Dye Solar Cells efficiency maps: a parametric study

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Fig. 1. A. Schematic representation of a DSC. B. Energy diagram of conversion processes: 1.Excitation of the dye, 2.Injection in the TiO_2, 3.Diffusion and collection at the anode. The recombination processes are: a. Decay of the dye in its ground state, b. Regeneration of the dye by TiO_2 conduction band electron, c. Reduction of the electrolyte occurring at the TiO2 interface.

Abstract—**In this work we present a numerical simulation of a Dye Solar Cell efficiency using a drift-diffusion model for the complete cell. The physical parameters such as the active layer thickness, the electron mobility and the dye spectrum are varied systematically in a range of values individuated experimentally, in order to obtain efficiency maps that reveal interesting features in this kind of devices.**

I. Introduction

Dye Sensitized Solar Cells (DSC) [1] are a very promising photovoltaic device reaching up to 11% efficiency, relatively recently discovered and with wide room for improvement. A DSC is essentially an electrochemical cell based on a thin nanoporous Titanium Dioxide layer (10-15 μm) where a monolayer of molecular organic dye (generally Ru-based) is chemisorbed.
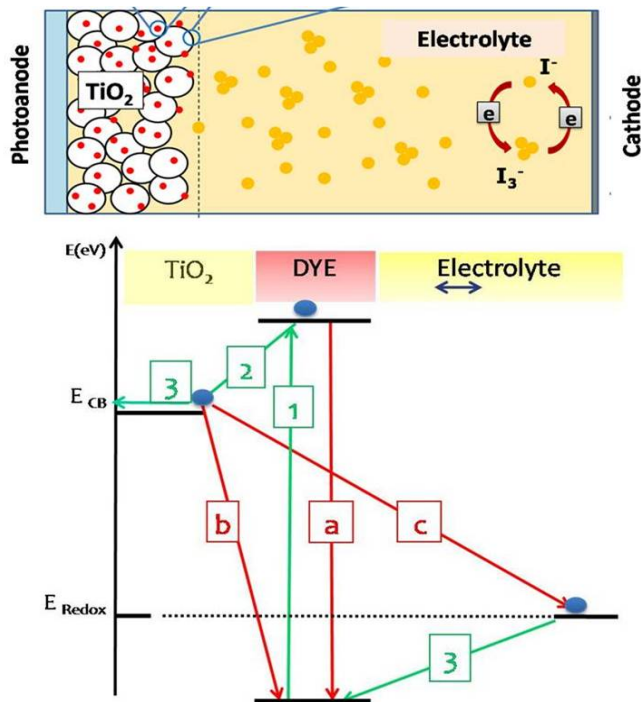

This hybrid organic-inorganic structure is dip in a liquid electrolyte where a redox couple is present (generally I_3^-, I^-). The whole system is sandwiched between two conductive glasses and encapsulated by a sealant (Fig. 1A). Once the light excite one electron in the dye (Fig. 1B, 1), this is fast injected to the TiO_2 conduction band (Fig. 1B, 2) and collected at the anode(Fig. 1B, 3). The ionized dye is regenerated by oxidation The redox reaction occurring in the cell is a two electrons process:
 The dark currents are represented by the dye electron decay in its ground state dye (Fig. 1B, process a), the regeneration of the dye by a TiO_2 electron (b) and the reduction of the electrolyte occurring at the TiO2/electrolyte interface (c).

We want to simulate the efficiency of a DSC varying the working conditions (direction of light), the paste used for the TiO2 (electron mobility), the molecule used to catch the light (dye spectrum) in order to create a parametric map of efficiency which is reliable and predictive for improving the light conversion of the device.
We implemented a specific module for DSC in the framework of TiberCAD [2], able to obtain complete IV curves and carriers density profiles. By varying the simulation parameters in a range of experimental values we calculate the output under different working conditions and present efficiency maps.

