Back-reflector optimization in thin-film silicon solar cells using 3D finite element simulations

Mark Blome[1], Kevin McPeak[2], Sven Burger[1], Frank Schmidt[1], and David Norris[2]

[1] Zuse Institute Berlin, Germany blome@zib.de, burger@zib.de, frank.schmidt@zib.de
[2] Optical Materials Engineering Laboratory, ETH Zürich, Switzerland kmcpeak@ethz.ch, dnorris@ethz.ch

Summary. We numerically optimize the light trapping efficiency of a periodic, pyramid structured back metal contact in thin-film amorphous silicon solar cells. Light propagation simulations are carried out by rigorously solving Maxwells equations in 3D space for a wide range of model geometry parameters. In using our optimization approach we have identified nanostructure back reflector geometries that display a significant increase in short circuit current density over flat back reflectors.

1 Introduction

Thin-film amorphous silicon based solar cells are an attractive design for providing cost-effective and efficient solar energy. Amorphous hydrogenated silicon (a-Si:H) can be deposited in thin layers on cheap substrate materials such as glass or plastic offering low fabrication costs suitable for mass production.

One of the major barriers to the widespread use of a-Si:H solar cells is their increased defect density under light exposure the Staebler-Wronski (SW) effect. To mitigate (SW) effects, low thickness absorber layers (in the range of a few hundred nanometers) that exhibit a high electric field are typically employed. Considering the large absorption length of amorphous silicon near its bandgap, these thicknesses necessitate light-trapping concepts for realizing efficient thin-film silicon solar cells [1].

2 Methodologies

Within this work we optimize geometry parameters of a periodic, pyramid structured back metal contact in a model (p-i-n type) thin-film solar cell. Our goal is to find optimal model parameters that considerably increase the solar cells light trapping efficiency compared to flat designs.

2.1 Finite element light propagation modeling

To judge the efficiency of different solar cell models we compute short circuit current densities

$$I_{sc} = \frac{q}{hc} \int_{\lambda_{\min}}^{\lambda_{\max}} \lambda \, QE(\lambda) \, S(\lambda) \, d\lambda \qquad (1)$$

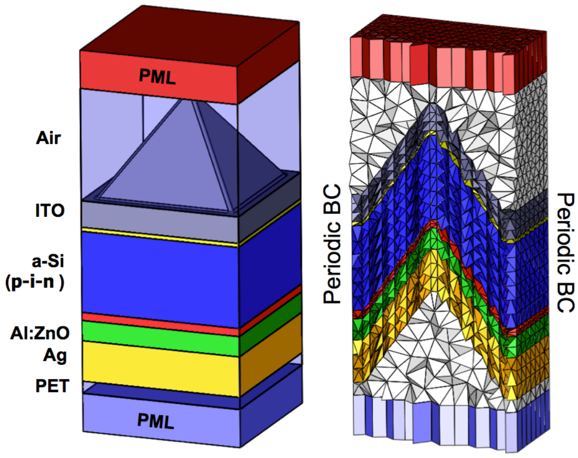

Fig. 1. Sample CAD representation of the model (p-i-n type) solar cell used (left) and vertical cut through a corresponding volume mesh (right). The computational domain is periodic in x,y directions; transparent boundary conditions are realized by adaptive perfectly matched layers (PML).

for the solar cell models under consideration. In (1) λ denotes the wavelength, q the elementary charge, h is Planck's constant, c is the speed of light and $S(\lambda)$ is the weighted sun spectrum (air mass 1.5 solar spectral irradiance). For each solar cell model short circuit current densities are computed over a wavelength range of 350 to 900 nanometers.

Estimating I_{sc} requires knowledge about the solar cells quantum efficiency $QE(\lambda)$ defined as the ratio of the number of generated charge carriers to the number of total incident photons:

$$QE(\lambda) = \frac{1}{P_o} \int 1/2cn \frac{4\pi k}{\lambda} |E(\lambda, \mathbf{r})^2| \, d\mathbf{r}. \qquad (2)$$

Here P_o is the optical input power, n and k are the real and imaginary parts of the complex refractive index and integration is carried out in the intrinsic a-Si solar cell layer.

$E(\lambda)$ in (2) is the electric field in the solar cells absorber layer, which, considering the involved length scales, needs to be computed by rigorously solving Maxwell's equations. For this purpose we employ a frequency domain finite element method. To assure a high solution accuracy we use higher order shape functions and adaptive perfectly matched layers for realizing transparent boundary conditions [4].

