Trapping Light in Organic Plastic Solar Cells with integrated Diffraction Gratings

Michael Niggemann[a], Benedikt Bläsi[a], Andreas Gombert[a], Andreas Hinsch[a], Harald Hoppe[c] Philippe Lalanne[b], Dieter Meissner[c] and Volker Wittwer[a]

[a]Fraunhofer Institute for Solar Energy Systems (ISE), Heidenhofstr.2 , 79110 Freiburg, Germany
[b] Laboratoire Charles Fabry de L'Institut d'Optique, Centre National de la Recherche Scientifique, BP 147, 91403 Orsay Cedex, France
[c]Linz Institute for Organic Solar Cells, Johannes Kepler University, Altenbergerstr. 69, A-4040 Linz, Austria

ABSTRACT: In this paper we investigate the potential of light trapping with diffraction gratings for organic solar cells. The architecture of the solar cell is based on conjugated polymers and a buckminsterfullerene derivative (PCBM), forming an interpenetrating donor-acceptor-network. The motivation for light trapping is the small absorptance of the photoactive polymer in the range of the solar spectrum and the limited thickness of the absorbing film. Integrated diffraction gratings offer the chance to increase the absorptance in a distinct range of the spectrum. The influence of the grating geometry on the absorption of the photoactive layer is simulated by calculations based on rigorous coupled wave analysis (RCWA), a method for describing the interaction between electromagnetic waves and diffractive structures. First experiments on the patterning of the diffraction grating are presented.

Keywords: Light Trapping - 1: Organic Solar Cell - 2: Diffraction Grating - 3

1 INTRODUCTION

Organic plastic solar cells have the potential of cost effectiveness. The mechanical flexibility and the low specific weight of the plastic materials opens a wide field of applications. One promising concept of an organic solar cell is based on a donor-type conjugated polymer (MDMO-PPV) and acceptor molecules (PCBM, a C_{60}-derivative) forming an interpenetrating donor/acceptor network. A power conversion efficiency of 3.0% under AM 1.5 illumination has been reported for these cells [1]. The efficiency is limited in this case by the small absorptance of the two components in the range of the solar spectrum combined with the necessity of a small film thickness of the absorbing layer (see figure 1). The maximum thickness of the absorbing layer (<200nm) is determined by the restricted mobility of the charge carriers. Thus a significant part of the light can not be absorbed.

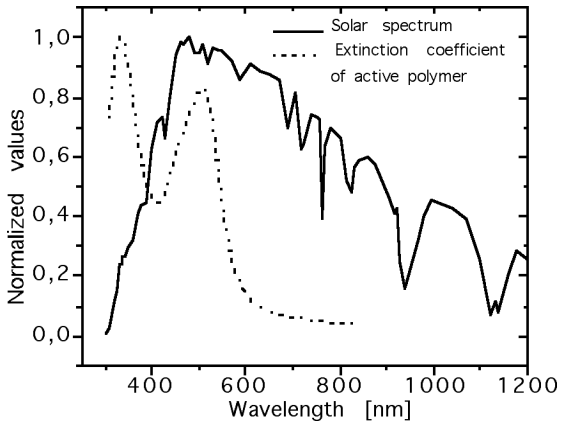

Figure 1: Normalized solar spectrum (AM1.5g) and normalized extinction coefficient of the active polymer (MDMO-PPV:PCBM)

Light trapping is one strategy to increase the gain of absorbed light. However it is no substitute for the development of new polymers whose absorption match the solar spectrum better. The integration of diffractive optical structures has been investigated for silicon solar cells [2]. This approach has been applied at polymer photodiodes and leads to promising results [3]. Depending on the geometric parameters of the diffraction grating, the absorption in the active polymer film can be significantly increased for a certain interval of the spectrum.
Simulations are essential for the optimisation of the diffractive structures. Calculations based on rigorous coupled wave analysis (RCWA) give information about the absorption of light inside of diffractive structures. In contrast to silicon solar cells the light trapping with diffraction gratings can be made in a simple embossing process which retains the advantage of cost effectiveness. If patterning is successful the availability of large patterned areas is a key issue in the long term. Holographic generation of microstructured surfaces on large areas is state of the art at the Fraunhofer ISE [4]. In a roll to roll-process, the patterning could be performed by roller embossing.

