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A sensitivity analyses of a p-i-n perovskite solar cell with a fixed band gap

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Abstract

Solar cell developers should have the theoretical knowledge how to best manipulate the solar cell properties in order to improve in a most effective way the solar cell efficiency. Such knowledge can be obtained by the simulation of the solar cells efficiency. Here a validated analytical model is used in order to simulate the model efficiency of the hybrid p-i-n solar cell in a multidimensional property space. The analytical model is based on a self-consistent stationary quantum simulation of the charge carrier generation and is established on the drift diffusion and the Poisson equations. The model simplifies the numerical simulation of the carrier generation as a function of the penetration deepness of the solar radiation, where the total charge generation is obtained by integration of local generated charges over the whole absorber layer thickness. Recombination currents at the p and n transport layers are considered as a function of (i) the diffusion coefficients of the free charges, (ii) the excess and the moderation of charges at the front and the back of solar cell, (iii) the effective surface recombination velocities of these charges and the (v) the solar cells built-in voltage. By use of a sensitivity analysis, it is shown how the properties of an ideal perovskite cell should be manipulated in order to improve its efficiency.

Keywords: *Perovskite Solar Cell (PSC), Analytical PSC Model, Sensitivity Analysis.*

1. Introduction

Whereas photovoltaic power plants based on the widely used silicon solar cells are already economically viable without subsidies in several countries [1] in residential applications and on the industrial scale, climate change problems demand the usage of renewable energy sources in very large scale [2], which stresses large investments. In order to reduce this investment cost photovoltaic modules should be available at lower costs in the future. Such an demand may be accomplished with the hybrid perovskite solar cells, as it combines potentially a low manufacturing cost with very high efficiency values in a multiple junction cell structure [10]. As discussed in [10] a triple junction solar cell combined with a crystalline silicon cell would lead to a cell efficiency of up to 50 %, which will result to the efficiency of photovoltaic modules of approximately 40 %. The first commercially available hybrid photovoltaic modules are based on Dye Sensitized Solar Cells (DSSC) [3], and they are commercially available by the company Solaronix[1]. In 2010, the photovoltaic effect of the hybrid Perovskite material was unveiled [4], which lead at the state of the art to much higher solar cell efficiencies than the one obtained by dye sensitized solar cells. Remarkable in the research with the

[1] http://www.solaronix.com/solarcells/

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Perovskite solar cell is the unprecedented and strong tendency to high efficiency values within the short time frame of the research with this cell[1]. Due to its recent discovery it seams that the efficiency of these cells degrades over time. However a very promissing way in order to improve the stability of the perovskite solar cell efficiency over time is the encapsulation of the perovskite layer with a metal-oxide layer in order to protect it from the humidity of the air [11]. As shown by these authors such a protection result to an initial degradation of 10 % of the PCE, which stabilize after approximating 30 days. The use of standardized module encapsulation should further reduce the degradation of this solar cell, if used in a solar module.

At the state of the art the improvement of the efficiencies of the hybrid solar cells is mostly based on the exhaustive cell prototyping and measurements of the efficiency values of the cells manufactured in laboratories. However the potential benefits from mathematical modelling of the solar cell efficiency, as shown in [5, 6], should be more exploited in order to foster the velocity of their development. By having a mathematical model at hand, which expresses most accurately the solar cell efficiency as a function of its material properties and other engineering parameters, it can be analyzed theoretically which of the parameters or properties do lead to the most significant improvement of the solar cell efficiency. Therefore a multidimensional sensitivity analysis of the model variables of a perovskite p-i-n solar cell is here accomplished based on the analytical model elaborated in [5].

2. Tuneability of the properties of the perovskite cell

Whereas the organic component of the hybrid perovskite material provides the viability of its deposition in a solution, which permits the printing of the cell in a roll to roll process, the inorganic component of the perovskite solar cell forms an extended framework of strong covalent interactions, ionic interactions, or both of them, which permits the advanced engineering of the cell properties. As stated in [9], the optical and electronic properties of the perovskite material can be tuned to a great extend by replacing the halide ion, the metal ion or the organic cation. Furthermore the perovskite material has an excellent tuneability of its band gap by adjustment of the relation of its chemical composition [10], making it therefore fit for the optimization of its efficiency in single, double or multiple junction cells. The details highlight the remarkable tuneability of the perovskite cell properties, which show its high potential for further improvement of its efficiency in the near future.

3. Model description of the perovskite p-i-n solar cell

Using as reference the results obtained by a detailed numerical simulation, the authors Sun et al. [5] elaborated a simplified analytical model for four different types of perovskite solar cells considering a fixed band gap. For the present analyses only the p-i-n solar cell is analyzed in more detail based on its analytical model as this cell resulted in [5] to the highest measured and modelled efficiency values of 15.7 %. The p-i-n solar cell consists of a p-type and a n-type charge conduction layer, an absorber layer, also denominated as intrinsic i-type layer, a transparent front electrode layer and a reflecting the back contact layer. As it is considered that the excitons are principally generated within the charge neutral depletion zone, the enlargement of this zone by use of the undoped intrinsic layer, constituted by the perovskite material, does improve the probability of the generation of the free charges by means of the solar radiation. Whereas the majority carriers account for the generation of the free charges, the minority carrier's results to the recombination effect under explosion to light. The electron and the hole transport layers of n-type and p-type are considered as perfect conductors for the majority carriers and as imperfect blocking layers for the minority carriers. Whereas the p-layer conducts the majority holes to the cathode and blocks the minority flux of electrons to this electrode, the n-layer conducts the majority electrons to the anode and blocks the minority flux of holes to this second electrode.

