Photon Management with Deterministic and Random Nanostructures for Photovoltaic Applications

Matthias Kroll and Thomas Pertsch
Institute of Applied Physics, Friedrich Schiller University Jena, Germany

Introduction

Photovoltaic power conversion is an important, steadily growing market within the field of green sustainable energy generation. Within this market 2nd generation thin film solar technologies are emerging since the last decade and starting to claim shares from crystalline wafer based technologies [1].
Most thin film solar cells have in common that the maximum achievable thickness of the active layers is limited for some technological reason. Therefore photon management is crucial to achieve a sufficiently high absorption of the incident light. Furthermore in case of inorganic thin film devices there are large refractive index contrasts that will lead to strong Fresnel reflections if not dealt with carefully.
Nanostructures with characteristic feature sizes comparable to or smaller than the wavelength of light can provide useful optical effects for light trapping and antireflection measures [2]. In Figure 1 some of these effects are illustrated. Thin film solar cells can be considered as a slab waveguide. Therefore a suitably designed periodic structure will provide wavevector matching to couple light into guided slab modes that are strongly confined. Even if no resonant coupling occurs, there will be a path length enhancement due to diffraction (periodic structures) or scattering (random structures). Sub wavelength structures with a continuous profile will provide a refractive index gradient that acts as an anti-reflection coating. Finally at metallic particles as well as at high index dielectric structures embedded in a low index host, localized resonances may occur and increase absorption due to an enhanced electric field.

Rigorous Numerical Modelling

A major difficulty in designing nanostructures for photon management is the complexity of optical modelling. Due to feature scales at the level of the wavelength of light, approximate theories like geometrical optics or scalar diffraction theory fail to provide a correct description of the interaction of light with such structures. Therefore Maxwell's equations have to be solved rigorously with wave optical methods to obtain correct results. Two

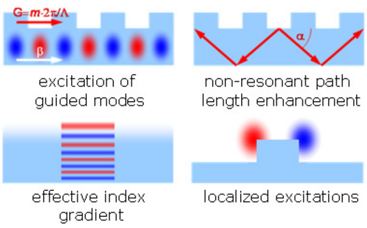

Figure 1. Optical effects at nanostructures that can be exploited for photon management.

methods which are especially useful for this purpose are the finite differences time domain (FDTD) method [3] and the Fourier modal method (FMM) [4]. With the FDTD method, the electric and magnetic fields are advanced in time on a discrete grid using a leap frog scheme. The method can handle arbitrary geometries and scales even for large problems. With the FMM the geometry is decomposed into layers with transversely periodic index profiles. Maxwell's equations are then solved in Fourier space by finding the Eigen modes in the individual layers and matching the boundary conditions. The FMM is especially useful if the considered geometry can be described by a low number of layers and exhibits a small periodic unit cell.
Besides reflectance and transmittance spectra both methods provide access to the electric and magnetic fields which are necessary to calculate the local power dissipation

$$\frac{dP}{dV} = \operatorname{div}\mathbf{S} = -\frac{\varepsilon_0\omega}{2}\Im(\varepsilon)|\mathbf{E}|^2$$

within the different materials of the solar cell. On this basis generation rates and theoretical short circuit currents are obtained by weighting with the AM1.5G spectrum [5].
In the following we present the application of both methods to investigate different nanostructures which have been fabricated and characterized experimentally.

Reactive Ion Etched Silicon Surfaces

Random rough nanostructured surfaces were prepared by reactive ion etching (RIE) of crystalline silicon with a mixture of SF_6 and O_2 [6]. These so called Black Silicon surfaces exhibit overlapping etch pits with a spacing of about 200 nm that leave sharp needle like silicon features with steep sidewalls and high aspect ratios. A typical example of a Black Silicon surface is depicted in Figure 2a. As can be seen from the optical spectra (Fig. 2c-d) Black Silicon exhibits a remarkably low reflectance in the absorbing spectral region of Si. The reflectance in the transparency region reveals strong scattering. A comparison to the theoretical reflectance of a wafer with perfect AR coating suggests the occurrence of total internal reflection at the polished rear side of the wafer. From the absorbance spectrum significant absorption enhancement at the Si absorption edge can be seen.
To gain insight into the light propagation within the Black Silicon layer, we obtained a three dimensional reconstruction of the surface topography by stepwise slicing with a focused ion beam and taking consecutive SEM micrographs of the surface cross section. The reconstruction process is illustrated in Figure 2b. The light propagation within the reconstructed surface was then simulated using the FDTD method.