2 DETERMINING OPTICAL CONSTANTS

Thin films of the active layer have been spin cast onto polished silicon or quartz wafers. Films cast on silicon were measured by spectroscopic ellipsometry (Uvisel ellipsometer, **Jobin Yvon S.A.,** 16-18 rue du Canal, 91165 Longjumeau Cedex, France). Films cast on quartz were measured with an UV-Vis spectrophotometer (Cary 3G, **Varian Australia Pty Ltd**, Mulgrave, Victoria, Australia). A dielectric function was then fitted to the ellipsometric as well as to the reflectance and transmittance data with the commercial software SCOUT (**M. Theiss - Hard- and Software,** Aachen, Germany).

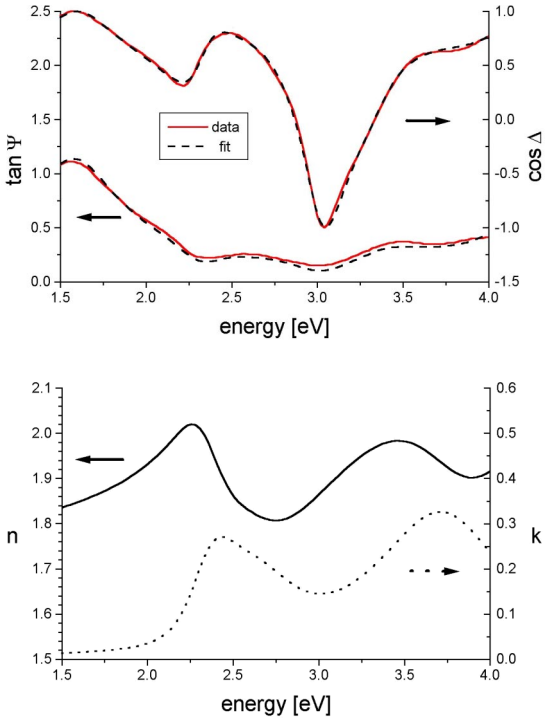

Figure 2: Measured and fitted reflection and transmission data obtained by ellipsometry (top) and the such determined optical constants of the photoactive composite film.

3 SIMULATIONS

3.1 Structure of the organic solar cell

The photophysics of the investigated device is presented in [1]. The structure of the organic plastic solar cell is as follows. An ITO coated glass substrate represents one electrode which is coated with a conducting polymer-PEDOT. The active layer is a conjugated polymer blend (MDMO-PPV:PCBM). The second Al-electrode is evaporated on top and represents the backside of the cell. The average thickness of the PEDOT- and MDMO-PPV-films are 100nm and 120nm respectively. The pursued approach is to pattern this active polymer layer. Figure 3 shows the structure of the cell.

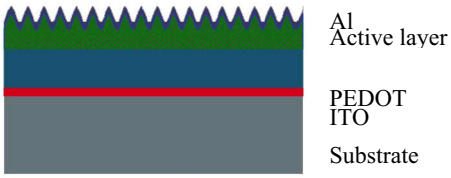

Figure 3: Cross-section of the patterned organic plastic solar cell

3.2 Simulation method

As the photoactive polymer is patterned with the diffractive structure, it is optical and charge generating element at the same time. Thus information about the absorption of light in the distinct layers of the device is important for a design of the diffraction grating.

Besides the dielectric function of the materials as determined experimentally (see above), the characteristics of the electromagnetic wave (wavelength λ, polarization, incident angle), the thickness of the different layers, the shape, depth and period Λ of the grating are decisive parameters for the absorption of light in the device.

The rigorous coupled wave analysis (RCWA) is one method for describing the diffraction of electromagnetic waves by periodic structures [5]. Based on this approach, the computation of the electromagnetic field distribution in the grating region and its vicinity is possible [6,7].