2.2 Model discretization using CAD techniques

To avoid discretization errors that would pollute the finite element solutions, investigated solar cell geometries need to be modeled and discretized with high accuracies. Furthermore, to be able to apply optimization algorithms for finding optimal back reflector geometries, it is essential that solar cell geometry models can be fully parameterized. For this purpose we have developed computer-aided design (CAD) techniques specifically tailored for the construction of parameterized nano-photonic device models.

A sample CAD representation of our model (p-i-n type) solar cell is displayed in Fig. 1. It consists of a nano-structured silver back contact deposited on a plastic substrate, followed by 50 nm of Al:ZnO, 200 nm of a-Si:H and a final layer of tin doped indium oxide. Edge rounding (fillet) is applied on sharp edges of the model geometry to avoid spurious reflections. The CAD model is parameterized by the period of the structure (in x,y directions) and the base width of the pyramids. In addition to these parameters other geometry parameters are currently being investigated.

A hybrid meshing scheme is used to discretize the model geometries with high quality structured/ unstructured tetrahedral cells. The periodicity of the computational domain is automatically enforced during volume meshing and prismatic cells are added for realizing transparent boundary conditions with perfectly matched layers (Fig. 1).

So far material interface layers within the solar cell stacks are modeled by extrusion of the pyramid structured PET-Ag interface layer in positive Z-direction (as displayed in Fig. 1). To achieve a more accurate representation of the topography of the individual material layers, a level-set based topography simulation method is currently being developed. The method relies on the ballistic transport and reaction model developed by [2] and employs the level-set method to evolve interface layers [3].

3 Results

Our simulation results reveal that the employed pyramid structured back-reflectors effectively increase the light path in the absorber by (i) exciting photonic waveguide modes in the absorber and (ii) coupling incident photons to surface plasmon polaritons (SPPs). Using our optimization approach, we have identified nanostructure back reflector geometries that display a significant increase in short circuit current densities compared to a flat solar cell design with identical material layer thicknesses.

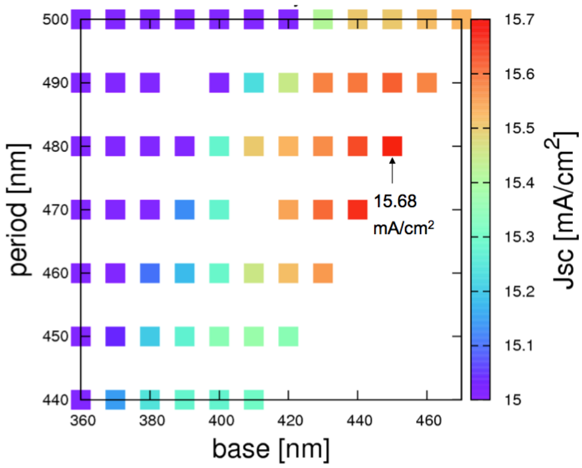

Fig. 2. Short circuit current densities I_{sc} computed for a series of solar cell models with varying cell periodicities and pyramid base widths. Displayed I_{sc} values are considerably larger than the value obtained for a flat back-reflector ($I_{sc} = 10.2\ mA/cm^2$).

Fig. 2 shows a map of computed short circuit current densities I_{sc} for a series of solar cell models with varying cell periodicities and pyramid base widths. A maximum value of $I_{sc} = 15.68\ mA/cm^2$ was identified for a solar cell model with a periodicity of 480 nm and a pyramid base width of 450 nm, which is considerably larger than the value obtained for a flat back-reflector ($I_{sc} = 10.2\ mA/cm^2$). Additional model parameters are currently being investigated. Furthermore, other type of back-reflector geometries are going to be analyzed in the framework of this ongoing research project.

Acknowledgement. The research presented here is the result of a multi-disciplinary, collaborative project headed by K. McPeak (OMEL, ETH Zürich). In addition to the authors of this abstract, the project relies on the work and contributions of: T. S. Cale (Process Evolution Ltd.), N. Wyrsch (EPFL, Lausanne) and M. Hojeij, Y. Ekinci (Paul Scherrer Institut).

References

1. H. A. Atwater and A. Polman. Plasmonics for improved photovoltaic devices. *Nature Materials*, 9:205–213, 2010.
2. T. S. Cale and V. Mahadev. *Thin Films: Modeling of Film Deposition for Microelectronic Applications*, volume 22, pages 176–277. Academic Press, 1996.
3. J. A. Sethian. *Level Set Methods and Fast Marching Methods*. Cambridge University Press, 2 edition, 1999.
4. L. Zschiedrich, R. Klose, A. Schädle, and F. Schmidt. A new finite element realization of the perfectly matched layer method for helmholtz scattering problems on polygonal domains in 2d. *J. Comput. Appl. Math.*, 188:12–32, 2006.