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

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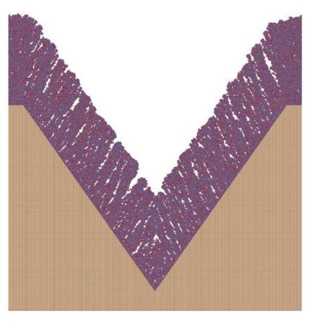
M Methodology
A Applications

Introduction: Transparent conductive oxides (TCO) present a large range of applications such as optoelectronic devices, especially transparent front-side contact for solar cells. In this last case, aluminum doped zinc oxide (ZnO:Al or AZO) can be a good alternative to indium tin oxide (ITO). Our work focuses on a full characterization process of crystalline silicon thin film solar cells structured by periodic inverted pyramids (wet etching). Such characterization is based on ① AZO film growth modelling by kinetic Monte-Carlo, ② effective electrical properties and ③ optical properties of the AZO coating (respectively by finite-elements and effective medium theory). Finally, ④ a full optimization by genetic algorithm, coupled to the RCWA optical tool, is done on the full multi-layered patterned solar cell.

⓪ Solar cell modelling and optimization: flowchart

AZO coating by kinetic Monte-Carlo

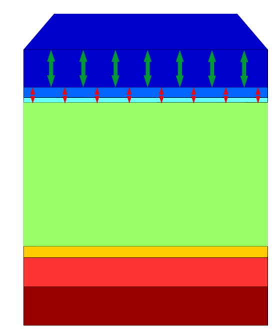


effective refractive index of AZO coating by **effective medium theory**

structure characterization:
- **thickness**
- porosity
- roughness
- **coating conformality**

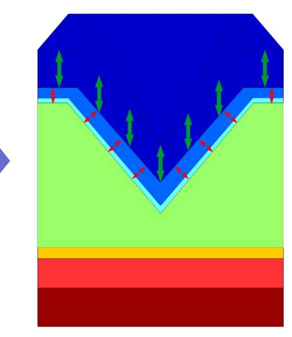
optical optimization by **RCWA*** and **genetic algorithm**

flat structure



c-Si active layer absorption → J_{sc}**

patterned structure



c-Si active layer absorption → J_{sc}**

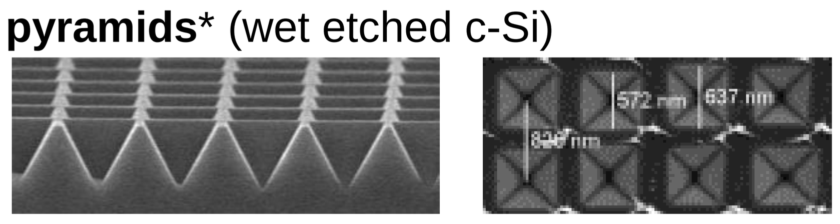
electrical characterization by **finite-elements**
- electrical conductivity
- structuration effect

Optimized solar cell

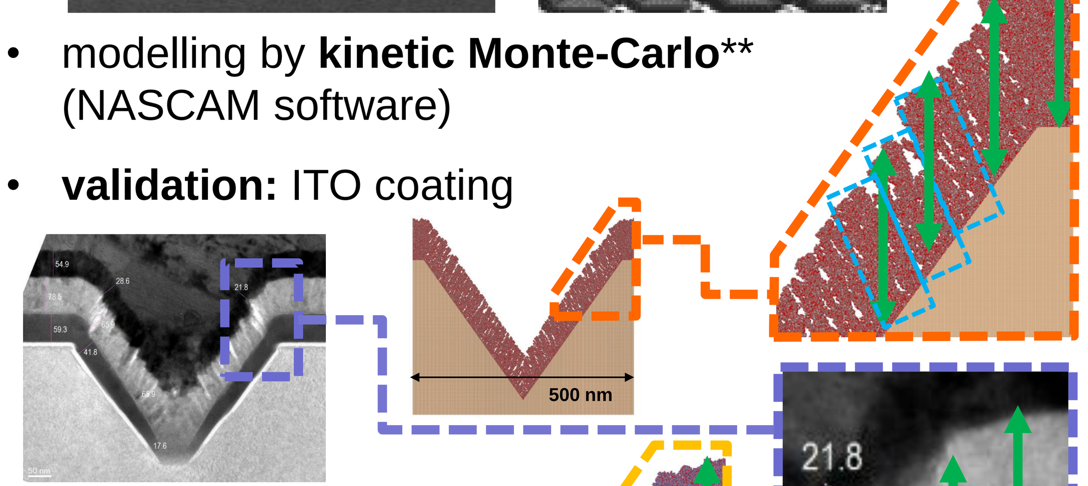
* rigorous coupled wave approximation ** short circuit current density