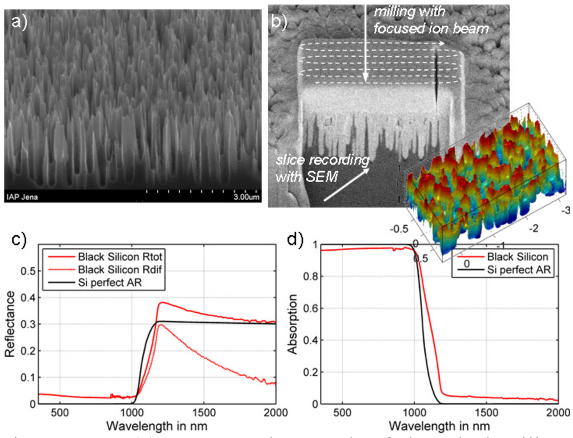

Figure 2. In (a) a SEM micrograph of the Black Silicon surface under investigation is shown, the surface reconstruction procedure and the recovered topography are depicted in (b). In (c) and (d) optical spectra measured with an integrating sphere are presented.

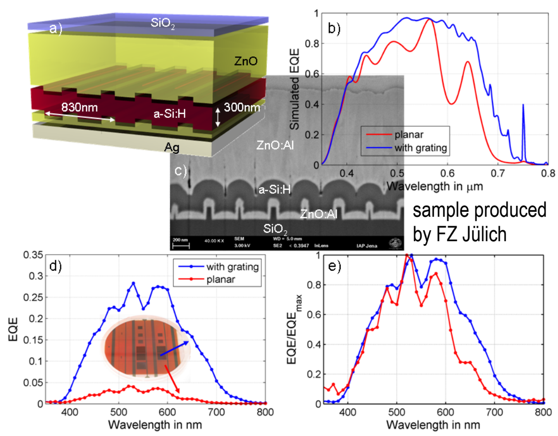

Figure 4. In (a) and (b) the considered thin film solar cell and the results from numerical optimization are presented. (c) shows the manufactured grating integrated into an a-Si:H solar cell. In (d) and (e) measured quantum efficiencies are presented.

From the field distribution below the structured surface we calculated the angular scattering distribution by the Fourier transforms of the electric and magnetic fields. An integrated angle distribution function (IADF) was defined that measures the fraction of transmitted energy which is scattered into a cone with a given opening angle. The obtained IADF is shown in Figure 3(left). As can be seen there, the Black Silicon indeed exhibits strong forward scattering into large propagation angles. Even at large wavelengths, more than 60% of the transmitted energy is scattered above the angle of total internal reflection, thus leading to a significant path length enhancement.

From the electric field within the Black Silicon structure the depth dependence of the optical carrier generation rate was calculated. As shown in Figure 3(right) there is a notable absorption enhancement resulting from resonances at individual silicon needles. However due to the small volume fraction of silicon within the structured layer the overall absorption is only slightly larger than that of an equally thick bulk silicon layer. We conclude that most of the light trapping can be attributed to the path length enhancement due to scattering and total internal reflection.

Gratings for Silicon Thin Film Solar Cells

One of the simplest nanostructures that can be integrated into a thin film solar cell is a periodic grating. However due to the broad spectral range of solar cell operation it is difficult to separate individual optical effects. Therefore we rigorously calculated the absorption of light within the active layer of a thin film a-Si:H solar cell incorporating a rear grating (Fig. 4a). For this the FMM was used. A genetic optimization algorithm was applied to determine the optimum grating parameters. The optimized solar cell exhibits a current enhancement of 37% when compared to a planar cell with the same active layer thickness. The simulated EQE is shown in Figure 4b. The optimum geometry was found to be an asymmetric grating with a depth of 70 nm that has two ridges of different width within a period of 830 nm.

