Double-pane Low-E glass window optimization - From optical optimization by Genetic Algorithm to multiscale thin film deposition modelling

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INNOVATIVE COATING SOLUTIONS
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Low-E glass: state of the art

- low-Emissivity coatings
  - reflect IR for energy saving purposes
  - stay transparent to visible light

- coating stack: silver-dielectric mix
  - silver layer(s): reflect the IR and reflect/absorb the UV
  - dielectric layers (oxide or nitride):
    - protect the Ag layer(s)
    - act like ARC
    - can be used to "tune" the optical response of the full stack

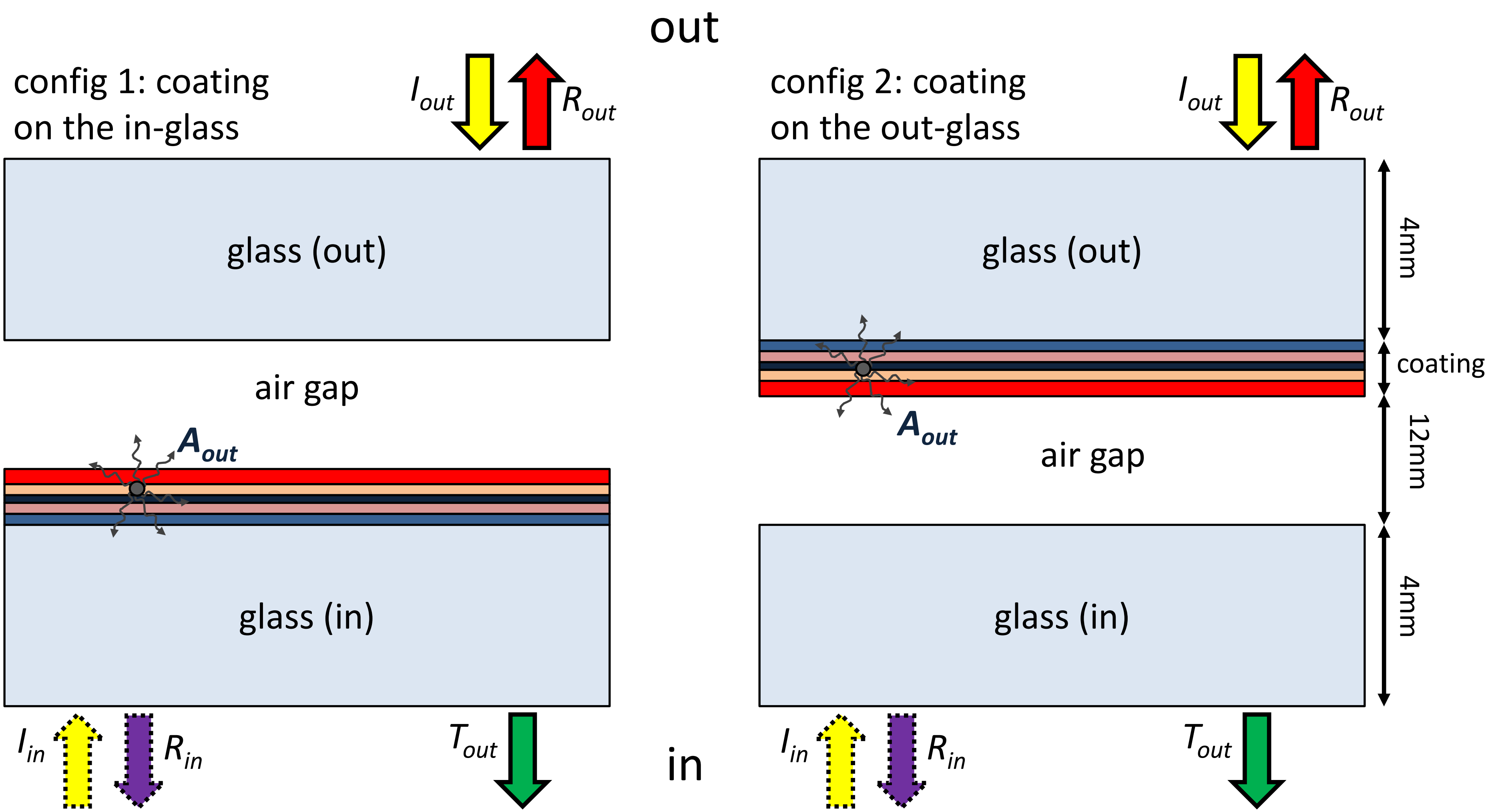
Goal of the Study

- Optimization of a low-E glass by genetic algorithm

- Film growth modelling of multilayers deposition by reactive magnetron sputtering with the software **Virtual-Coater™**
  - deposition parameter investigation to reproduce the optimum found by GA
  - film properties characterization (porosity, roughness, optical,...)

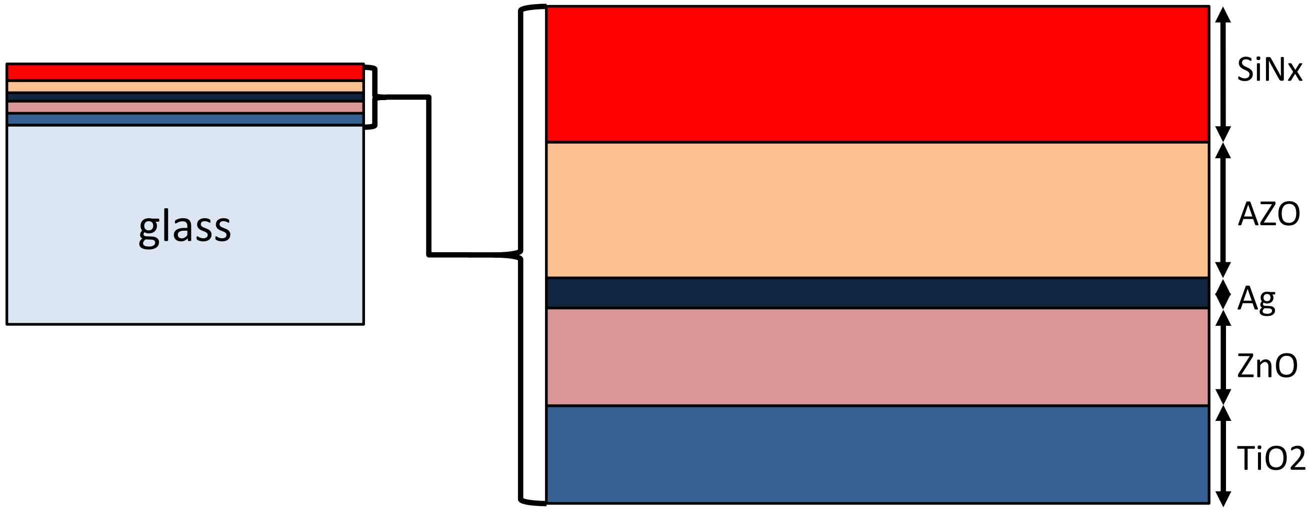
Studied low-E glass

- double-pane glass
- 2 possible positions for the coating



Studied low-E glass

- coating: 5 layers stack (**single Ag layer**)
- each layer can be deposited by **Reactive Magnetron Sputtering** with different deposition parameters (pressure, speed,...)