Taking the diffraction efficiencies in the far field and the near field-intensity pattern EE* into account one can calculate the absorption in a distinct area by considering the following relation between absorption density a(x,z) and the field intensity EE*.

$$a(x,z) = \frac{\sigma}{2}\left|EE^*\right|^2(x,z)$$

Where x,z are the coordinates in the 2-dimensional cross section of the device, σ conductivity of the material and E(x,z) amplitude of the electric field. The plane of incidence is stretched by the normal of the grating plane and the grating vector. The calculations are made for classical mounting, where the wave vector is parallel to the plane of incidence. For this situation, two polarizations of the electromagnetic wave can be distinguished. In the case of transversal electric (TE)-polarization, the electric-field vector is perpendicular to the plane of incidence. The case of the transversal magnetic polarisation (TM), with the electric field vector parallel to the plane of incidence, is not considered yet.

3.3 Results

The calculations are valid for coherent light. This condition is fulfilled for the thin layers, but not in the glass-substrate plate. Therefore we assume the incident wave coming from a space with the dielectric function of glass.

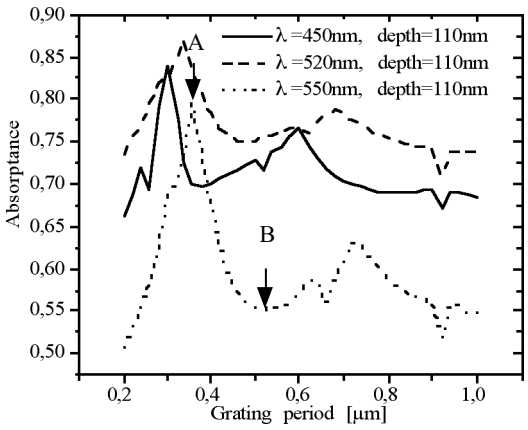

Figure 4: Absorptance inside the active layer versus the period of the diffraction grating with a constant depth of the grating. (Normal incidence)

Figure 4 shows the calculation of the absorption inside the active layer depending on the period with a constant depth of the diffraction grating. Two distinct absorption peaks can be observed at each wavelength. The second absorption peak occurs at the twofold grating period of the first peak. This indicates that the coupling of the 1st and 2nd diffraction order occur at the 1st and 2nd peak respectively. The local minima of the absorption are caused by local absorption maxima in the PEDOT and ITO layers.

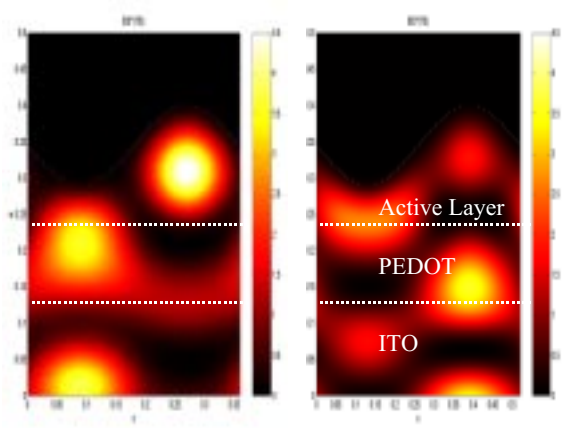

Figure 5: Near-field intensity EE* in the cross section for the cell with Λ=360nm (Situation **A** of Figure 4)

Figure 6:Near-field intensity EE* in the cross section for the cell with Λ=520nm (Situation **B** of Figure 4)

Examples of near-field intensities EE* in the cross section of the cell are shown in figures 5 and 6. These correspond to the situations A and B marked in figure 4. The higher field intensities in the grating area and thus the higher absorption in the case A is obvious.

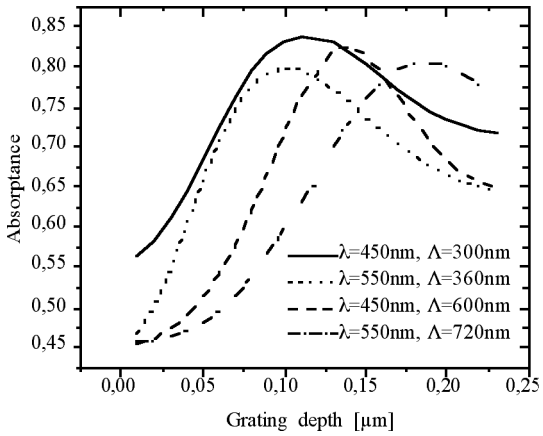

Figure 7: Absorptance versus the grating depth for the 1st and 2nd order coupling at the wavelengths 450nm and 550nm.