To verify the feasibility of such a grating a test solar cell was deposited at Forschungszentrum Jülich onto a pre structured fused silica wafer covered with a thin conductive ZnO layer. A cross sectional view of the fabricated sample is shown in Figure 4c. It can be seen that the rear grating is replicated by the amorphous silicon layer. Though a smoothing of the steep grating features occurs that was not consider in the optical model.

Due to shunts and poor conductivity of the thin ZnO layer on top of the insulting grating, the first fabricated test cell exhibited poor quantum efficiency (Fig. 4d). However a comparison of the normalized EQEs (Fig. 4e) suggests a light trapping effect due to the grating. Also an anti-reflection effect indicated by the reduced modulation depth of the Fabry Perot oscillations can be seen.

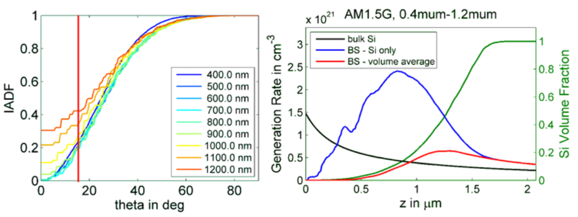

Figure 3. On the left the integrated angle distribution of the forward scattered energy is shown. The vertical red line indicates the angle of total internal reflection at the Si-air interface. On the right the simulated carrier generation rate within the structured surface is plotted.

Silicon Nanowires for Organic Photovoltaics

Silicon nanowires with diameters in the range of 25 nm to 150 nm exhibit scattering resonances in the visible and near infrared wavelength range that can be used for light trapping in thin film devices. Such nanowires were prepared using vapour-liquid-solid CVD method [7]. A sample grown at the Institute of Photonic Technologies Jena (IPHT) is shown at the top of Figure 5. The measured reflectance of the fabricated sample was compared to the calculated backscattered energy normalized to the totally scattered energy for random arrangements of parallel nanowires with different mean distances <d>. For the calculations semi analytical Mie theory was used

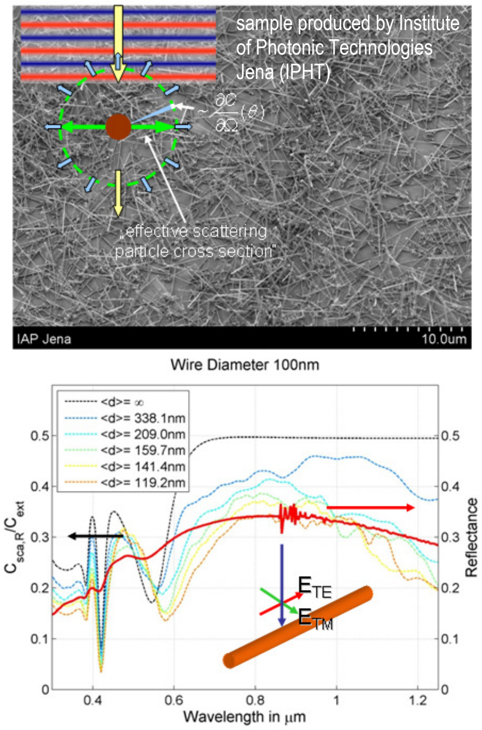

Figure 5. In the top a SEM micrograph of random nanowires prepared on a glass substrate is shown. In the bottom a comparison of the measured reflectance with numerical results for random parallel nanowires is given. The inset on the top illustrates the quantities that can be obtained from scattering calculations.

[8]. Measurements and calculations were found to be in good agreement. All spectral features could be reproduced without adjustment of any parameters (see bottom of Fig. 5).

