Report on 3-D simulation of a-Si:H solar cells
(in the frame of European FP7 Silicon-Light project)

Optical simulator

To analyze the effects of 2-D textures, a 3-D simulator MEEP was employed. The MEEP is based on the finite-difference time-domain (FDTD) method of electromagnetic simulations. It enables us to simulate general dispersive, anisotropic and nonlinear materials in up to three dimensions. The wavelength dependent complex dielectric (permittivity) functions ($\varepsilon = \varepsilon_1 - j\varepsilon_2$) of dispersive materials can be modelled as a sum of Lorentz oscillators. Computation of reflectance and absorptance spectra is made by Fourier transformation of the response to a Gaussian pulse of light. Here fluxes are computed by integrating Fourier-transformed electric and magnetic fields on various surfaces which depend on the shape of the scattering object. To validate the simulator, selected structures with 1-D periodic gratings were simulated by MEEP and the results were compared to the ones obtained by FEMOS simulator. Simulation results agreed very well. Also comparison tests on realistic structures were done.

To obtain the output characteristics of the solar cells related to the improved optics, a simplified electrical analysis was employed for all optical simulators. The short-circuit current density (J_{SC}) and wavelength dependent external quantum efficiency (*QE)*, of the solar cells were determined directly from the absorrptance in the absorber layer by considering ideal extraction of electrons and holes from the intrinsic absorber layers (i-a-Si:H, i-μc-Si:H) and neglecting the contribution from the p- and n- doped layers. In this case the *QE* is represented by the absorptance curve of the corresponding absorber layer. This assumption holds very well for state-of-the-art thin-film silicon solar cells. The reference AM1.5 (IEC60904) solar spectrum was used for the determination of J_{SC} from *QE* (wavelength range of 350 nm – 800 nm for a-Si:H solar cells and 350 nm – 1100 nm for μc-Si:H based solar cells).

Simulations with 3-D optical simulator

The presented results so far were based on 2-D optical simulations, considering both, TE and TM polarizations . For 3-D simulations one has to point out first that they are much more time consuming than 2-D simulations, thus, less study cases can b analyze effectively. Some selection based on 2-D simulations is appreciable. The 3-D MEEP simulator that was used for 3-D simulations is based on FDTD method, which can suffer convergence problems if realistic (measured) optical properties of layers, especially the metal layers (i,e. Ag back contact in thin-film solar cells). Also absorption in the layers, for which the interfaces cannot be approximated with a few horizontal planes, are not possible to be calculated straightforwardly. For these reasons our strategy was to carry out a broad range of simulations with the 2-D simulator and then based on the obtained optimized values for surface textures make a selection of structures for 3-D simulations. However, it was found out that 3-D simulations gave similar trends regarding optimal lateral and vertical texturization parameters as 2-D.

First measured optical properties of layers that were described by wavelength-dependent real and imaginary part of complex refractive index were described by complex dielectric

functions (epsilon). Several Lorenz oscillators were used to fit the real and imaginary part of epsilon in different regions of the wavelength spectrum separately. Optimization of the structure mesh-grid, boundary conditions, convergence tests and, later on, simulations were carried out on HP server with two Intel Xeon E5520 2.26GHz four-core processors with 12GB of memory.

Selection of the results of the a-Si:H solar cell with 2-D rectangular texturization (see difference between 2-D and 1-D texturization in Fig. 1) are presented in Figs 1 and 2. Comparison to the results obtained with 2-D simulations (1-D rectangular texturization) is given for specific case. In this simulations fully perpendicular left and right side of the texturization shape were considered and ideal metal was used at the back. Otherwise the structure and layers of the solar cell structure is the same as in section 3.1. Basically, with these simulations we wanted to check/confirm

- whether the same optimal values regarding the parameters *P* and *h* are observed in 3-D simulations (for 2-D textures) that were obtained for 2-D simulations (1-D textures) and
- what are expected further improvements in J_{SC} if 2-D textures are used instead of 1-D.

