Ultra-thin CIGS: 1D/2D modelling methodology and impactful results for cell design

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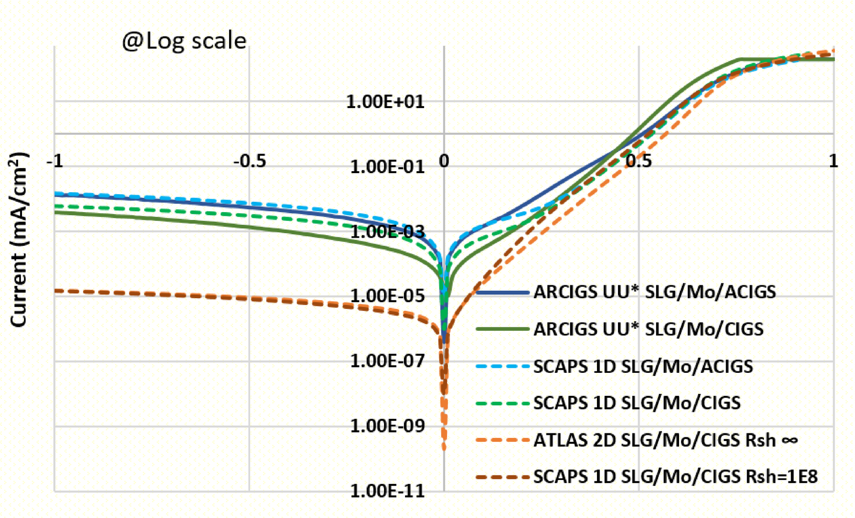
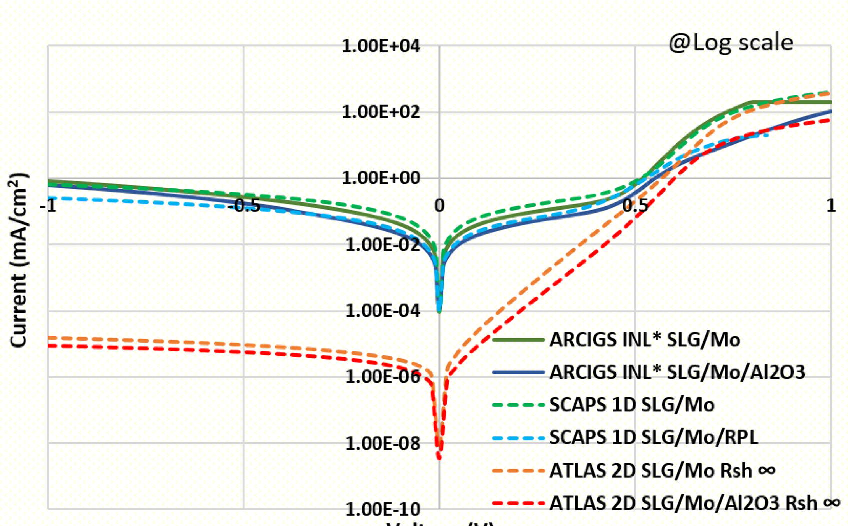
Abstract

We present the 1D/2D modelling methodology, using SCAPS and ATLAS software to simulate ultra-thin CIGS solar cells, and their impactful results on optical and electrical properties of Al_2O_3-passivated with point contact structure and unpassivated cells with and without back optical reflector.