The light trapping performance of silicon nanowires embedded into a bulk heterojunction solar cell was evaluated using the FMM. The considered geometry is depicted in Figure 6b. As can be seen from Figure 6a, silicon nanowires can lead to an enhancement of the photo current for a certain range of wire diameters and densities. To understand the influence of the wire diameter, we calculated the angular far field scattering distribution of the silicon nanowires embedded in pure polymer blend for the points marked in Figure 6a. Overlaid in green is the imaginary part of the dielectric function of the polymer blend. From the scattering distributions we conclude the following: For thin wires only the first, isotropic scattering resonance occurs. However the strength and bandwidth is small, therefore the interaction with the polymer blend is weak. For the optimum wire diameter there is a good overlap between higher order resonances and the visible absorption band of the blend. For thick wires, the resonance strength and overlap gets smaller again. Furthermore due to the increased silicon volume fraction, parasitic absorption gets significant.

Summary

We presented rigorous numerical investigations on different kinds of nanostructures for photon management. We demonstrated how those simulations can be used to gain a deeper understanding of the light interaction with

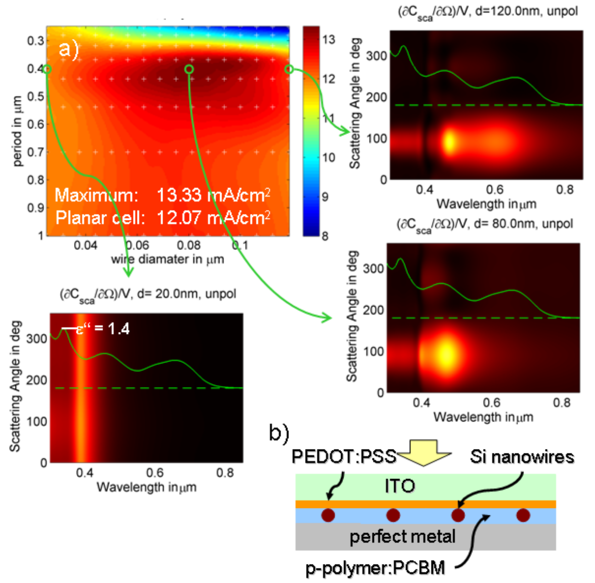

Figure 6. In (a) the simulated photo current of Si nanowires embedded in 125nm polymer blend is shown. The geometry under investigation is given in (b).

such structures. The calculations give access to quantities that cannot be observed with experimental techniques like the distribution of propagation angles within the absorbing material. Furthermore the local absorption within the different materials of a solar cell can be calculated as an important figure of merit for optimization of light trapping geometries.

We thank Dr. Vladimir Sivakov at the IPHT Jena for the preparation of nanowire samples as well as Dr. Reinhard Carius and Dr. Jürgen Hüpkes at Forschungszentrum Jülich for solar cell deposition. The authors gratefully acknowledge financial support by the German Ministry of Education and Research (PHIOBE, HypoSolar) and the German Research Foundation (PAK88).

References

[1] Green, M. (2006) *Prog. Photovoltaics Res. Appl.* **14**, 383–392.

[2] Kroll, M., Fahr, S., Helgert, C., Rockstuhl, C., Lederer, F., and Pertsch, T. (2008) *Phys. Status Solidi A* **205**, 2777–2795.

[3] Oskooi, A. F., Roundy, D., Ibanescu, M., Bermel, P., Joannopoulos, J. D., and Johnson, S. G. (2010) *Comput. Phys. Comm.* **181**, 687–702.

[4] Whittaker, D. M. and Culshaw, I. S. (1999) *Phys. Rev. B* **60**, 2610–2618.

[5] Ann. Book of ASTM Standards chapter G173-03e1 – Standard Tables for Reference Solar Spectral Irradiances: Direct Normal and Hemispherical on 37° Tilted Surface ASTM (2003).

[6] Jansen, H., deBoer, M., Legtenberg, R., and Elwenspoek, M. (1995) *J. Micromech. Microeng.* **5**, 115–120.

[7] Wagner, R. S. and Ellis, W. C. (1964) *Appl. Phys. Lett.* **4**, 89–90.

[8] Felbacq, D., Tayeb, G., and Maystre, D. (1994) *J. Opt. Soc. Am. A* **11**, 2526–2538.