II. Modeling

A. Physical model and equations

We use a Finite Element Method for solving our calculations in 1-dimension. The cell is divided into two parts: a homogeneous photoactive part where TiO_2 and electrolyte are intermixed and a part of bulk electrolyte.
Modeling DSC requires to handle four different charge carriers: e electrons, I_3^- and I^- ions and positive C cation necessary to assure the neutrality of the system.
For the charge transport we use a drift diffusion equation for each carrier, coupled with the continuity and the Poisson equation:

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$$\nabla \boldsymbol{j}_\gamma = \Lambda_\gamma (G - R)$$
$$\boldsymbol{j}_\gamma = -D_\gamma \nabla n_\gamma + \mu_\gamma n \nabla \varphi$$
$$\in \nabla^2 \varphi = e(n_c + N_D^+ - n_{I^-} - n_{I_3^-} - (n_e - \bar{n}_e))$$

Where μ_γ is the carrier mobility n_γ is the charge density for each carrier. In particular for electrons we implement a model for diffusion which include trapped electrons [3].

B. *Parameters*

Our complete model of DSC requires a very careful selection of the parameters to be implemented in the code. In order to achieve the most reliable comparison between simulations and real cells, we derive the most parameters from experimental results, even if it is often not straightforward. We extract the electron mobility and the recombination constant ranges starting from a set of experimental cells with different efficiencies (3-8%): by means of a IV characteristic fitting procedure, where the non-electronic simulation parameters are fixed by the experiment (i.e. dye, ions diffusion coefficient), the mobility and recombination rate values are recursively varied until the complete experimental curve is reproduced. We applied this procedure to a wide samples of cells, fabricated with different geometries and treatments. In this work we summarize the results obtained in the experimental comparison, presenting a pure theoretical efficiency estimation when the parameters are varied in the range of values found experimentally.

C. *Map of Efficiency*

The fine tuning of the light absorption, transport parameters and the geometry of the active layer, allow us to define a consistent parameterization of the simulator which is then used as a predictive tool to calculate maps of efficiency for different working conditions and different directions of incoming light.
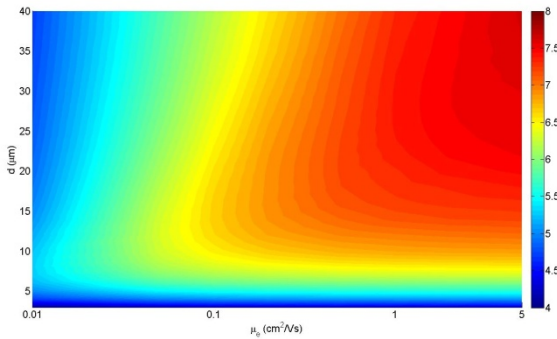
In Fig. 2 A map of efficiency is shown for a typical dye spectrum N719 in function of the active layer thickness and of the mobility. Every point of the map has been obtained by a calculating the efficiency and the color bar represents its scale of values.

The performance are strongly influenced by changing the experimental conditions of a working DSC. In Fig. 4 we present a comparison of efficiency maps when the direction of illumination is varied(A,B photo-anode side, C,D electrolyte side) and the absorption coefficient of the dye is changed from a dye with low absorption coefficient and 0.7 sun(A,C) to a dye with high absorption coefficient (B,D) for 1 sun.
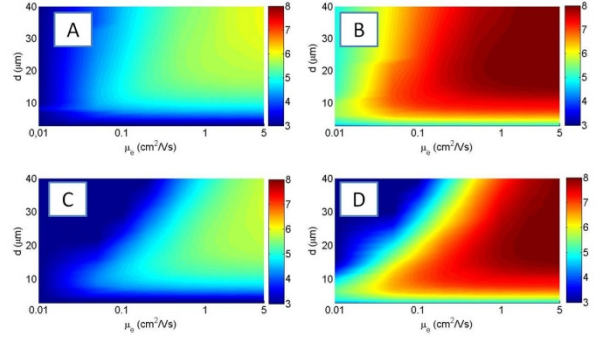
Fig. 5 The varying color represents the simulated efficiency for increasing active layer thickness (y-axis) and electron mobility (x-axis), representing different working conditions. A and B are front-illuminated , while C and D are back- illuminated for Dye N719 for 0.7sun (A , C) and (D,B) TiCl4 treated for 1sun.

III. BIBLIOGRAPHY

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