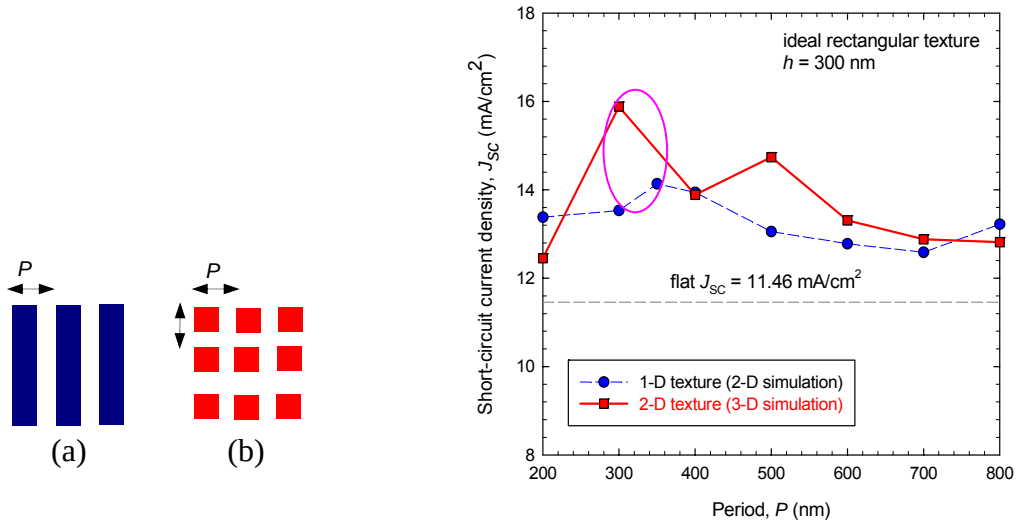
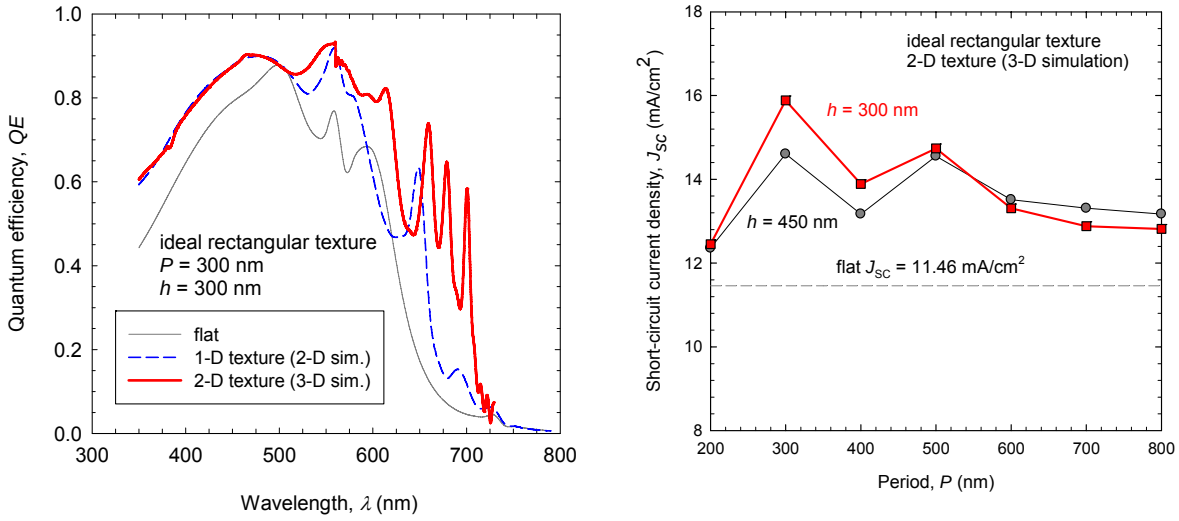


Figure 1. Top view of (a) 1-D texture and (b) possible realization of 2-D texture on the left and the plot with J_{SC} gains corresponding to a-Si:H solar cell with 2-D textures (3-D simulations) and 1-D textures with ideal rectangular shape.

The analyzed case of rectangular periodic surface-texture in a-Si:H solar cell demonstrate that approx. the same optimal values of lateral dimensions (*P*) are obtained for 2-D texture as for 1-D (Fig. 1). However, the gain in J_{SC} for the case of optimal P ≈ 300 nm is for 2-D texture much larger than the gain obtained with 1-D texture. The corresponding *QE* curves (*P* = 300 nm, *h* = 300 nm) are shown in Fig. 2 (a). One should note that the J_{SC} and *QE* results cannot be directly compared to the ones presented in section 3.1, since ideal metal was used at the back and since ideal rectangular shape was considered here.

Results in Fig. 2 (b) show that also concerning vertical dimensions of texturization features the same values of *h* (~ 300 nm) as in case of 1-D textures appear to be more optimal.



(a) (b)

Figure 2: (a) Simulated *QE* of a-Si:H solar cell with 1-D texture (2-D simulations) and 2-D texture (3-D simulations).
(b) Simulated J_{SC} for different values of *h* parameter – results of 3-D simulations.