- goal: optimize the optical response of the coating

➡ by genetic algorithm

Genetic Algorithm Optimization

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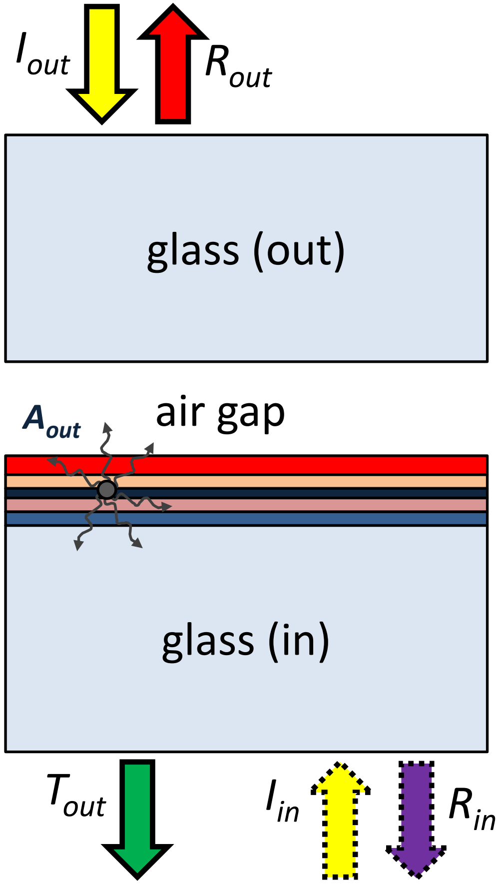
Optimization goal

- Parameters to optimize for each layer
  - thickness (0-50nm per layer)
  - porosity (5-15%)
  - interlayer thickness (0-5nm - due to roughness)
- Objectives
  - maximization of visible Transmittance (*Tout*)
  - maximization of IR Reflectance (*Rin* and *Rout*)
  - maximization of UV Absorptance (*Aout*)
  - neutral color for the visible Transmittance (a* and b* near 0)
  - minimization of total thickness (low production cost)
- Constraint
  - total thickness lower than 100nm



GA Optimization Flowchart

Input parameters

Multi-layers optical stack
- thickness t_1
- porosity p_1
- thickness interlayer $t_{1|2}$
- ...
- thickness interlayer $t_{n-1|n}$
- thickness t_n
- porosity p_n

Multi-Objectives GA by global constrained normalized fitness

- multi-Obj.: RWGA*

$\boldsymbol{F} = \sum w_i^{\mathrm{r}} w_i^{\mathrm{u}} \tilde{f}_i$

w_i^{u} = user weight (def:1)

w_i^{r} = random weight (0<<1)

- constraint: dynamic penalties on thickness

$\boldsymbol{F_c} = \boldsymbol{F} - (C.g)^{\alpha}\mathrm{SVC}^{\beta}$

$\mathrm{SVC} = \max[0; \frac{\mathrm{T_{tot}} - \mathrm{T_{max}}}{\mathrm{T_{max}}}]$

g = generation id

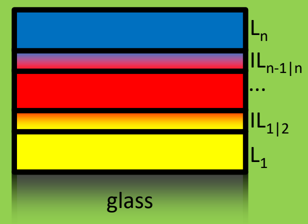
$C = 0.5$

$\alpha = \beta = 2$

*Random Weights GA

Fitness function

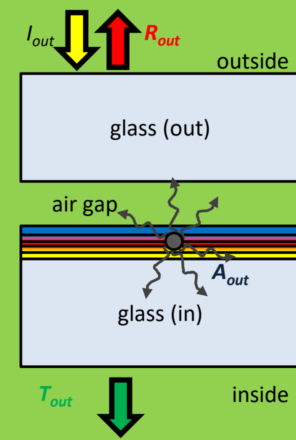
Structure construction



Optical modelling

Models
- effective optical index (with porosity) by **Effective Medium Approximation**
- reflectance, transmittance and absorptance by **Transfer-Matrix**

Illumination from outside



Illumination from inside

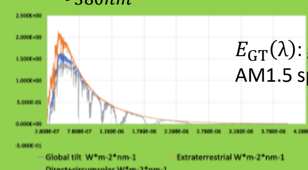
Objectives

- IR reflectance efficiencies:

$$\mathrm{LR_{out}} = \frac{\int_{780nm}^{2.5\mu m} R_{out}(\lambda) E_{\mathrm{GT}}(\lambda) d\lambda}{\int_{380nm}^{780nm} E_{\mathrm{GT}}(\lambda) d\lambda} \quad \mathrm{LR_{in}} = \frac{\int_{780nm}^{2.5\mu m} R_{in}(\lambda) d\lambda}{\int_{380nm}^{780nm} d\lambda}$$

- Visible transmittance efficiency:

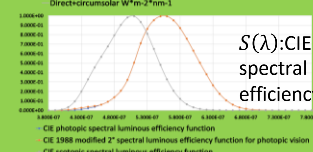
$$\mathrm{LT_{out}} = \frac{\int_{380nm}^{780nm} T_{out}(\lambda) S(\lambda) E_{\mathrm{GT}}(\lambda) d\lambda}{\int_{380nm}^{780nm} S(\lambda) E_{\mathrm{GT}}(\lambda) d\lambda}$$



$E_{\mathrm{GT}}(\lambda)$: global tilt AM1.5 spectra

- UV absorptance efficiency:

$$\mathrm{LA_{out}} = \frac{\int_{200nm}^{380nm} A_{out}(\lambda) E_{\mathrm{GT}}(\lambda) d\lambda}{\int_{200nm}^{380nm} E_{\mathrm{GT}}(\lambda) d\lambda}$$



$S(\lambda)$:CIE photopic spectral luminous efficiency function

- Lab(T_{out}(λ),D65,10°): a_T, b_T
- Total Thickness: $\mathrm{T_{tot}} = \sum_{i:1}^{n} t_i + \sum_{i:1}^{n-1} t_{i|i+1}$

