

Innovative Structure for Dye Solar Cells

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Abstract—In this work we present a Computer Aided Design (CAD) software, called TiberCAD, to simulate Dye Sensitized Solar Cells (DSC). DSC are particularly interesting devices due to their high efficiency (more than 12% on small area and 8% on large area) and long stability. Since their first development, much progress has been made in terms of efficiency, stability, lifespan and engineering of the device. However, the field of DSCs still lack a complete model able to simulate the entire device including all its components. In our model a drift-diffusion set of equations for the different charge carriers coupled to Poisson equation has been implemented within finite element method. The model takes into account also trap assisted transport for electrons in the mesoporous titanium dioxide with a phenomenological model derived from multi-trapping model.

An application of the code presents an innovative topology for a DSC using a 3D geometry. A cell where contacts and illuminated surface are completely decoupled.

I. INTRODUCTION

In recent years third generation solar cells has appeared. Differently from the previous two generations, this last group is oriented towards a completely different class of materials, like polymers, small molecules materials and nanostructured materials. Their efficiency is still lower than that of semiconductor devices and some of them, like polymeric solar cells, lack also the needed stability to be commercialized. However, the technology is rapidly growing.

Among third generation solar cells Dye-sensitized solar cells (DSCs) [1] are the most promising devices.

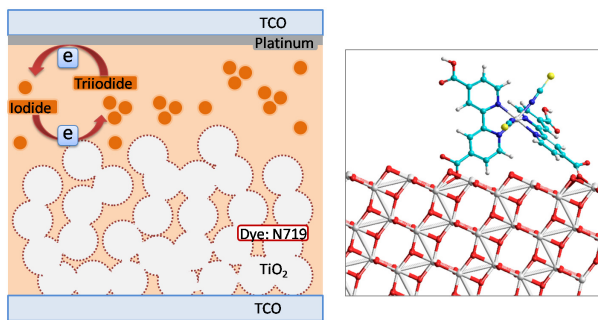


Fig. 1: (color online) On the left, scheme of a DSC. At the bottom the TiO_2 (white circles) with the chemisorbed dyes (red dots) between the two transparent conductive oxides (TCO) and the thin platinum layer at the counter-electrode (cathode). The cell is filled by an electrolyte with a redox couple I^-/I_3^- (orange). On the right, scheme of a typical dye (an organic ruthenium complex) chemisorbed on the TiO_2 nanoparticles.

A DSC (fig. 1, left) is fundamentally an electrochemical device. A mesoporous dye-covered semiconductor is plunged into a liquid electrolyte containing a redox couple. The standard semiconductor used in DSCs is titanium dioxide (TiO_2) made of nanoparticles, 10-20 nm in size, sintered together to create a connected network. The titania paste is deposited on a transparent conductive oxide (TCO) that works as one contact for the device. The surface of the mesoporous material is covered by a monolayer of molecules, the dye, chemisorbed on the surface. This molecular layer makes the device photoactive in the visible range. The mesoporous material has a very large effective area allowing for a high density of chemisorbed dye. The electrolyte usually contains a iodide/triiodide (I^-/I_3^-) redox couple. Finally, the cell is closed by a counter-electrode formed by a TCO covered by a thin layer of platinum acting as catalyst, in contact with the electrolyte. Under illumination, at the counter-electrode, the iodide acts as the reducer and triiodide as the oxidant.

II. SIMULATION MODEL

The DSC simulation model implemented in TIBERCAD uses the drift-diffusion approximation to describe carrier transport in the cell [2], [3], [4]. Five carriers are needed to describe a DSC, namely electrons (in the TiO_2), iodide, triiodide, and cations. The cations are needed for charge neutrality in the electrolyte, although they do not participate in the electrochemical processes. The complete model describing the cell reads as follows:

$$\nabla(\mu_e n_e \nabla \phi_e) = G - R \quad (1)$$

$$\nabla(\mu_{I^-} n_{I^-} \nabla \phi_{I^-}) = -\frac{3}{2}(G - R) \quad (2)$$

$$\nabla(\mu_{I_3^-} n_{I_3^-} \nabla \phi_{I_3^-}) = \frac{1}{2}(G - R) \quad (3)$$

$$\nabla(\mu_c n_c \nabla \phi_c) = 0 \quad (4)$$

$$\nabla(\varepsilon \nabla \varphi) = q[n_c + N_D^+ - n_I - n_{I_3^-} - (n_e - \bar{n}_e)] \quad (5)$$

Here, μ_α , n_α and ϕ_α are the mobility, the density and the electro-chemical potential of the particle α . G is the electron generation term due to illumination, and R is the recombination rate. φ is the electrostatic potential, and N_D^+ is the density of ionized dyes, given by the generation rate G divided by the dye regeneration rate. For each carrier we assume local thermal equilibrium, and we assume the TiO_2 to be non-degenerate so we can write all particle densities using Boltzmann statistics as

$n_{\alpha} = \bar{n}_{\alpha} \exp(\pm \frac{q\varphi - q\phi_{\alpha}}{k_B T})$, where the barred quantities are the densities in thermodynamic equilibrium (dark condition and no external bias applied).