① AZO film growth modelling

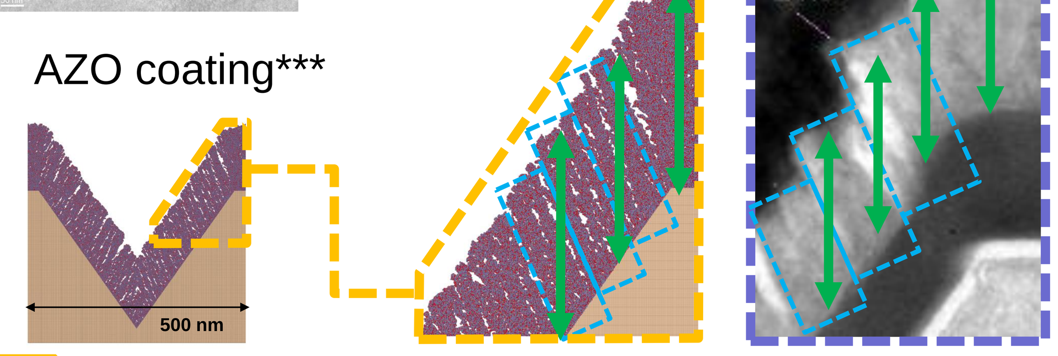
- deposition by reactive sputtering on **inverted pyramids*** (wet etched c-Si)



- modelling by **kinetic Monte-Carlo**** (NASCAM software)
- **validation:** ITO coating



- AZO coating***

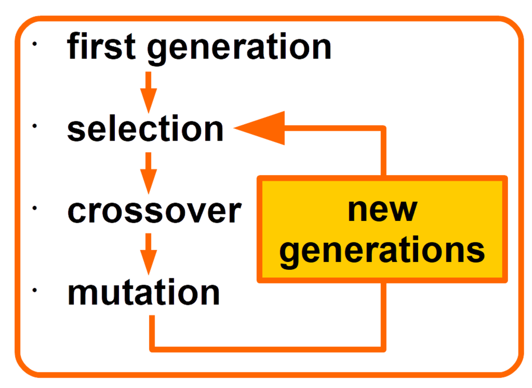


- **thickness constant** in the vertical direction
- **higher porosity** in the tilted zone

* 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.

Tool Genetic Algorithm*

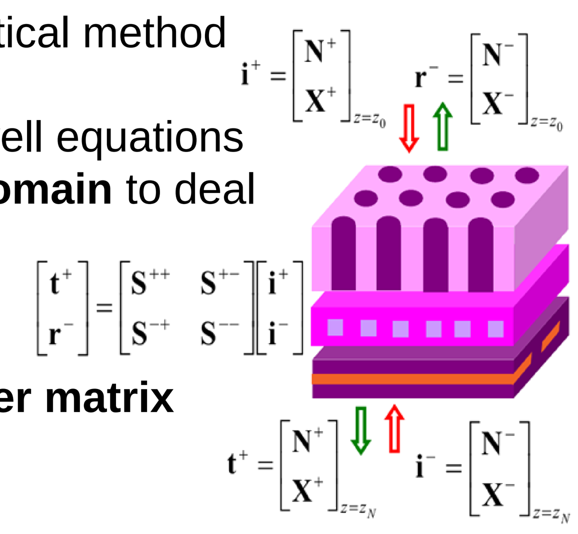
- **optimization** algorithm inspired by the natural selection process
- powerful tool for optimization of a **large number of parameters** (≥3)



* A. Mayer and M. Lobet, *UV to near-infrared broadband pyramidal absorbers via a genetic algorithm optimization approach*, Proceedings of SPIE, vol. 10671, p.1067127 (2018).

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



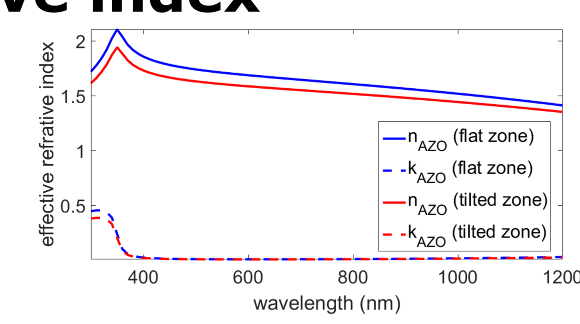
- possible to have access to the electric field maps and then to the **local absorption**

* 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.