Dimensionless objectives: $f_i \rightarrow 0 < \tilde{f}_i < 1$*

- $\widetilde{\mathrm{LT}}_{\mathrm{out}} = \mathrm{LT_{out}}$
- $\widetilde{\mathrm{LR}}_{\mathrm{out}} = \mathrm{LR_{out}}$
- $\widetilde{\mathrm{LA}}_{\mathrm{out}} = \mathrm{LA_{out}}$
- $\widetilde{\mathrm{LR}}_{\mathrm{in}} = \mathrm{LR_{in}}$
- $\tilde{a}_T = 1 - abs(a_T)/128$
- $\tilde{b}_T = 1 - abs(b_T)/128$
- $\tilde{T}_{tot} = 1 - p(\mathrm{T_{tot}}/\mathrm{T_{max}})$, p=0.1

Constraint:

$\mathrm{T_{max}} = 75\mathrm{nm}$

(* 1 is the optimum for each normalized objective)

Results storage for data mining/deep learning

GA Optimization results

	case	coating on in-glass	coating on out-glass
	parameters		
TiO2	thickness (nm)	14.9	17.2
	porosity (%)	14.9	6.5
	interlayer thickness (nm)	4.2	0.5
ZnO	thickness (nm)	**0.6**	**2.6**
	porosity (%)	15.4	9.3
	interlayer thickness (nm)	2.9	0.8
Ag	thickness (nm)	**18.3**	**18.3**
	porosity (%)	5	8.8
	interlayer thickness (nm)	0.6	2.1
AZO	thickness (nm)	**3.2**	**2.0**
	porosity (%)	19.6	11.6
	interlayer thickness (nm)	0.6	4.2
Si3N4	thickness (nm)	29.7	27.3
	porosity (%)	16.4	7.9
	Tout (%)	68.0	68.5
	Rout (%)	62.6	60.7
	Rin (%)	61.2	62.3
	a_T	**-6.9**	**-6.8**
	b_T	**-6.1**	**-5.9**
	thickness (nm)	74.9	74.8

stable Ag thickness

really thin ZnO and AZO layers

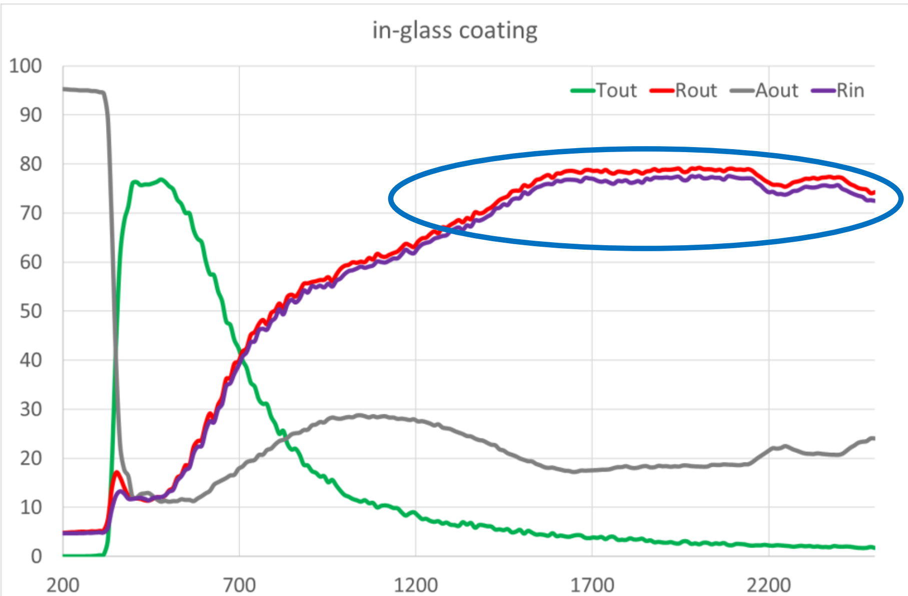
blue tinted glass

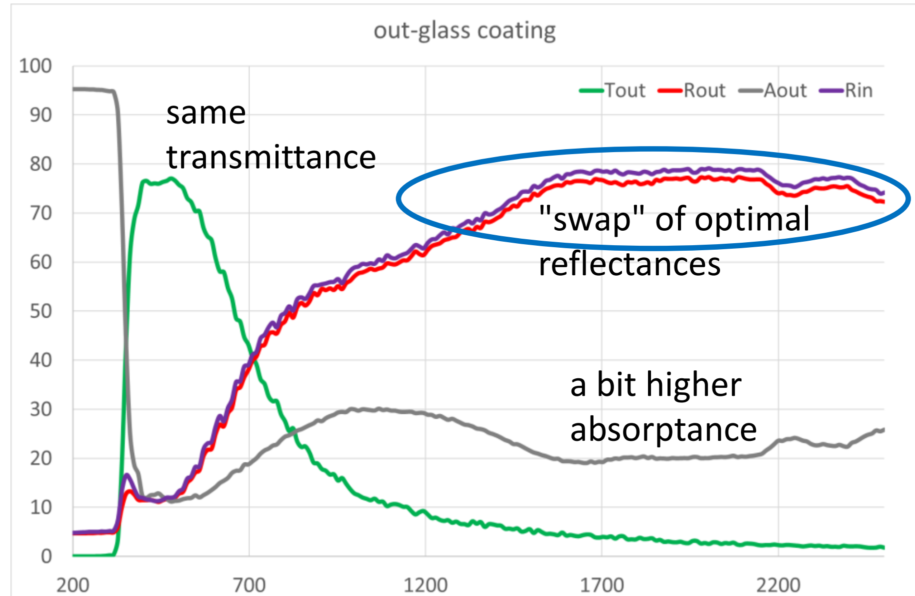
GA Optimization results

<u>config: coating on the in-glass</u>

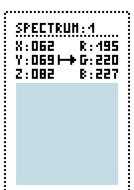
<u>config 2: coating on the out-glass</u>

- Spectra

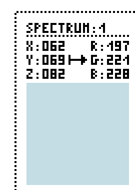




- Colors



L	a	b
86.3	-6.9	-6.1



L	a	b
86.5	-6.8	-5.9

not enough "neutral": two much red light reflected. Possibility to improve it by adding a weight to the color fitness