The local generation rate G is related to the photon flux and the absorption in the active TiO_2 . It is calculated considering the absorption spectrum of the dye used for the DSCs (usually a Ruthenium complex called N719, Fig.1, right inset) and using the spectral power flux of the illuminating source (standard solar illumination at AM 1.5 G of 100 mW/cm^2).

III. NEW TOPOLOGIES FOR DSCS

In this paragraph we show a 3D application of the simulator for an innovative geometry of the cell. The discussed device is shown in figure 2. It is a cell where the metallic contact for the anode is on one side of the device spatially separated from the transparent surface for light absorption.

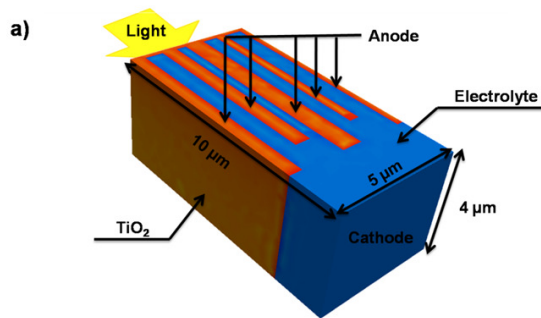


Fig. 2: (color online) Grid used for the simulations. $10 \mu\text{m} \times 4 \mu\text{m} \times 5 \mu\text{m}$.

The presence of the metallic fingers overlapping the illuminated side of the cell, reduces the overall absorption and has a big impact on the final efficiency. A new concept could be the one proposed here where the metallic fingers are not a problem anymore for light harvesting. In figure 3 the electron generation (a) and the recombination (b) are shown. The decoupling of illumination regions changes the density distribution inside the cell, in fact the main photogeneration of electrons is concentrated close to surface from where photons come, but the electrons generated far from the metallic fingers partially recombine before reaching the contact and in fact recombination is mainly located at the bottom of the cell. In figure 3 (b) the current lines are plotted to show the path followed by the electrons. Another simulation has been done for a similar cell with the difference that the collection contact is on the same surface used for illumination and it is not located on top of the cell. The I-V characteristics are compared in figure 4. The current for the cell with the top contact (TOP), red broken line, is larger than the current of the cell with the side contact (SIDE) because the electron path in the TOP case is smaller than in the SIDE case allowing a better collection.

REFERENCES

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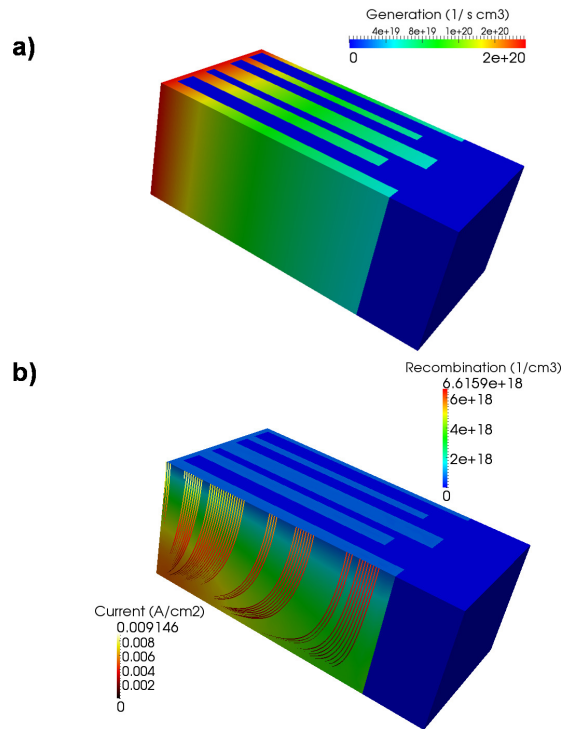


Fig. 3: (color online) a) Generation of electrons in the cell b) Electron recombination and electron current lines at short-circuit condition.

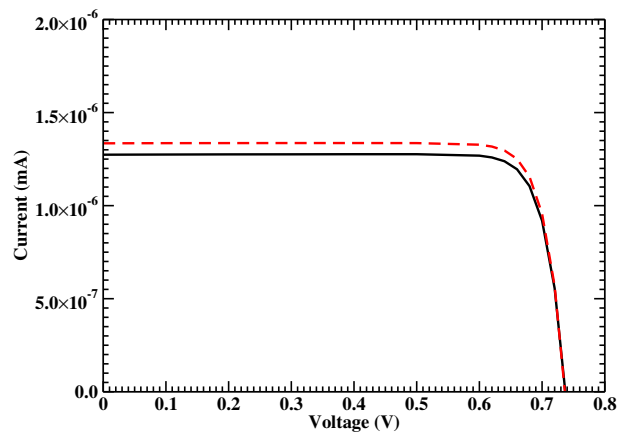


Fig. 4: (color online) I-V characteristics for the two positions of the anode (TOP and SIDE). SIDE anode: continuous black line, TOP anode: red broken line.

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 [3] A. Gagliardi, M. Auf der Maur, D. Gentilini and A. Di Carlo, *J. Comp. Elec.*, **8**, 398 (2009).
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