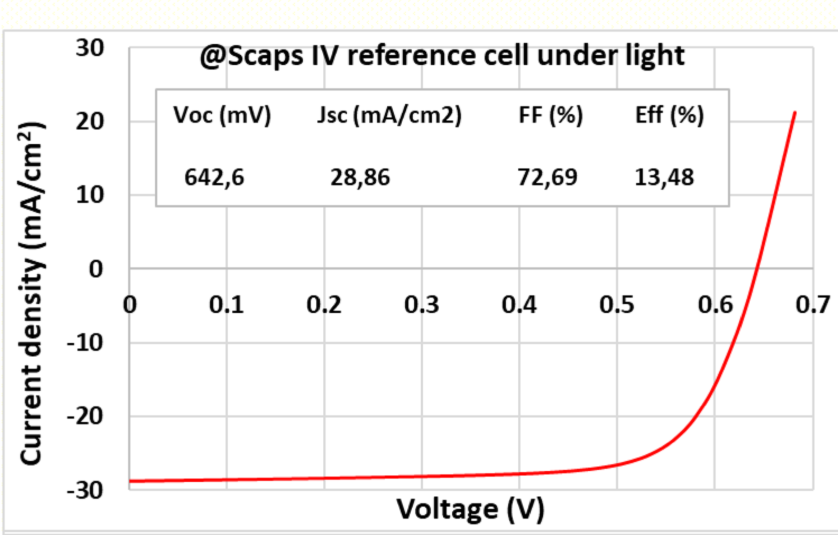
These simulations help predict optimum conditions compared to different parameters like geometry of contact hole openings (W), oxide charges density (Qf), surface recombination velocity (SRV) and back reflector (BR). The impact of the results of these simulations are very significant for cell design and fabrication.