- Total thickness

75 nm

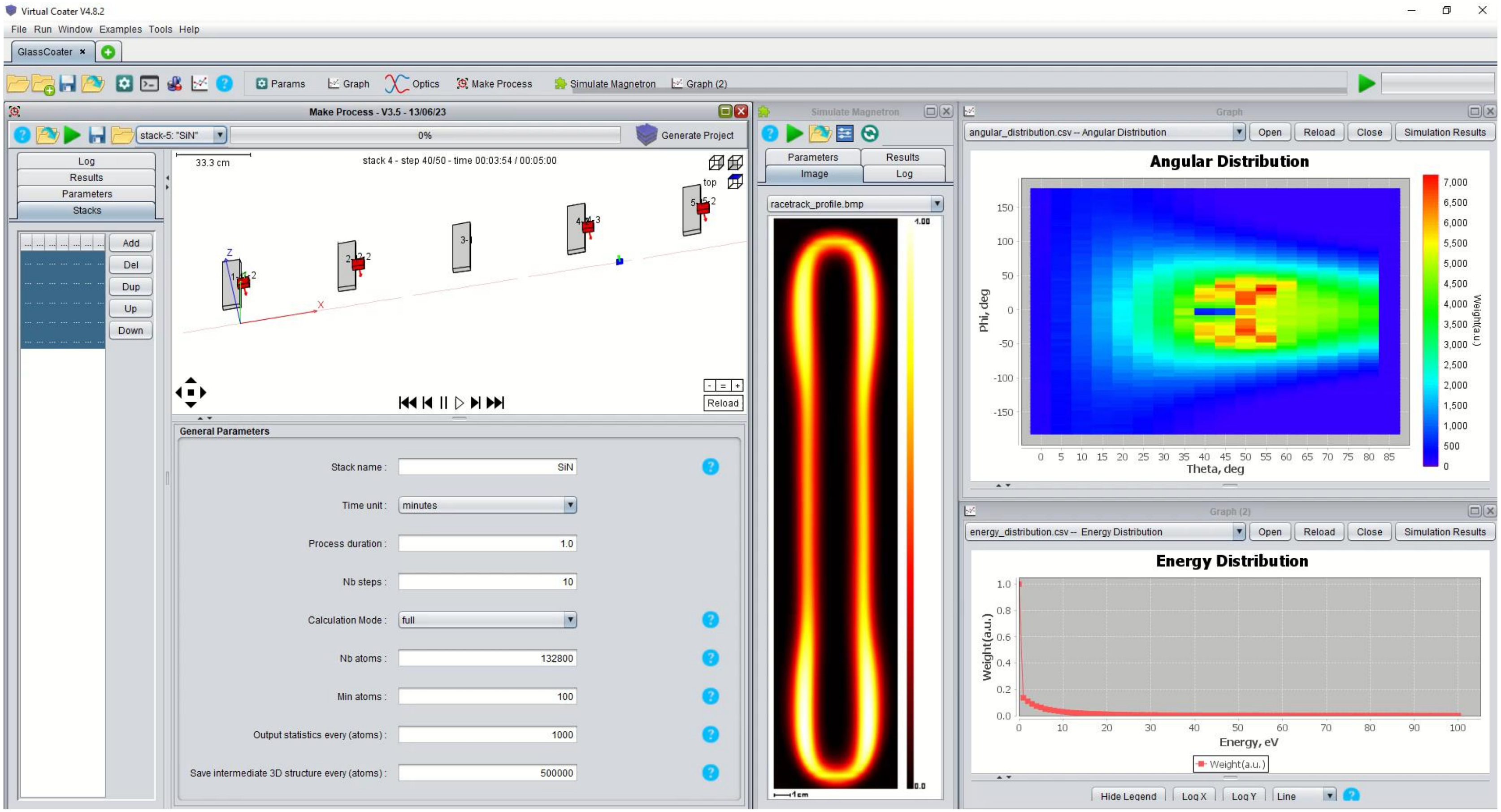
75 nm

coating thin enough for industrial applications

Film growth modelling

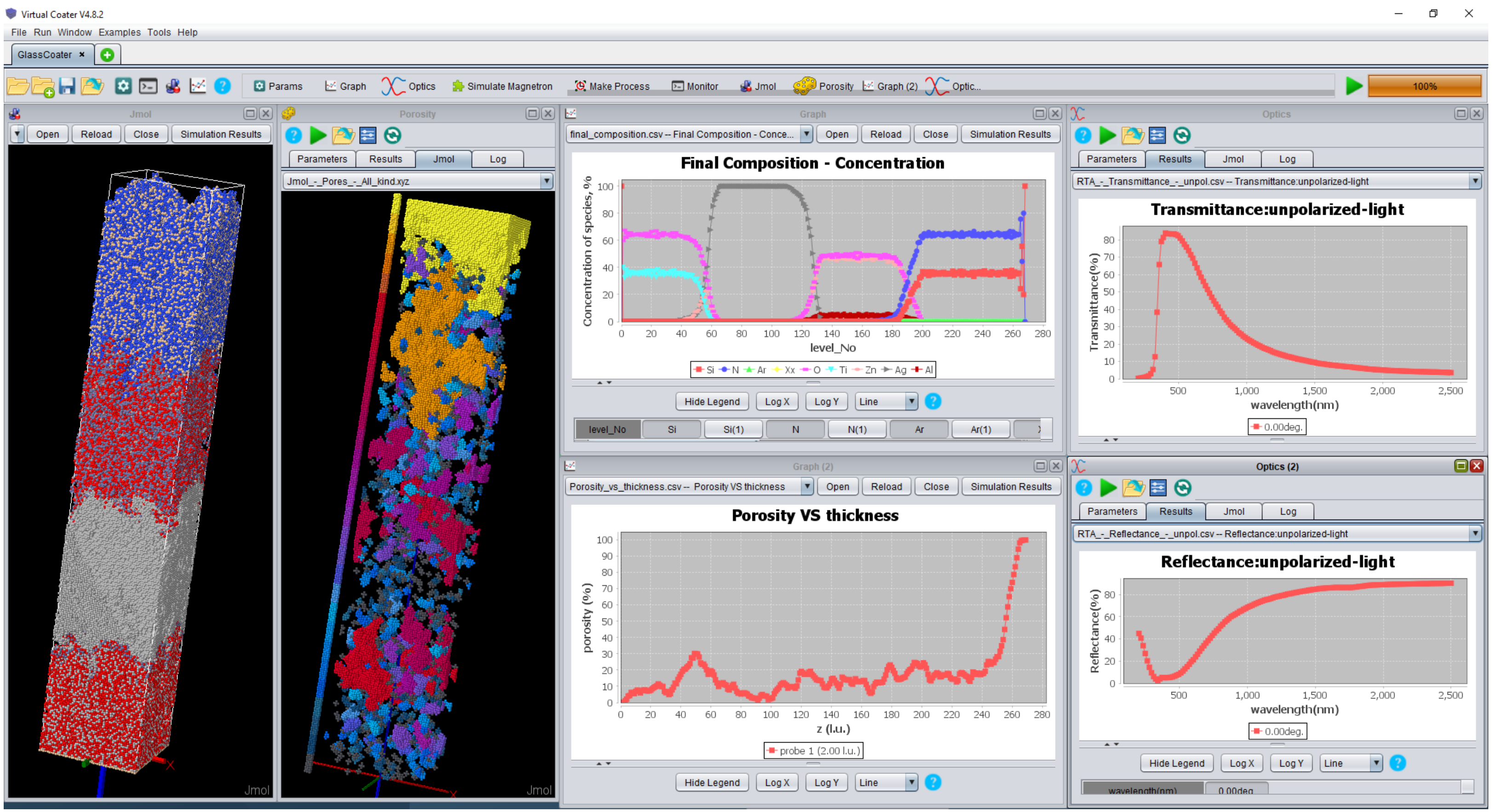
Film growth modelling tool 1/2 - industrial scale

