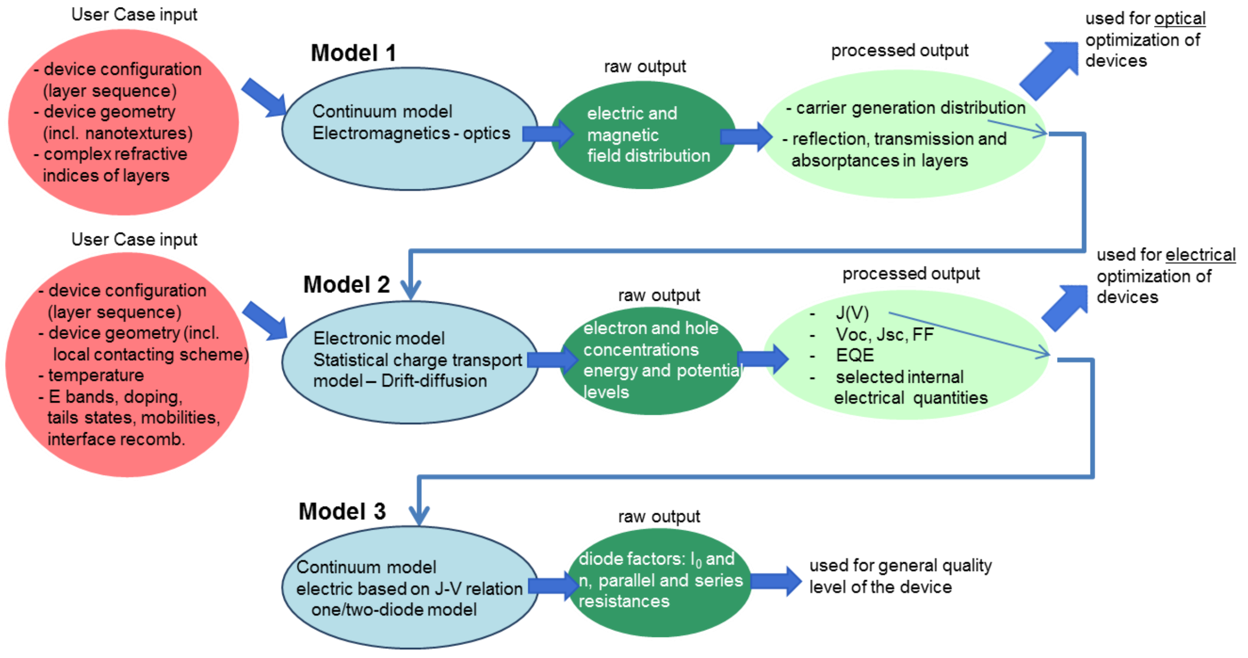
Modelling data documenting one simulation - MODA

Project ARCIGS-M

Optical and electrical device simulation

OVERVIEW of the simulation			
1	**USER CASE**	The user wants to simulate (ultra-thin) CIGS solar cells with different contacting schemes. Concepts such as additional passivation layers, highly reflective back reflector, local back contacting are included. The purpose of simulation is to understand and analyse opto-electronic behaviour of the device and to optimize it with respect of optical (light management) and electrical (layer and interface quality, contacting scheme) point of view.	
2	**CHAIN OF MODELS**	**MODEL 1**	Continuum model: electromagnetic wave propagation in the device, propagation of light in (semi) absorbing material, interface reflection, transmission, scattering included. **4.6 in RoMM.**
		MODEL 2	Electronic model: statistical drift-diffusion transport model used in continuum material, transport of charge carriers (electron and holes) in semiconductor and contacting layers, optical and thermal carrier generations and recombinations, interface recombinations, **1.4 in RoMM**.
		MODEL 3	Continuum model: simple one- or two-diode electrical model, describing relationship between electrical voltage and current of the device, theory behind is the drift-diffusion model , **4.6 in RoMM**.
3	**PUBLICATION ON THIS ONE SIMULATION**		
4	**ACCESS CONDITIONS**	The specified models are widely used in opto-electronic simulations of semiconductor devices and are implemented in commercial software such as COMSOL, Sentaurus T-CAD and others.	
5	**WORKFLOW AND ITS RATIONALE**	Thicknesses of the CIGS absorber is in the range of a few hundred nanometers, thus, no special quantum effects need to be included in these simulations. First, optical simulation is performed to determine charge-generation distribution in layers as input parameter for the electrical simulation. These two models are linked. Additionally, well known one- and two-diode model of a solar cell is then linked further to get additional information about the quality of the solar cell device. (input J(V) characteristics)	