The influence of the grating depth on the absorption is depicted in figure 7. The grating period and wavelength correspond to the maximum values of figure 6 for the wavelengths 450nm and 550nm. The influence of the grating depth on the absorption is uncritical in terms of slight variations. For the 1st order coupling, a depth of 110nm is a good compromise. For the 2nd order coupling the optimum depth is in a range between 140nm and 200nm. The effect of the grating depth on the absorptance depending on the period can be observed in Figure 8. The chosen depths correspond to the optimum depths for 1st and 2nd order coupling at λ=550nm (see figure 6).

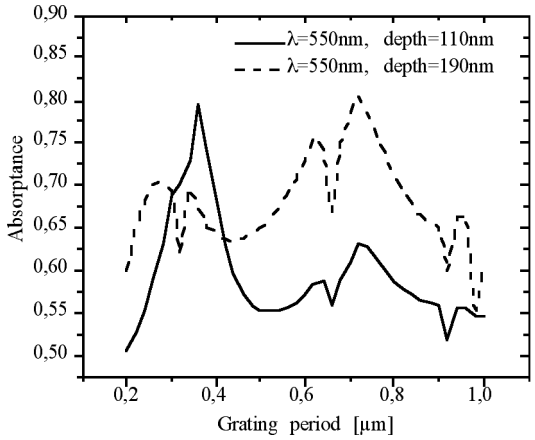

Figure 8: Absorptance inside the active layer versus the period of the diffraction grating for two different depths of the grating. (Normal incidence)

The dependence of the absorption on the incident angle is an important issue as the normal incidence of the light is only a special case, which can not be assumed in later applications. Figure 8 shows the angle dependent absorption for the parameters of case A in figure 4.

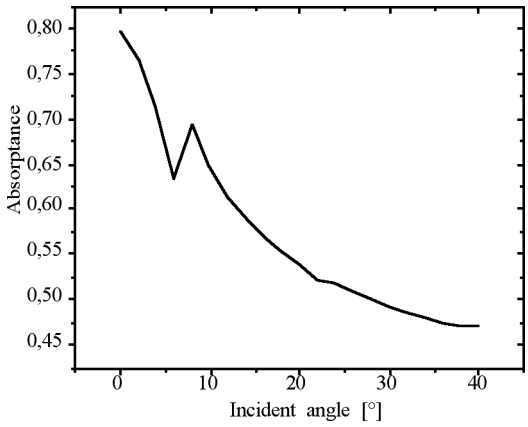

Figure 9: Absorptance versus the incident angle (λ=550nm, Λ=360nm, Grating depth = 110nm)

4 INITIAL EXPERIMENTS

Initial experiments were carried out to investigate the pattern generation in the photoactive layer. The masterstructure of the surface relief grating was made by holographic exposure of a photoresist coated glass substrate [8]. The thickness of the photoresist layer determines the depth of the grating. A grating period of 300nm was chosen.

From this photoresist structure, a copy in silicon rubber was made [3,9]. The patterning of the spin coated active layer was performed by embossing with the silicon rubber stamper. Figure 10 shows an AFM image of the embossed grating and a height profile plot. The obtained mean depth is 16nm. An electrical characterization of the structured cells did not seem to be promising at this point because the experiments were carried out under ambient conditions at temperatures of 60-80°C. A fast degradation of the active polymer can be assumed under those circumstances.