- multiscale modelling with the **VirtualCoater™** software
  - full linear glass coater (industrial scale) with **Make-Process**
  - take as input parameters like pressure, target racetrack,...
  - compute the energy and angular distributions of incident species for each step of the deposition process

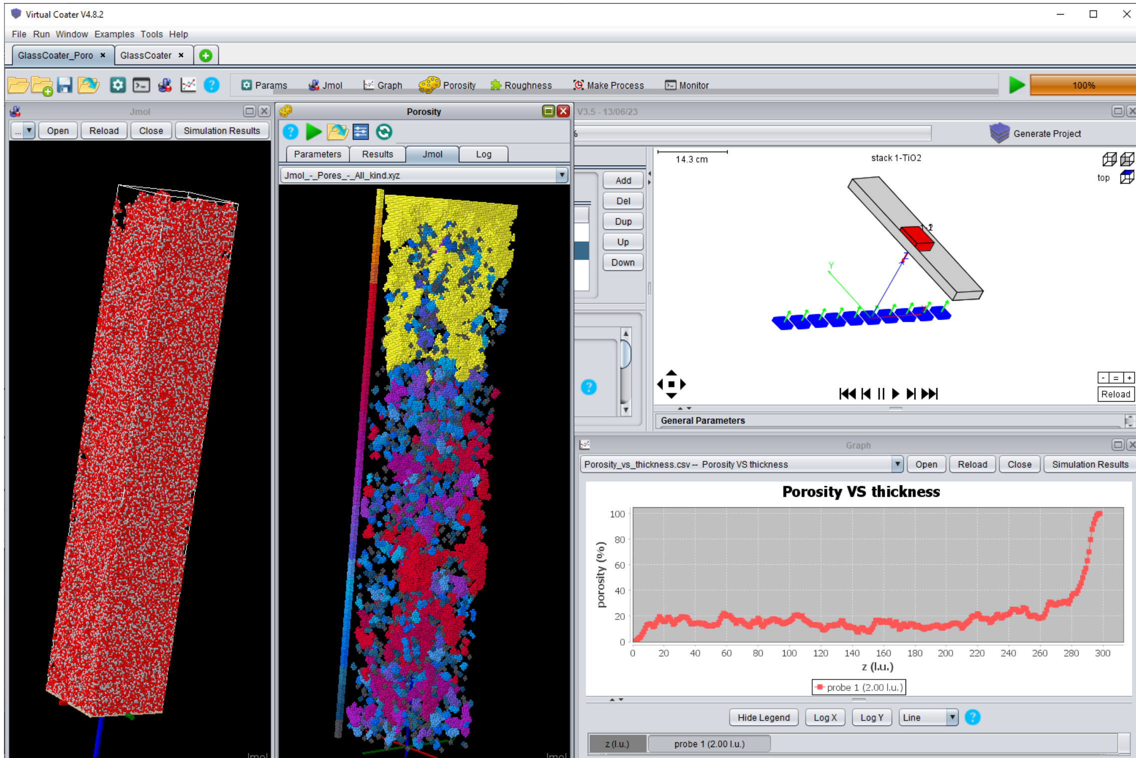


Film growth modelling tool 2/2 - atomic scale

- multiscale modelling with the **VirtualCoater™** software
  - thin film growth modelling with **Nascam**:
    - atomic scale kinetic Monte-Carlo model
    - take as input the energy and angle distributions given by **Make-Process**
  - optical/structural characterization



How to master the layer density

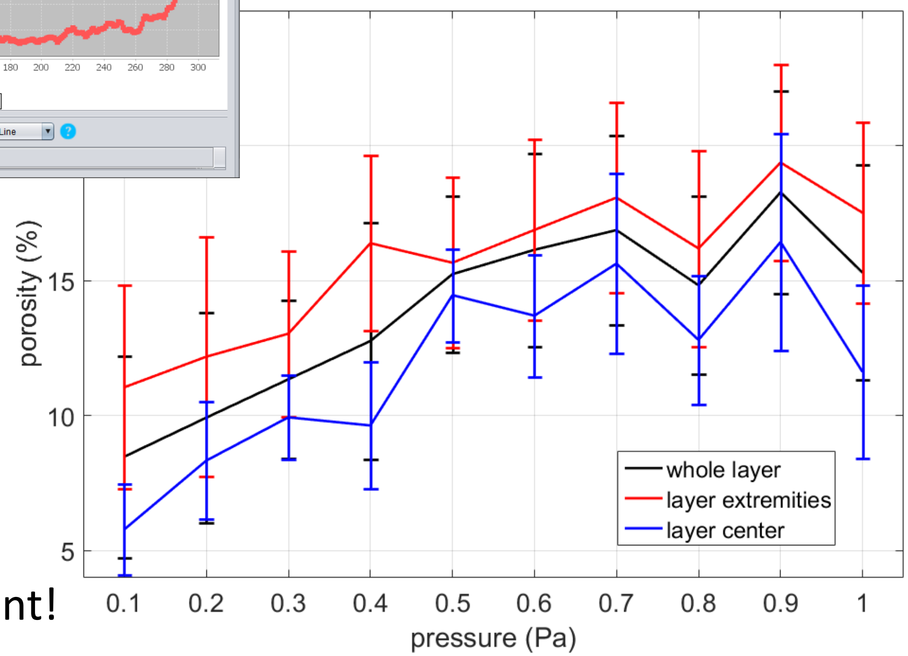


e.g.: TiO2 deposition at 0.5Pa

- the chamber pressure influence the porosity
  - pressure: from 0.1 to 1Pa
  - porosity: from 8 to 18%
- E.g.:
  - TiO2: 1Pa for 15% porosity
  - Ag*: 0.1Pa for 5% porosity