[1] http://www.nrel.gov/ncpv/,

4. Initial parameter configuration based on measured results

Sun et al., 2015 [5] defined by use of the Optical Transfer Matrix method first the fundamental optical parameter of the analyzed cell, which are (i) the generation of free charges G_{max} = 1.4356 x 10^{23} $cm^{-2}s^{-1}$ (qG_{max} = 23 mA/cm²), and (ii) the average optical decay length λ_{ave} = 100 nm for the presented p-i-n solar cell. Wereas G_{max} gives the charge generation rate at the surface of the solar cell as function of the band gap λ_{ave} gives a measure of how the radiation intensity decays as it pentrates into the solar cell. Then, in order that the p-i-n model UI curves at AM1.5 irradiation $J_{light}(U)$ and in the dark $J_{dark}(U)$ fit to the measured UI curves, these obtained optical parameters and the measured ambient temperature T_a = 27.41 °C, were used in a regression using the algorithm 'lscurvefitt' of the Mablab™ program. This algorithm minimizes the sum of the least square deviations in-between the measured and the modeled UI curves and leads to the perovskite material properties considering a fixed solar cell thickness. Then, using the obtained model specification the cell efficiency for different absorber layer thicknesses was modeled in a unidimensional optimization process. The optimized cell was manufactured and its efficiency was validated with the optimized model efficiency. The authors obtained the following model properties: Diffusion coefficient of charges $D_n = D_p \approx$ 0.05 cm^2/s, front and back surface recombination velocities of charges s_f = 2 x 10^2 cm/s, s_b = 19.2 cm/s, number of charges participating at the recombination process Δn = 8.426 x 10^6 cm^{-3}, Δp = 1.3003 x 10^8 cm^{-3}, front and back surface recombination currents J_{f0} = 2.7 x 10^{-13} mA/cm^2, J_{b0} = 4.0 x 10^{-13} mA/cm^2, built-in voltage V_{bi} = 0.78 V, absorber layer thickness of t_0 = 450 nm, average optical decay length λ_{ave} = 100 nm. This optimization resulted to an cell efficiency of η = 15. 7% [5].

5. Results and discussion

As graphically shown in [5], the efficiency is a function of the recombination velocities of charges trough the front and the back transport layers s_f and s_b and the absorber layer thickness t_0. A reduction of s_f and s_b , and principally the front surface recombination velocity s_f , would improve the cell efficiency also by approximately 3 % (figure 4 in [5]). However, as given from the model equations the cell efficiency is sensible to more than those three variables. Therefore, in the present sensitivity analysis the efficiency is shown as a function of an increased number of model variables. The following material properties are considered as additional variables of which the efficiency is a function: (i) the average optical decay length (λ_{ave}) in context with the thickness of the intrinsic absorber layer (t_0), (ii) the diffusion coefficients of electrons and holes D_f and D_b, the built-in voltage V_{bi} .

Whereas the cell thickness seems to be the main factors in order to improve the cell efficiencies (see figure 3 is [5]), the melioration of the average optical decay length seems to be insignificant leading to an improvement of only 0.05…0.1 %, if a fixed optical decay length is considered. However, showing these two variables in a bi-dimensional space, while the other variables are are being fixed to the values in item 4, it can be seen that the efficiency can be considerably improved if it would be possible to reduce the optical decay length (Figure 1). As shown by the vertex line in this figure, the active layer thickness t_0 has to be adjusted as a function of the average optical decay length λ_{ave} in order to obtain the best efficiency values. In the best case this results to the augmentation of the efficiency from 15.7 % to around 17 % (Figure 1). Further improvement of the efficiency values can be obtained by manipulation of the diffusion coefficients and principally the diffusion coefficient of the holes D_p , which lead to an improvement of up to approximately 3 % of the efficiency (Figure 2). The variation of the built-in voltage resulted to an increase of the efficiency of approximately 1.8 % at V_{bi} of 1.4 eV. As to see from the Shockely-Quaisser efficiency curve the a band gap adjustment would improve the efficiency by less then 2 %.

Recommendations for the improvement of the efficiency of the p-i-n perovsktite cells

The perovskite material with the lowest average optical decay length λ_{ave} should be selected as this results to the conversion of the solar irradiance by use of smaller values of the cell thickness t_0 . The cell thickness t_0 should be adjusted as a function of the attained average optical decay length of the synthesized Perovskite absorber layer as shown by the blue vertex line in Figure 8, which shows the highest solar cell efficiency values within this function space. The perovskite material should be modified in order that the diffusion coefficients of the electrons and holes D_n and D_p are coming as high as possible. Especially high improvements can be obtained by the improvement of D_p , if D_n is at least higher than approximately 0.3 m^2/s (Figure 2). The perovkite material and the organic conduction layer material should be selected in order to obtain the highest possible built-in voltage V_{bi} .