Modelling Workflow



MODEL 1

1	ASPECT OF THE USER CASE/SYSTEM TO BE SIMULATED
1.1	ASPECT OF THE USER CASE TO BE SIMULATED	To perform detailed optical simulation of (ultra-thin) CIGS solar cell. To analyse and understand optical behaviour, to generate input for linked electrical simulation, to optimize device optically (proposed light management strategies).
1.2	MATERIAL	Simulated device consists of the following basic layers: front transparent contact: ZnO:Al + ZnO window layer: CdS (n-type) absorber layer: (ultra-thin) Cu(In, Ga)Se2 (p-type) passivation layer: Al2O and MgF2 back contact: Mo substrate: thin steel foil / soda lime glass
1.3	GEOMETRY	vertical dimensions of device (W/o substrate): ~ μm, lateral dimensions: mm to several cm
1.4	TIME LAPSE	not applicable
1.5	MANUFACTURING PROCESS OR IN-SERVICE CONDITIONS	incoming light
1.6	PUBLICATION ON THIS ONE SIMULATION	

2	GENERIC PHYSICS OF THE MODEL EQUATION		
2.0	MODEL TYPE AND NAME	RoMM 4.6 Continuum model - Electromagnetism - Optics	
2.1	MODEL ENTITY	finite volumes	
2.2	MODEL PHYSICS/ CHEMISTRY EQUATION PE	Equation	PE: Maxwell's equations $\nabla \cdot \boldsymbol{E} = \frac{\rho}{\varepsilon}$ $\nabla \cdot \boldsymbol{B} = 0$ $\nabla \times \boldsymbol{E} = -\frac{\partial \boldsymbol{B}}{\partial t}$ $\nabla \times \boldsymbol{B} = \mu \boldsymbol{J} + \mu\varepsilon \frac{\partial \boldsymbol{E}}{\partial t}$ which present the basis for wave equation, describing the propagation of electromagnetic waves.
		Physical quantities	ρ – space charge density E – electric field B – magnetic flux density J – electrical current density
2.3	MATERIALS RELATIONS	Relation	MR: $\boldsymbol{D} = \varepsilon \boldsymbol{E}$, $\boldsymbol{B} = \mu \boldsymbol{H}$ ε and μ describe material properties and directly determine complex refractive indices of layers
		Physical quantities/ descriptors for each MR	D – electric flux density E – electric field B – magnetic flux density H – magnetic field ε - permittivity (material property) μ - permeability (material property)
2.4	SIMULATED INPUT		

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3	SOLVER AND COMPUTATIONAL TRANSLATION OF THE SPECIFICATIONS		
3.1	NUMERICAL SOLVER	Finite element method (FEM)	
3.2	SOFTWARE TOOL	COMSOL Multiphysics	
3.3	TIME STEP	not applicable, frequency domain	
3.4	COMPUTATIONAL REPRESENTATION ,	PHYSICS EQUATION, MATERIAL RELATIONS, MATERIAL	PE: Maxwell's equations (see above) applied to each discrete element in the mash-grid. MR: connections between E and H and D and B via permittivity and permeability, permittivity is linked to complex refractive indexes which are actual input parameters of simulation
3.5	COMPUTATIONAL BOUNDARY CONDITIONS	top and bottom side of the device: Perfectly matched layers (PML), Absorbing boundary condition (ABC), other sides of the device: Periodic boundary condition (PBC), Symmetry boundary condition (SBC)	
3.6	ADDITIONAL SOLVER PARAMETERS	mesh-grid: > 5 discrete elements per effective wavelength	