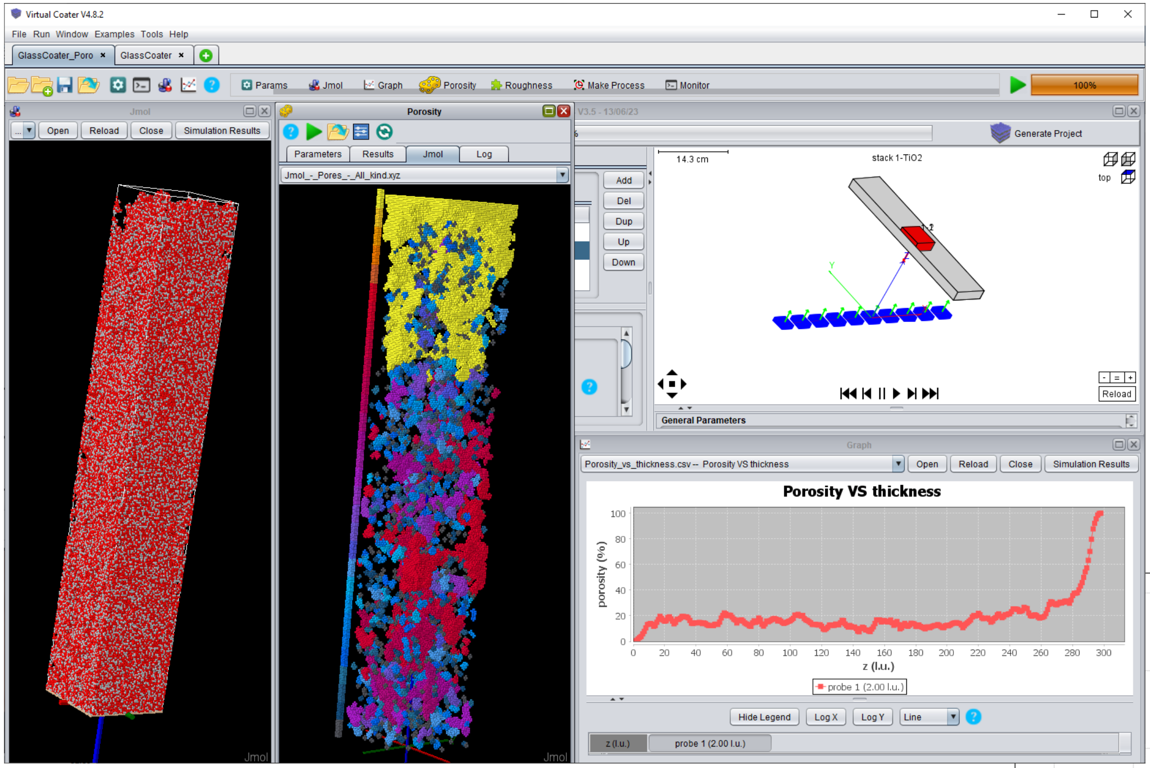
Achtung: the porosity depends on the position of the sample

- front of the target: low porosity
- far from the target: high porosity due to GLAD deposition



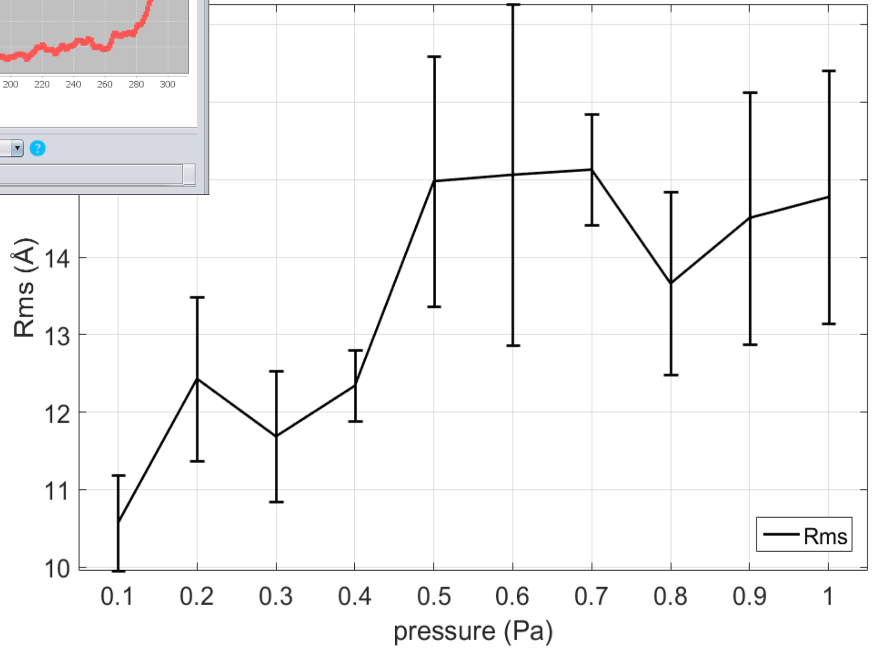
***Achtung**: Ag diffusion is not taken into account!