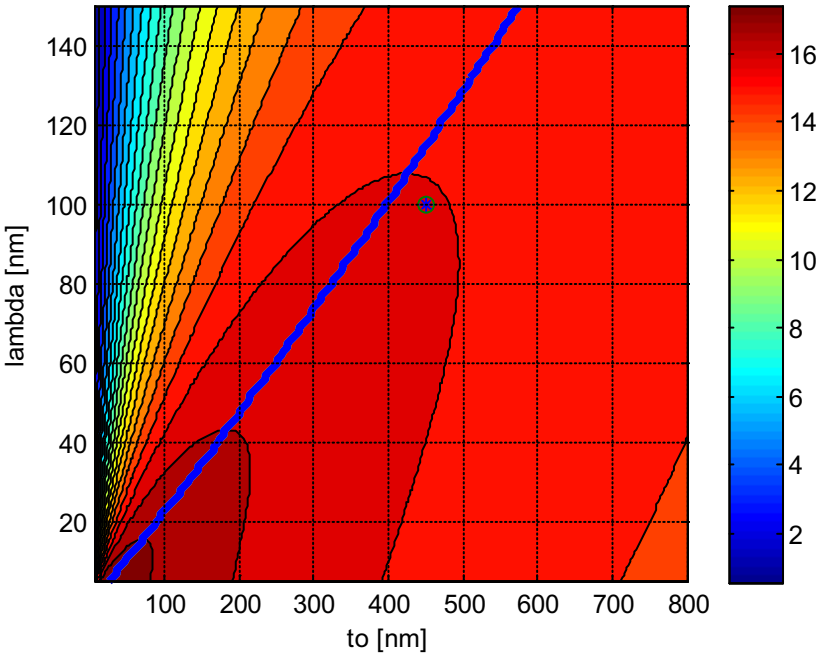

Figure 1: Modeled efficiency for a current generation of q x G_{max} = 23 mA / cm² as a function of the thickness of the absorber layer t_0 and the average optical decay length λ_{ave} with a vertex line of the maximal efficiency points (blue line) and the measured efficiency obtained in [5] (blue star surrounded by a circle).

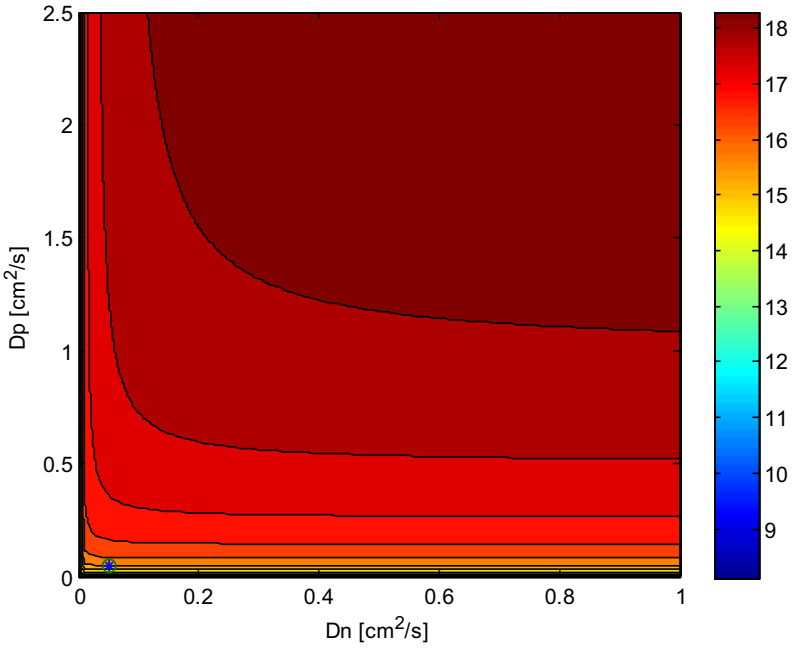

Figure 2: Cell efficiency for a current generation of q x Gmax = 23 mA / cm² as a function of the diffusion coefficient of holes D_p and diffusion coefficient of electrons D_n with maximum value of the efficiency of 18.8 % within the upper right part of the presented graphic and the measured efficiency in [5] (blue star surrounded by an circle).

6. Conclusions

In the present publication the perovskite cell efficiency is shown as a function of an extended variable space determined by the cell properties and manufacture parameters. The obtained results lead to a better understanding on how the efficiency of the p-i-n perovskite solar cell can be improved and results into recommendations to show how to modify these variables, in order to increase most successfully the solar cell efficiency. Whereas the melioration of each one of the single variables lead to a lower improvement of the efficiency the interplay or interdependence of the model variables in an nonlinear space lead to more substantial improvements, which are much higher than the improvements obtained by single variable variations.

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