Post processing

4	POST PROCESSING	
4.1	THE PROCESSED OUTPUT	charge carrier generation distribution, optical reflection, transmission and absorption in individual layers for Model 2
4.2	METHODOLOGIES	Volume averaging; applying Poynting vector to electric and magnetic field
4.3	MARGIN OF ERROR	numerical error < 1 % in post-processing

MODEL 2

1	ASPECT OF THE USER CASE/SYSTEM TO BE SIMULATED	
1.1	ASPECT OF THE USER CASE TO BE SIMULATED	To perform detailed electrical simulation of (ultra-thin) CIGS solar cell. To analyse and understand electrical behaviour, to optimize device electrically (layers, interfaces, contacting schemes).
1.2	MATERIAL	Device consists of the following basic layers: front transparent contact: ZnO:Al + ZnO window layer: CdS (n-type) absorber layer: (ultra-thin) Cu(In, Ga)Se2 (p-type) passivation layer: Al2O and MgF2 back contact: Mo substrate: thin steel foil / soda lime glass energy bandgaps, electron affinities, doping, tails states, mobilities, interface recomb.,
1.3	GEOMETRY	vertical dimensions (w/o substrate): µm, lateral dimensions: mm to several cm
1.4	TIME LAPSE	steady state analysis
1.5	MANUFACTURING PROCESS OR IN-SERVICE CONDITIONS	voltage bias, temperature
1.6	PUBLICATION ON THIS ONE SIMULATION	

2	GENERIC PHYSICS OF THE MODEL EQUATION		
2.0	MODEL TYPE AND NAME	RoMM 1.4 Electronic model, Statistical charge transport model – Drift-diffusion applied to continuum material	
2.1	MODEL ENTITY	finite volumes	
2.2	MODEL PHYSICS/ CHEMISTRY EQUATION PE	**Equation**	PE: basic semiconductor equations (represented for 1D, can be extended to 2D and 3D): $J_n = q\mu_n n E + q D_n \frac{dn}{dx}$ $J_p = q\mu_p p E - q D_p \frac{dp}{dx}$ $\frac{\partial p}{\partial t} = G - R - \frac{1}{q}\frac{\partial J_p}{\partial x} = -\frac{p-p_0}{\tau_p} - \frac{1}{q}\frac{\partial J_p}{\partial x}$ $\frac{\partial n}{\partial t} = G - R + \frac{1}{q}\frac{\partial J_n}{\partial x} = -\frac{n-n_0}{\tau_n} + \frac{1}{q}\frac{\partial J_n}{\partial x}$ $\frac{\partial E}{\partial x} = \frac{\rho}{\varepsilon} = \frac{q}{\varepsilon}(p - n + N_D - N_A)$
		Physical quantities	J – electrical current density (n- of electrons and p - holes) n – electron concentration p – hole concentration E – electric field ρ – space charge density G – charge generation rate R – charge recombination rate N_D – donor concentration N_A – acceptor concentration µ – mobility coefficient of carriers D – diffusion coefficient of carriers q – elementary charge
2.3	MATERIALS	**Relation**	Einstein relation: $\mu_{n(p)} = \frac{qD_{n(p)}}{k_B T}$

	RELATIONS	Physical quantities/ descriptors for each MR	relation between mobility $\mu_{n(p)}$ and diffusion coefficient $D_{n(p)}$ to each other; T = temperature
2.4	SIMULATED INPUT	charge carrier generation distribution from Model 1	

3	SOLVER AND COMPUTATIONAL TRANSLATION OF THE SPECIFICATIONS		
3.1	NUMERICAL SOLVER	Finite difference / Finite element method	
3.2	SOFTWARE TOOL	SCAPS (1D) / ASPIN3 (2D) / ATLAS / SENTAURUS T-CAD (3D) decision made upon specifics of the problem	
3.3	TIME STEP	not applicable, steady state simulation	
3.4	COMPUTATIONAL REPRESENTATION	PHYSICS EQUATION, MATERIAL RELATIONS, MATERIAL	Above mentioned semiconductor equations are applied to discrete elements of the device structure
3.5	COMPUTATIONAL BOUNDARY CONDITIONS	ohmic contact, selective, schottky, perfect isolation surface, periodic	
3.6	ADDITIONAL SOLVER PARAMETERS	mesh-grid: order of diffusion length	