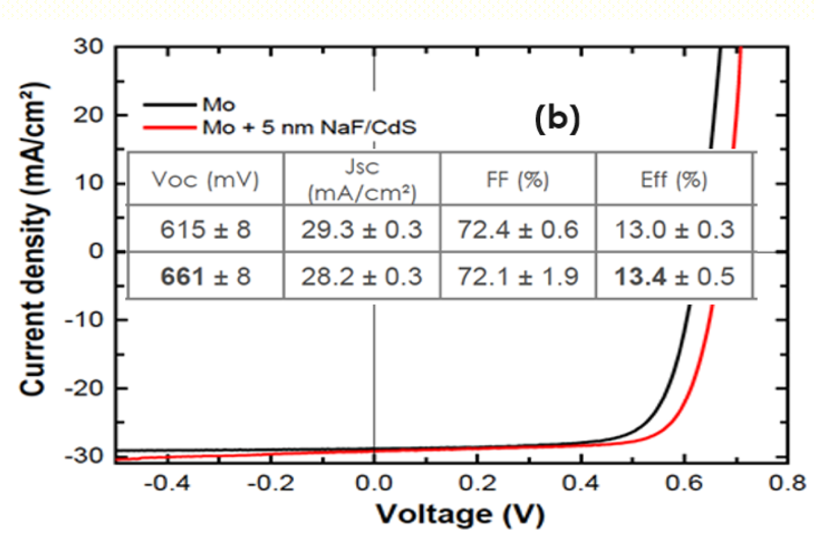
Simulations vs. Measurements





Dark IV curves comparison, ARCIGS samples vs. Simulations



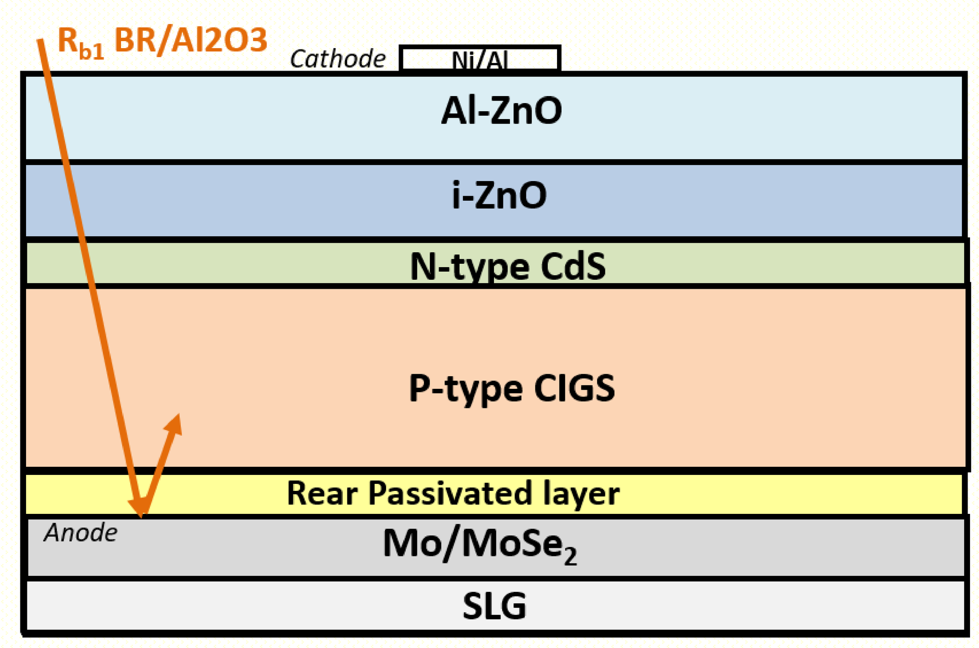


Light IV curves comparison, ARCIGS samples vs. Simulations

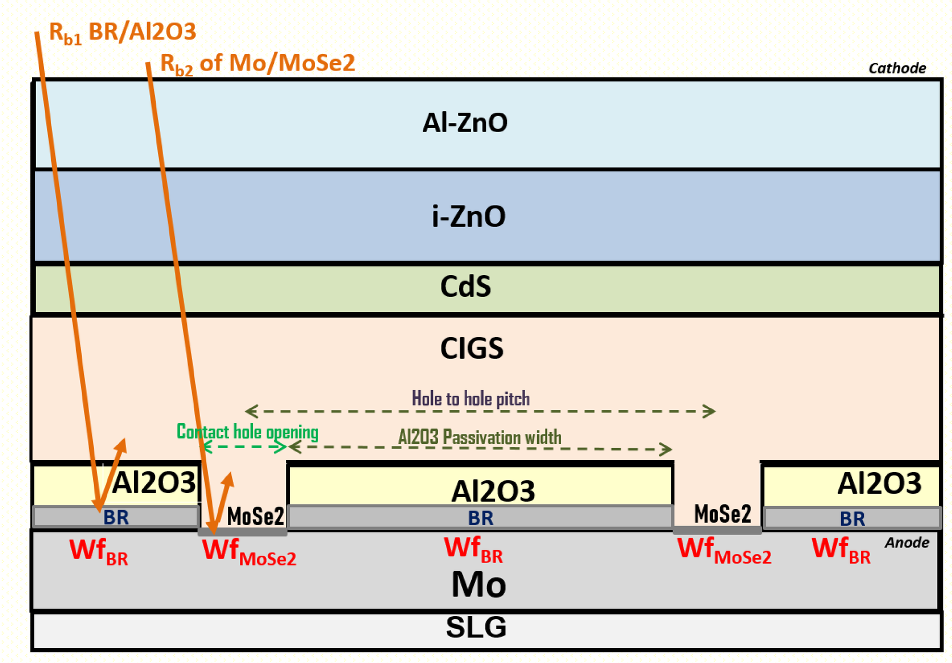
Simulations results reproduce as close as possible the experimental results on real devices

*Acronyms: *UU stand for Uppsala University*
**INL stand for International Iberian Nanotechnology Laboratory*
**UL stand for Ljubljana University*

Description of 1D/2D models



ARCIGS 1D cell model designed in SCAPS



ARCIGS 2D cell model designed in ATLAS

Our 1D and 2D models consist of an unpassivated (reference) and a passivated ultra-thin CIGS cell.

Passivation is realized in 1D by a rear passivated layer (RPL) with the properties of CIGS and with negative charge density (Qf) and interface trap density (Dit). No opening (contact holes) through RPL

Passivation is realized in 2D by an Al_2O_3 dielectric layer with contact hole openings (W) with fixed hole to hole pitch width (P).