How to master the interlayer thickness



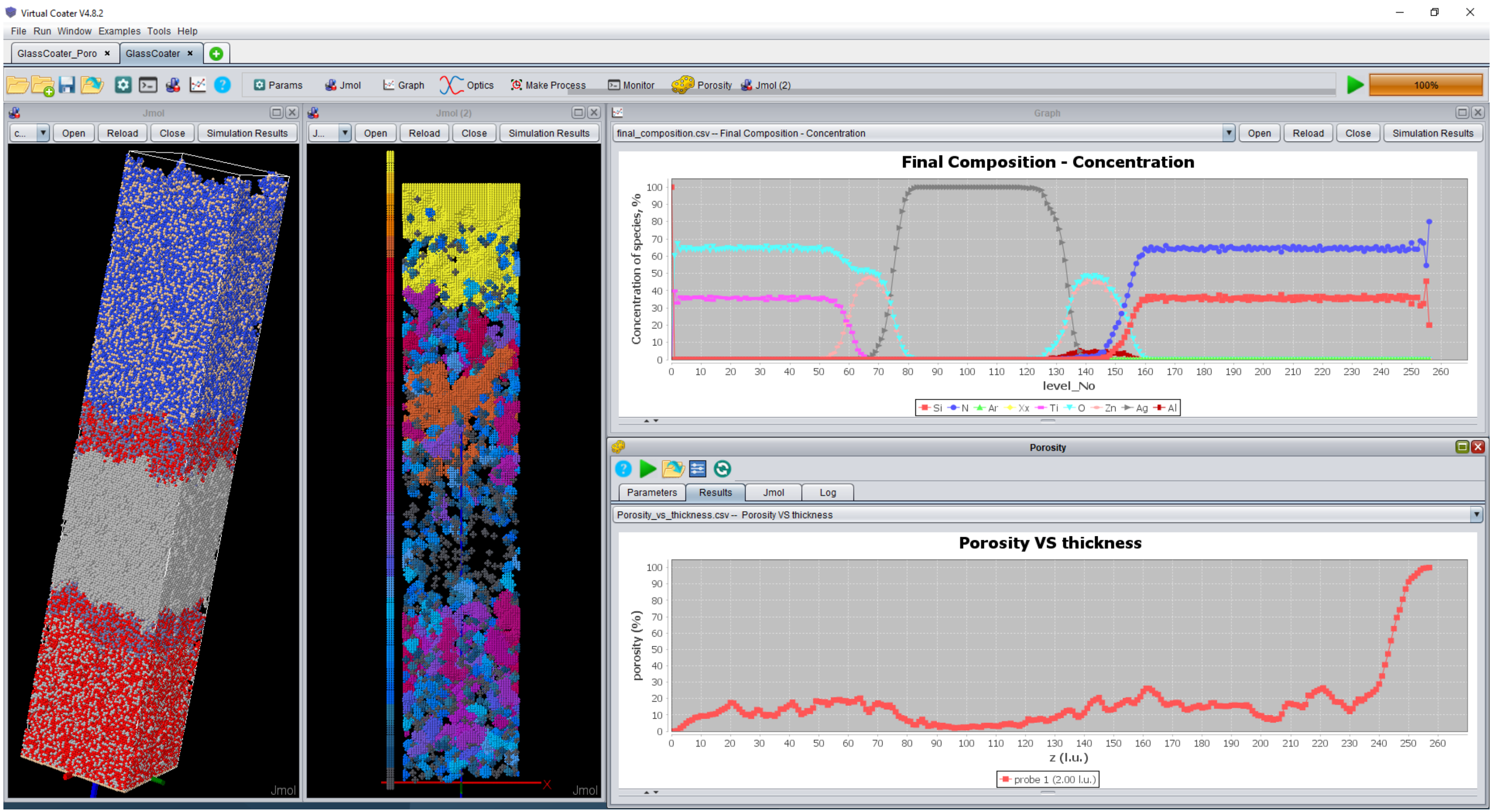
e.g.: TiO_2 deposition at 0.5Pa

- the chamber pressure influence the roughness, and then the interlayer thickness
  - pressure: from 0.1 to 1Pa
  - Rms: from 10 to 15Å



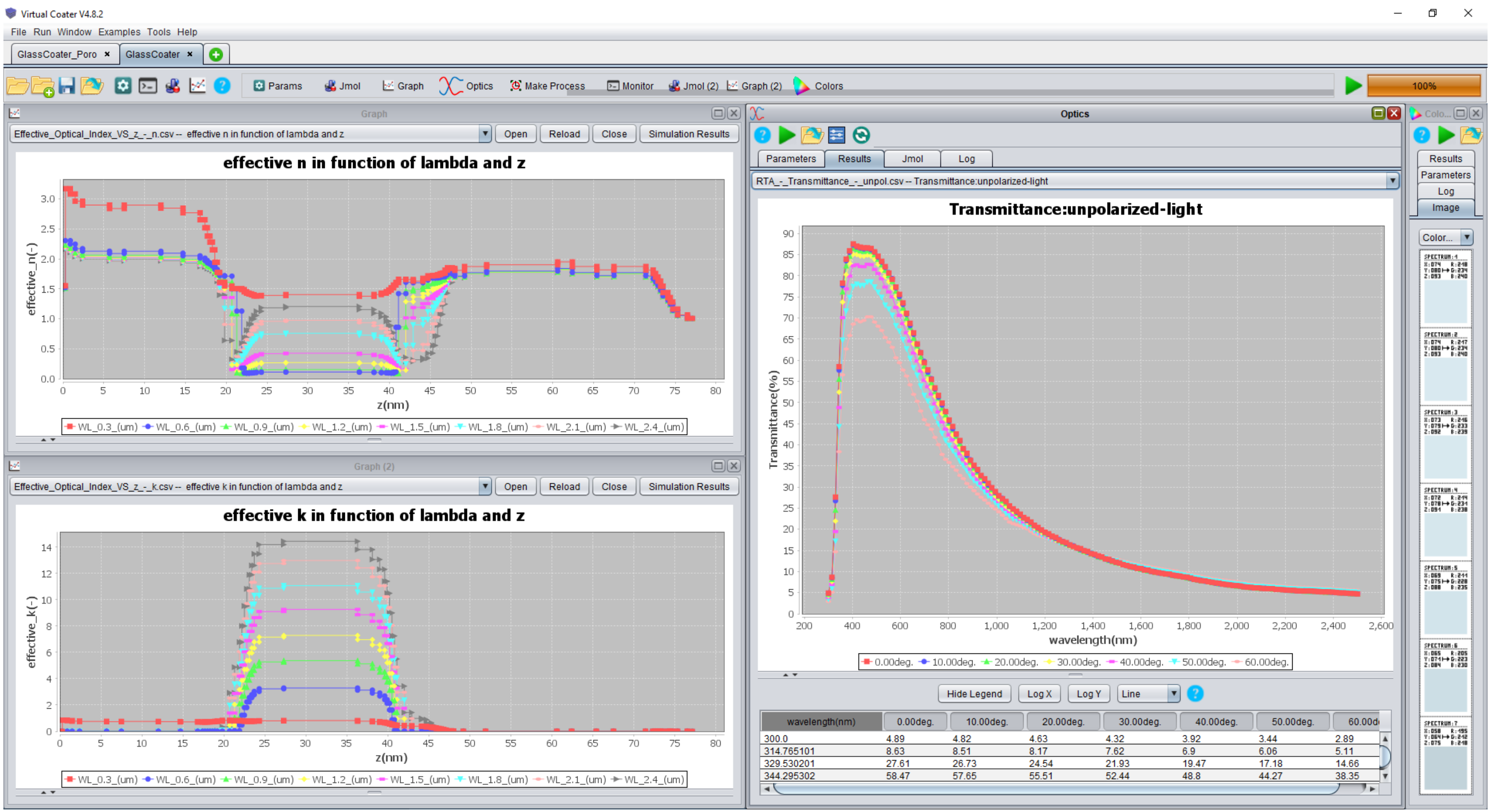
Optimal coating - full stack modelling

- Structural properties
  - porosity respected (low for Ag, high for other layers)
  - hard to master the interlayer thicknesses!



