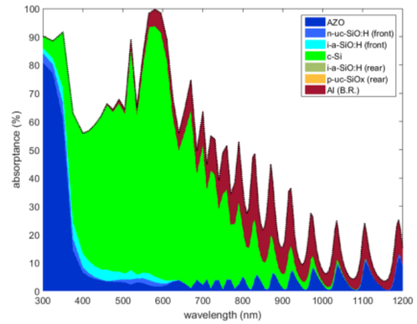
- Jsc for all parameters investigated by the genetic algorithm



optimization of the flat stack



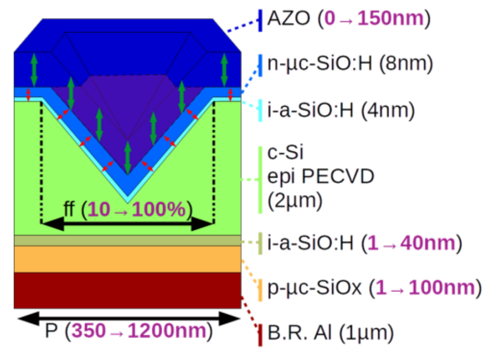
- **absorptance** spectra of each layer



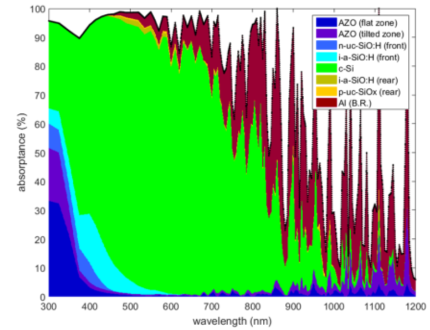
- **optimal short circuit current**:

$$J_{sc} = 17.6\text{mA/cm}^2$$

optimization the patterned stack



- **absorptance** spectra of each layer



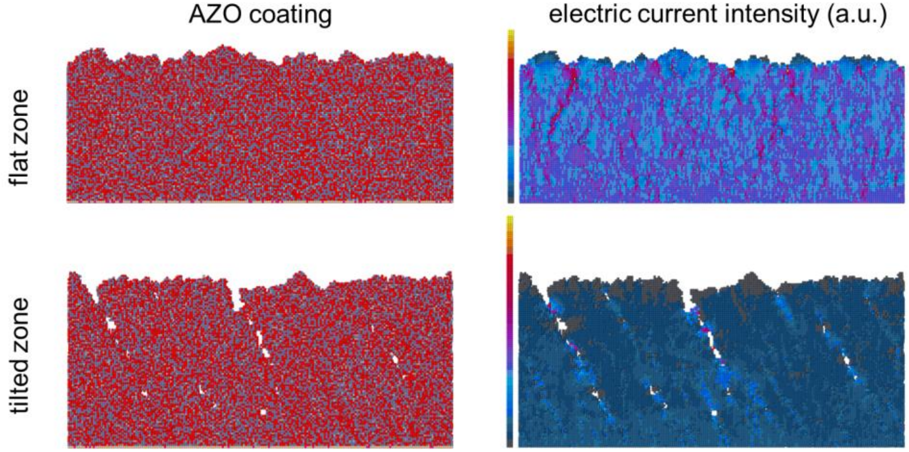
- **optimal short circuit current**:

$$J_{sc} = 24.3\text{mA/cm}^2$$

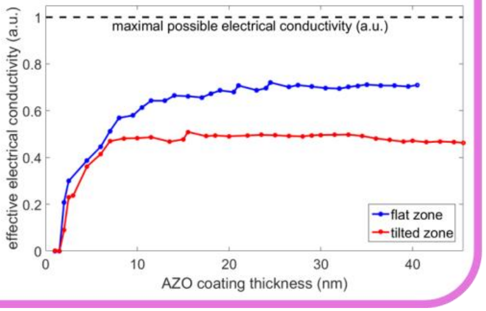
Electrical characterization

2 Electrical characterization

- finite-elements model
  - solve the Maxwell-Faraday equation (hypothesis: near-absence of varying magnetic field)
  - compute the voltage field in the whole structure allowing a minimal dissipated power
- electrical current intensity in AZO coating



- effective conductivity
  - high impact of the porosity in the tilted zone
  - no evolution after 15nm



note about the a.u. : 1 represents the conductivity of a perfectly dense coating

Conclusion and prospects

Conclusion

- numerical modelling, by kMC, of atomistic deposition by reactive sputtering of AZO on a structured substrate
- full characterization process performed to estimate the electrical and optical properties of the AZO coating
- global optimization by genetic algorithm used to enhance the efficiency of a multi-layered structured solar cell
- however, this study pointed the high impact of the substrate pattern on those physical properties, especially the decrease of the electrical conductivity

Thanks