No series and shunt resistance is implemented in this version of ATLAS model.

Rs is approximated by the contact resistance. Shunt resistance is assumed infinite

Optic parameters from UL simulations on UU samples	
Front interface	Reflectance spectrum Air/Al-ZnO
TCO optic files	Al-ZnO, i-ZnO absorption spectrum
P/N Junction	CdS, CIGS absorption spectrum
Back side reflection	Different metal stack reflection spectrum
Front internal reflection	10% of the reflected light

Contacts	Back contact	Front contact
Work function (eV)	**5.38** ($MoSe_2$)	**4.7** (Al/Ni)
Barrier height (eV)	**0.27** ($MoSe_2$)/CIGS	**0.15** (Al/Ni/ZnO)
SRVe (cm/s)	**1E7** for Reference and **1E2** for Passivated	**1E7**
SRVh (cm/s)	**1E7** for Reference and **1E2** for Passivated	**1E7**
Resistances	**Rs** and **Rsh** Calibrated with measurements	

ARCIGS input parameters for SCAPS 1D simulations

Optic parameters from UL simulations on UU samples	
Front interface	n, k spectrum Al-ZnO
TCO optic files	Al-ZnO, i-ZnO (n, k) spectrum
P/N Junction	CdS, CIGS (n, k) spectrum
Back side reflection	Different metal stack reflection value
Mo/CIGS reflectance	20% (UL simplified model value)
MoAl2O3/CIGS Reflectance	45% (UL simplified model value)
Mo/Metal(Ag)/Al2O3/CIGS	100% (UL simplified model value)

Contacts	Back contact	Front contact
Work function (eV)	Wf_{Mo}; Wf_{MoSe2}; Wf_{RBC}	**4.7**
Barrier height (eV)	**0.27**	**0.15**
SRVe (cm/s)	1E7 UnPass and 1E2 (Pass)	1E7
SRVh (cm/s)	1E7 UnPass and 1E2 (Pass)	1E7
Contact Resistance	$Rc_{Mo/CIGS}$ (Ωcm^2)	-
Resistances	**Rs** and **Rsh not implemented!**	

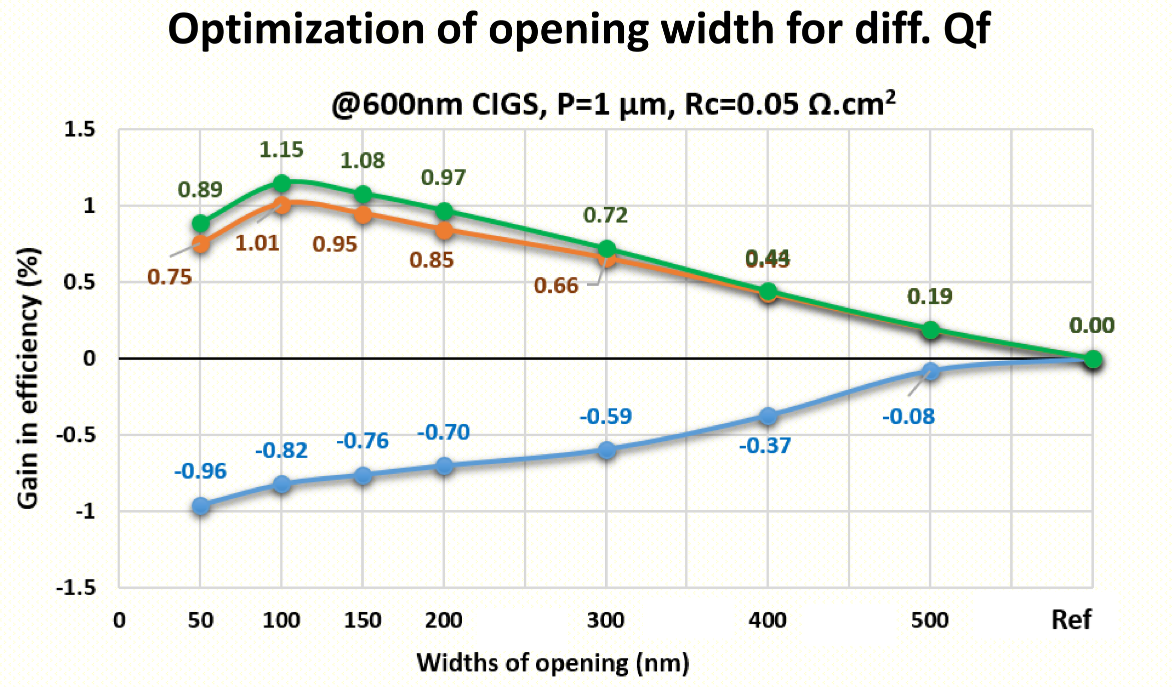
ARCIGS input parameters for ATLAS 2D simulations