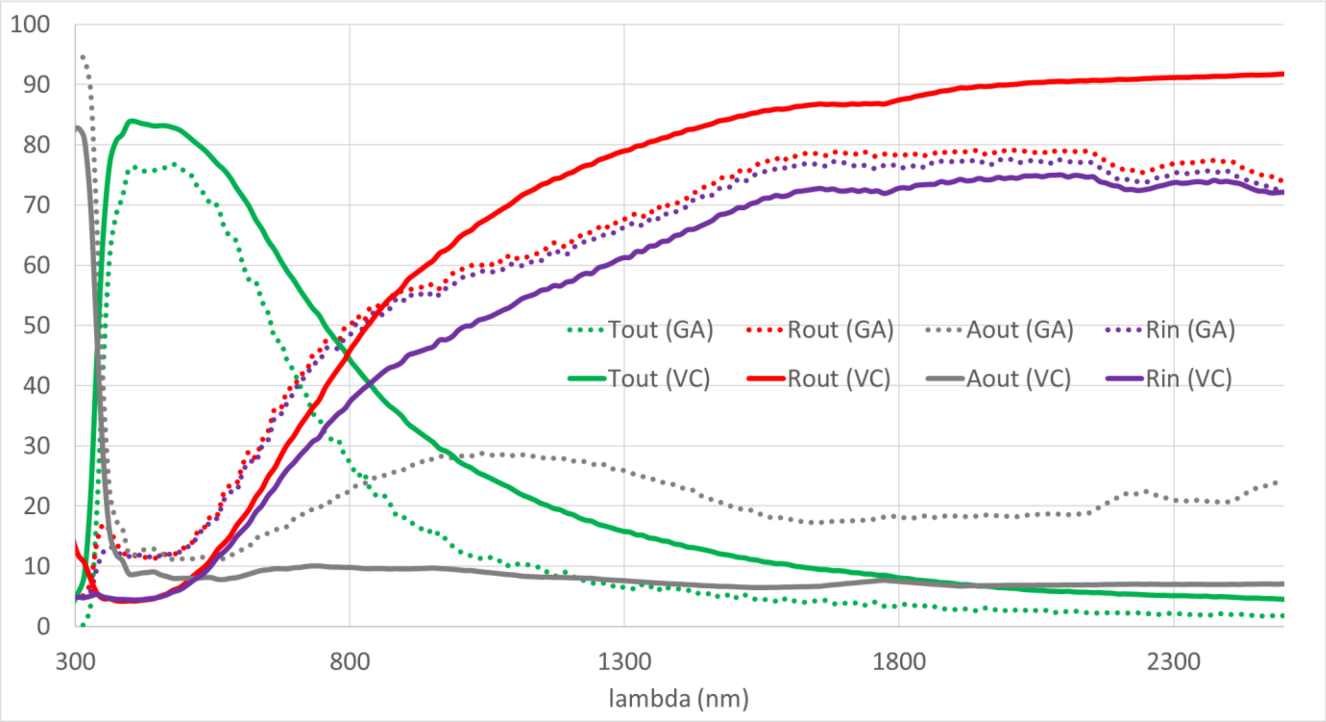
Optimal coating - full stack modelling

- Optical properties
  - computation of the effective indices: good description of interlayers
  - little influence of the incidence angle on the optical response



Optimal coating - full stack modelling

- Optical properties
  - comparison: **GA** optimum VS **Virtual-Coater™** model
  - lower absorptance predicted by **VC** (factor 2) providing better visible transmittance and IR reflectance
  - main explanation: better description of the coating structure, with better variation of the effective indices taking into account the deposition process



Conclusion

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Conclusion

- Virtual Coater is a tool available to model the deposition process and the resulting properties of coatings
- We added Genetic Algorithm for full process optimisation
- We applied this simulation chain to perform global optimization of a single Ag low-E double pane glass.

➢ We demonstrated that it allows to better describe the optical structure and then its optical response

Prospects

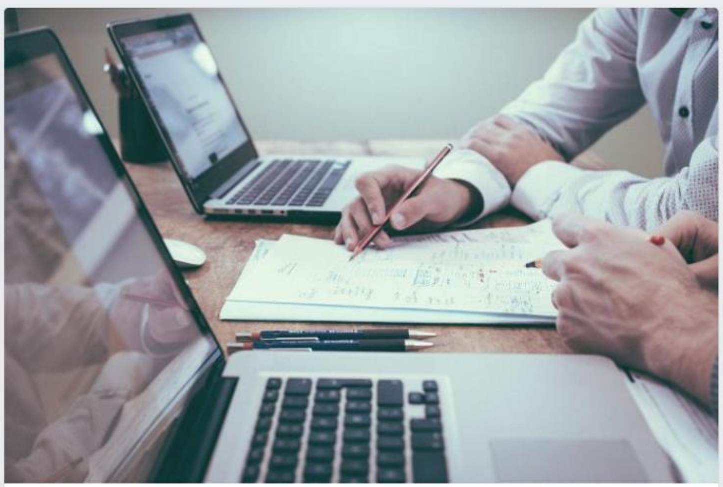
- extend the study to double, triple end quad-silver coatings
- extend the study to other dielectric materials

Interested by Virtual Coater ?

slu@incosol4u.com / www.incosol4u.com

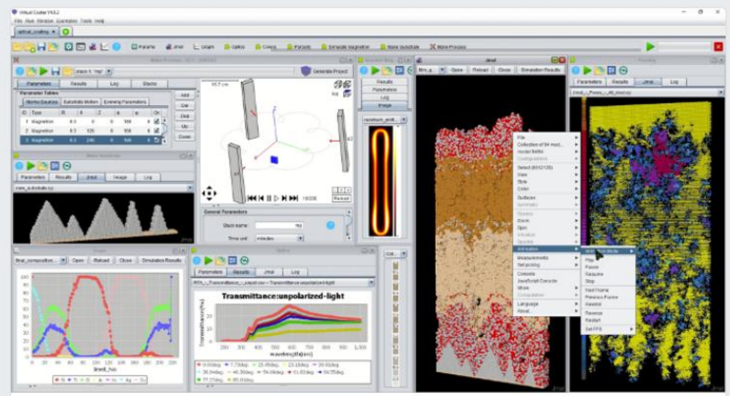
Modeling and simulation

Do you want to outsource modeling or buy a state of the art film growth simulation software ?



Service

We provide services in simulation of coating deposition by PVD



Software sales

ICS is the exclusive dealer of VIrtual Coater simulation suite