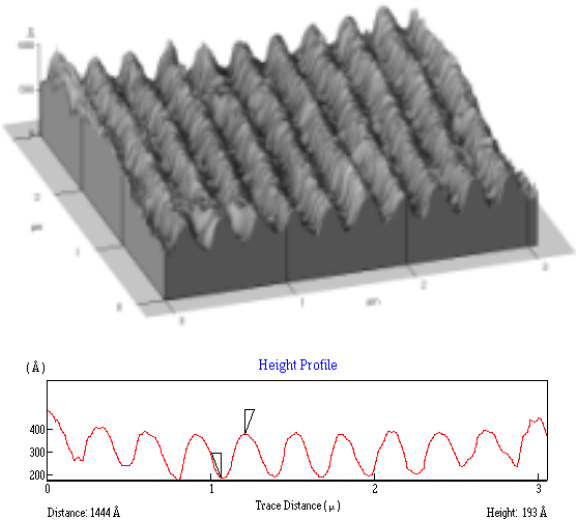

Figure 10: AFM-image and height profile of an embossed diffraction grating in the active polymer layer

2. CONCLUSIONS AND OUTLOOK

The simulation calculations show a significant effect of the diffraction grating on the absorption in a distinct range of the spectrum depending on the chosen grating parameters. 1st and 2nd order coupling are observed. General statement in terms of optimum grating parameters can not be made until TM polarisation is considered. An optimum grating design will be a compromise between the optimum values for TE and TM polarisation. The choice for 1st or 2nd order coupling depends not only on the absorption but also on the changing geometry of the active layer. The deep structures for 2nd order coupling lead to larger maximum diffusion length of the charge carriers and may cause problems in the manufacture process.
The described simulations present only a few cases. More aspects have to be considered. The conical mounting is the most general case of the incident angle. The boundary between air and the glass-plate and reflections inside the glass-plate have to be taken into account by applying the fresnel equations. Other shapes of the grating like rectangular or blazed gratings are worth investigating.
The initial experiments show that embossing of the grating in the active layer is possible. However the depths in the range of 100nm demanded by the first simulations is not achieved yet. Furthermore the effects of the mechanical stress and the applied temperature on the performance of the active polymer it have to be investigated.

ACKNOWLEDGEMENTS

We like to thank J.C.Hummelen from University of Groningen for the delivery of the chemical components and Michael Klicker for the comparative measurements.

REFERENCES

[1] C.J.Brabec, N.S.Sariciftci, and J.C.Hummelen, „Plastic Solar Cells“,Adv. Funct. Mater. 2001, 11, No. 1, February, pp.15-25; S. E. Shaheen, C. J. Brabec, N. S. Sariciftci, F. Padinger, T. Fromherz, J. C. Hummelen, „2.5 % Efficient Organic Solar Cells”, Appl. Phys. Lett. 78: 841-843 (2001)

[2] Heine, C.; Morf, R.H., „Submicrometer gratings for solar energy applications“, Applied Optics, Vol.34, No.14, 10 May 1995, pp.2476-2482.

[3] Roman, L.S.; Inganäs, O.; Granlund, T., Nyberg, T., Svensson, M.; Andersson, M.R., Hummelen, J.C., „Trapping Light in Polymer Photodiodes with Soft Embossed Gratings“, Adv. Mater.200, 12, No.3, pp.189-195.

[4] A.Gombert, „Future Steps Towards Large-Area Microstructured Surfaces“, in: M. Weck (Ed.), „Precision Engineering and Micro Technology“, 195-203, Aachen (2000).

[5]M.G Moharam and T.K. Gaylord, “Diffraction analysis of dielectric surface-relief gratings”, J.Opt.Soc.Am.,Vol.72, 1385-1392 (1982).

[6]Ph. Lalanne, G.M. Morris, “Highly improved convergence of coupled-wave method for TM polarisation”, J.Opt.Soc.Am. A 13,779-784 (1996).

[7]Ph. Lalanne, M.P. Jurek, “Computation of near field pattern with coupled-wave method for TM polarization”, J. Mod. Opt. 45, 1357-1374 (1998).

[8] www.funktionale-oberflaechen.de

[9] Y. Xia , J. J. McClelland, R. Gupta, D. Qin, X. M. Zhao, L. L. Sohn, R. J. Celotta, and G. M. Whitesides, „Replica Molding Using Polymeric Materials A Practical Step Toward Nanomanufacturing“, Adv. Mater. 1997, 9, No.2, pp.147-149.