Simulation of Electron and Electrolyte Transport in Dye- sensitized Solar Cells.

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Dye-sensitized nanocrystalline solar cells (DSNC cells) have achieved solar-to-electrical energy conversion efficiencies of 12% in diffuse daylight. The cell is based on a thin film of dye sensitized nanocrystalline TiO_2 interpenetrated by a redox electrolyte. Photoexcitation of the dye is followed by fast (<100fs) electron injection into the conduction band of the TiO_2 nanoparticles. The injected electrons travel through the nanocrystalline TiO_2 to the anode and the redox mediator (I^-/I_3^-) acts as a shuttle to permit constant current operation under illumination. A simplified schematic of the DSNC solar cell structure is shown below in Fig, 1.

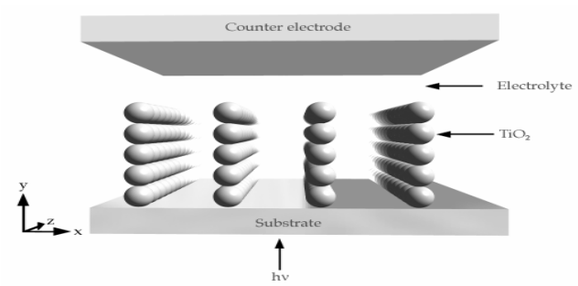


Fig. 1. ***Schematic cell diagram showing the TiO_2 grains as spheres, aligned as rows parallel to the z-axis, interpenetrated by an electrolyte phase.***

Whilst much effort has been made to elucidate the nature of electron transport in the TiO_2 films using empirical, analytical or numerical techniques, few studies have focused on the role of the electrolyte. In this communication we examine a 2 dimensional finite difference model incorporating both a solid (TiO_2) and liquid (electrolyte) phase. For the purposes of illustration the following mechanism was examined

$$dye \xrightarrow{hn} dye^*$$

$$dye^* \longrightarrow dye^+ + e^-_{TiO_2}$$

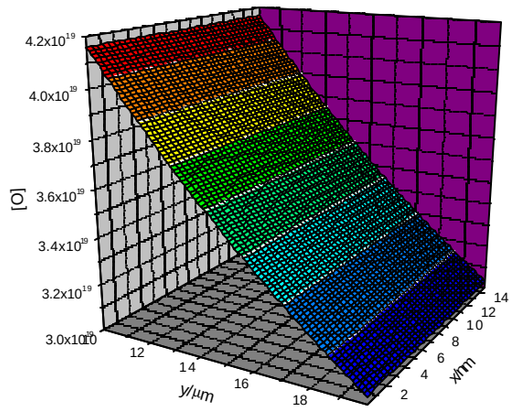
$$dye^+ + R \longrightarrow dye + O$$

$$O + e^-_{TiO_2} \longrightarrow R$$

$$dye^+ + e^-_{TiO_2} \longrightarrow dye$$

where O/R represents the redox mediator (typically iodide/tri-iodide in a DSNC cell), e^-_{TiO2} the conduction band electron density within the TiO_2 and dye/dye^+ the reduced/oxidised form of the surface adsorbed dye. The flexibility of our numerical approach permits the calculation of the O/R concentration distribution as a function of the TiO_2 framework (eg grain size, periodicity of the TiO_2 structure and grain/counter electrode separation) for a large range of illumination and back reaction rates. Results will be presented to assess the role that electrolyte transport plays in the operating efficiency of the DSNC cells. Figure 2 shows a typical set of electrolyte concentration data obtained for species O and R within the cell. Here, the cell thickness was 20 μm, the radius of the TiO_2 grains 15 nm, the electrolyte region extends 15 nm in the x-direction, the diffusion coefficient was $1x10^{-5}cm^2s^{-1}$ for species O and R and the electrons, the back reaction rate was $1x10^{-25}cm^{-4}s^{-1}$ and the light absorption coefficient was $2300x10^{-7}cm^{-1}$ A short circuit condition was used where $k_{ext} = 1x10^5\ s^{-1}$.

(a)



(b)

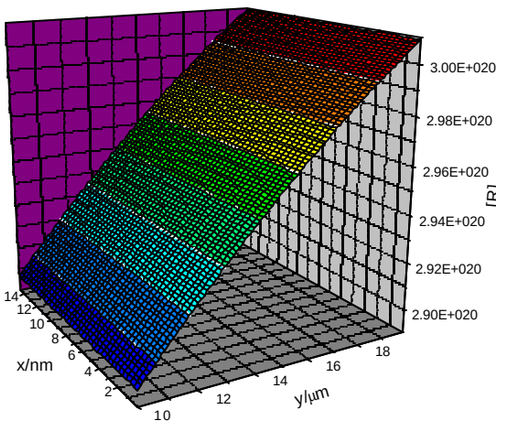


Fig. 2 ***Concentration profile of the oxidised species O (panel a) and reduced species (panel b) in the gap between the TiO_2 grains and the anode.***