Post processing

4	POST PROCESSING
4.1	THE PROCESSED OUTPUT	current density – voltage (J(V)) curve, external quantum efficiency (EQE) and any internal parameter distribution upon user request
4.2	METHODOLOGIES	applying different voltages to device in simulation and calculate current densities, separate application of charge generation by light to obtain spectral responses such as EQE
4.3	MARGIN OF ERROR	numerical error < 2 % in post-processing

MODEL 3

1	ASPECT OF THE USER CASE/SYSTEM TO BE SIMULATED
1.1	ASPECT OF THE USER CASE TO BE SIMULATED	To extract basic parameters of the one- and two-diode model of (ultra-thin) CIGS solar cell and to generally evaluate the quality of the solar cell
1.2	MATERIAL	CIGS solar cell represented by equivalent electrical circuit with two electrical connection ports
1.3	GEOMETRY	complete solar cell area
1.4	TIME LAPSE	steady state analysis
1.5	MANUFACTURING PROCESS OR IN-SERVICE CONDITIONS	temperature
1.6	PUBLICATION ON THIS ONE SIMULATION	

2	GENERIC PHYSICS OF THE MODEL EQUATION		
2.0	MODEL TYPE AND NAME	RoMM 4.6 Continuum model – Electromagnetism - electrical	
2.1	MODEL ENTITY	complete device volume	
2.2	MODEL PHYSICS/ CHEMISTRY EQUATION PE	**Equation**	PE1: one-diode equation $I = I_L - I_0 \left\{ \exp\left[\frac{V + IR_S}{nV_T}\right] - 1 \right\} - \frac{V + IR_S}{R_{SH}}.$
		Physical quantities	I – device electrical current I_L – photocurrent V– device voltage R_S – series resistance R_{SH} – shunt resistance I_0 – diode saturation current n – diode ideality factor
		Equation	PE2: two-diode equation $I = \left\{ \begin{array}{l} I_L - I_{01} \left[\exp\left(\frac{q(V_L + I\ R_s)}{n_1 kT} \right) - 1 \right] \\ - I_{02} \left[\exp\left(\frac{q(V_L + I\ R_s)}{n_2 kT} \right) - 1 \right] \\ - \left[\frac{(V_L + I\ R_s)}{R_{sh}} \right] \end{array} \right\}$
		Physical quantities	I – device electrical current I_L – photocurrent V– device voltage R_S – series resistance R_{SH} – shunt resistance I_0 – diode saturation current (of first and second diode) n – diode idelaity factor (of first and second diode)

2.3	MATERIALS RELATIONS	Relation	$I_0 = AkTn_i^2(\frac{\mu_p}{L_p N_D} + \frac{\mu_n}{L_n N_A})$
		Physical quantities/ descriptors for each MR	I_S – diode saturation current A – area k – Boltzmann constant n_i – intrinsic concentration of electrons μ – mobility coefficient of carriers (e-electrons, p-holes) L – diffusion length of carriers N_D – donor concentration N_A – acceptor concentration
2.4	SIMULATED INPUT	current density – voltage (J(V)) curve	

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3	SOLVER AND COMPUTATIONAL TRANSLATION OF THE SPECIFICATIONS		
3.1	NUMERICAL SOLVER	method for solving the system of non-linear equations (e.g. Newton)	
3.2	SOFTWARE TOOL	Matlab	
3.3	TIME STEP	not applicable, steady state simulation	
3.4	COMPUTATIONAL REPRESENTATION ,	PHYSICS EQUATION, MATERIAL RELATIONS, MATERIAL	depending on the selected method of solving the system of non-linear equations
3.5	COMPUTATIONAL BOUNDARY CONDITIONS	none	
3.6	ADDITIONAL SOLVER PARAMETERS	accuracy tolerance	

Post processing

4	POST PROCESSING	
4.1	THE PROCESSED OUTPUT	There is no post-processing related to this model. I_0 and n values as well as the values for parallel (shunt) and series resistances of realistic diodes are already the raw output data of Model 3.
4.2	METHODOLOGIES	
4.3	MARGIN OF ERROR	