The input database is calibrated with material, electrical and optical parameters extracted from experimental devices.

Optical simulations performed by UL* partner with SunShine simulator have provided significant optical inputs for full cell modelling of light management within the cell.

Simulation results

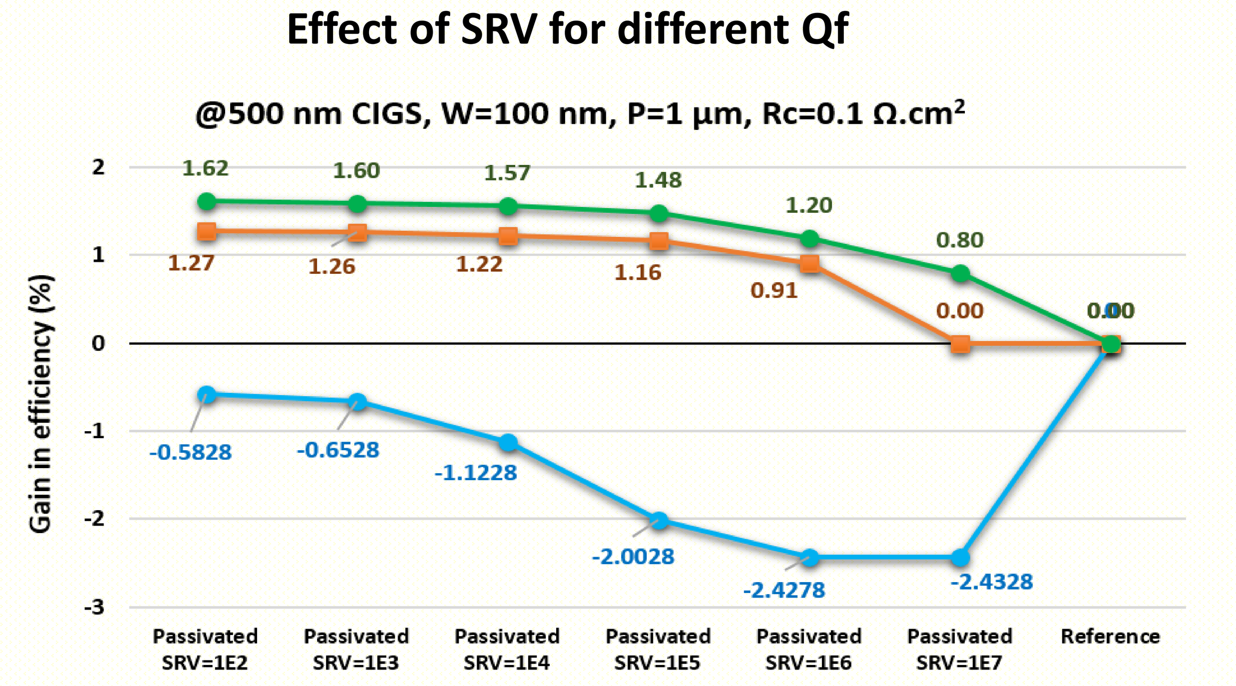
Optimization of opening width for diff. Qf



A passivation layer with a very low density of Qf degrades the performances of the cell under the reference while a high density of negative Qf improves the performance over the reference.