③ AZO effective refractive index

- effective medium theory based on Maxwell-Garnett method:

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



④ Optical optimization

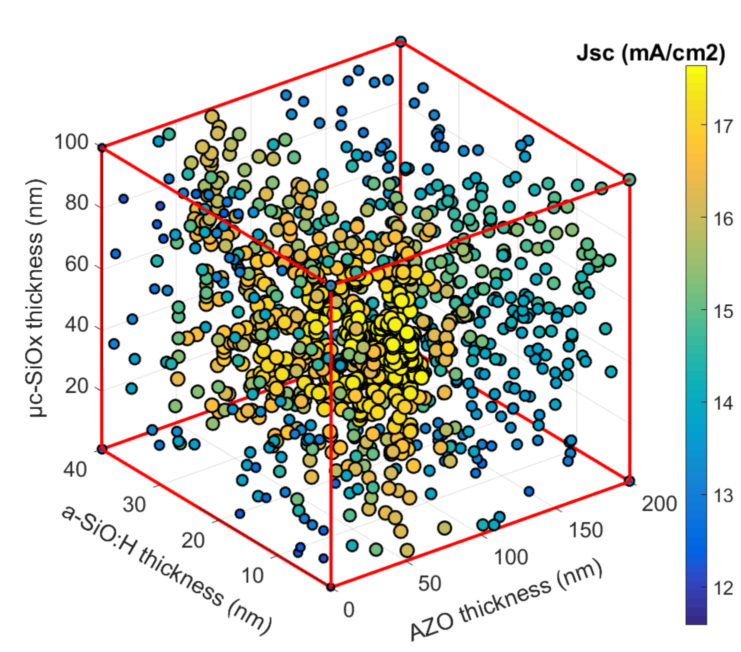
- computation for absorbance spectrum in the active layer (A_{cSi}) computation of the **short circuit current**:

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

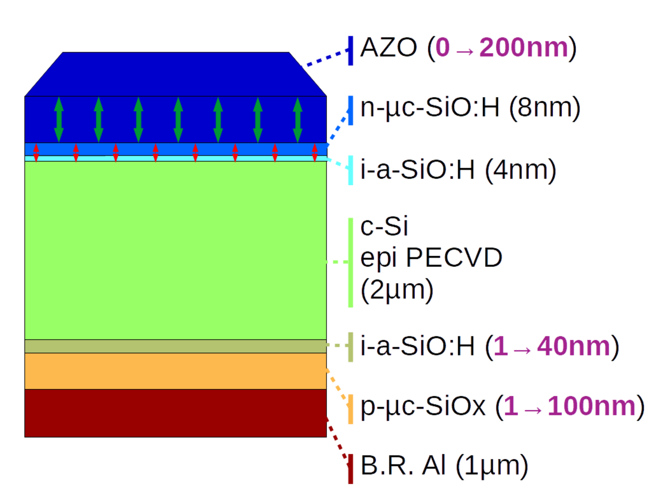
- optimization by **genetic algorithm**

* 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.

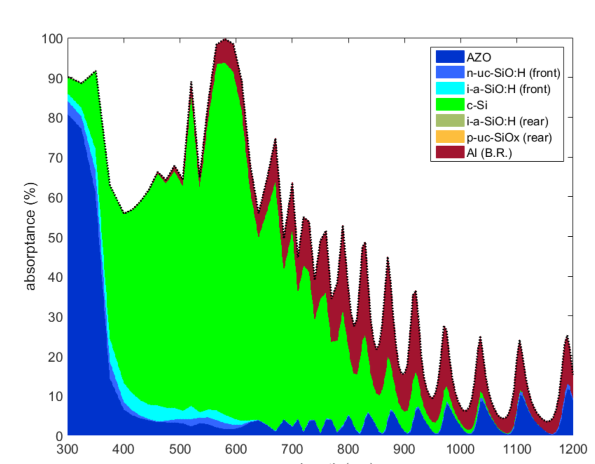
- Jsc for all parameters investigated by the genetic algorithm