Presence of an optimum related to the width of the opening and the contact resistance.

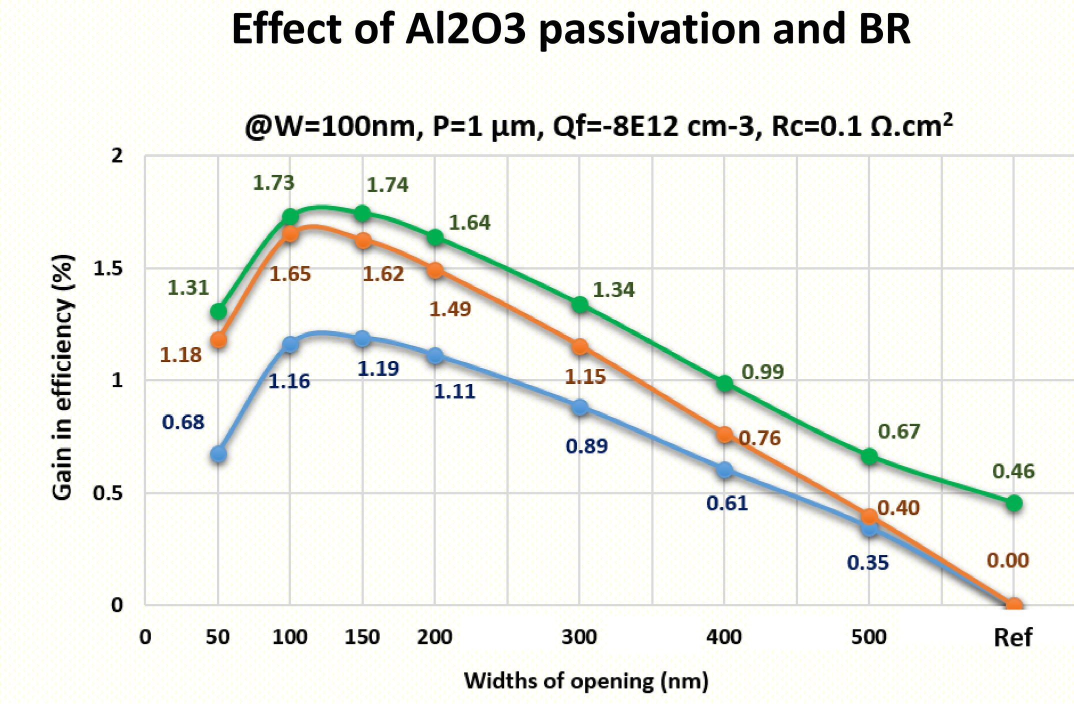
Effect of SRV for different Qf



The oxide passivation layer helps to reduce the effective recombination by field effect and improve the performances of the cell.

For a low density of Qf, reducing the SRV maintains the performances below the reference. For a high density of Qf (> 5E12 cm-3), the gain is over the reference and does not vary significantly for SRV below 1E4 cm/s.

Effect of Al2O3 passivation and BR



Introduce a back optical reflector helps to increase the performance of the cell.

Increasing the CIGS thickness from 500nm to 600 nm helps to improve more the performance without loosing the passivation effect.

Conclusions

- Our SCAPS 1D and ATLAS 2D models simulate as fairly as possible the measurements on real devices.
- ATLAS 2D model helps to guide cells processing for passivated cells and predict optimum conditions for different parameters.
- Simulations show that ensuring an excellent passivation with a high density of negative oxide charges is more relevant than reducing the SRV to very low values.
- The influence of the geometry of contact hole openings on the performance is critical for pattern design of the passivated cell structures.

Acknowledgements

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