optimization of the flat stack



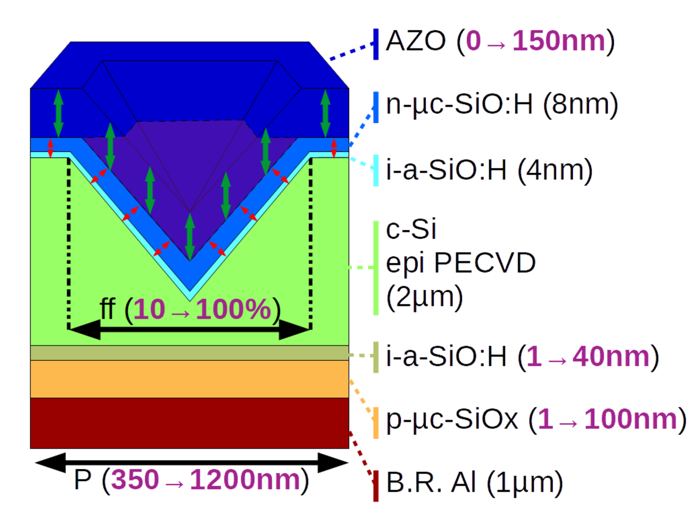
- **absorptance** spectra of each layer



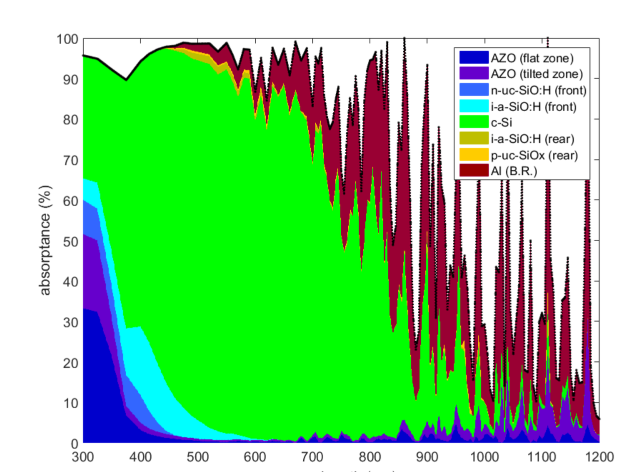
- **optimal short circuit current**:

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

optimization the patterned stack



- **absorptance** spectra of each layer

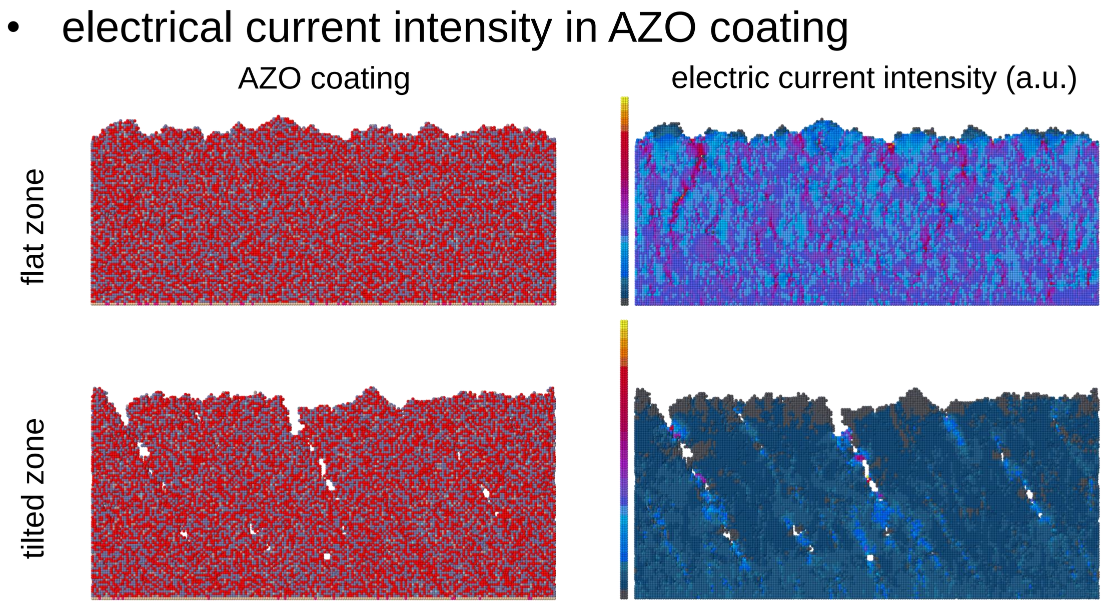


- **optimal short circuit current**:

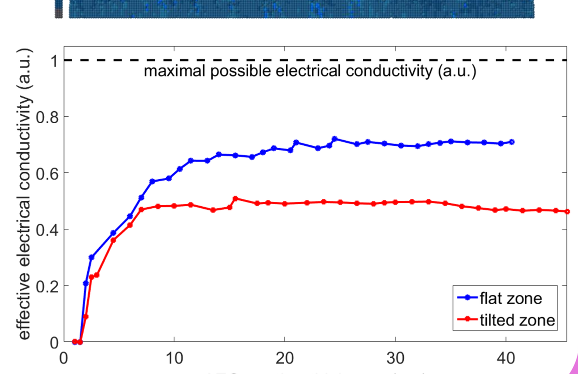
$J_{sc}=24.3\mathrm{mA/cm^2}$

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: In this work based on the numerical modelling of atomistic deposition by reactive sputtering of AZO on a structured substrate, a full characterization process was performed to estimate the electrical and optical properties of a crystalline silicon solar cell using this AZO coating as a front transparent conductive oxide. Such study pointed the high impact of the substrate pattern on those physical properties, especially the decrease of the electrical conductivity. Moreover, a global optimization by genetic algorithm was used to enhance the efficiency of such multi-layered structured solar cells.

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