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Monte Carlo simulation for optimization of a simple and efficient bifacial DSSC with a scattering layer in the middle

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ABSTRACT

Bifacial dye sensitized solar cells (DSSCs) show potential for use in diffuse and low light environments, but their photoanode light scattering properties have not been optimised. We examine DSSC photoanodes composed of a mixed scattering layer (made by blend of 18NR-T and WER2-O pastes), sandwiched between nanostructured TiO_2 layers (made by 18NR-T paste). WER2-O paste was chossen after accessing scattering properties: scattering coefficient (S), forward scattering ratio (FSR) and forward path length enhancement (FPLE) of the solid TiO_2 particles of different shapes and sizes. Monte Carlo simulations of light harvesting indicate the optimal volume fraction of scattering particles (f_{vsca}) in the sandwiched layer to be 5–30%. The proposed photoanode absorbs light effectively and the DSSC with scattering layer made by blend of 60% of 18NR-T and 40% of WER2-O paste showed the power conversion efficiency (PEC) of 8.54% and 5.26%, when illuminated from photoanode (PA) and counter electrode (CE) side, respectively. The effective sorting criteria and optimization routine used in this work can also be used for other devices like perovskite solar cells.

1. Introduction

This study concerns the optimisation of light harvesting in bifacial dye-sensitized solar cells (DSSCs). DSSCs are an alternative photovoltaic technology which show particular promise relative to conventional solar cells for energy harvesting in low and diffuse light conditions such as those found in cloudy climates and indoors (Ito et al., 2008a; Vignati, 2012). Steadily increasing performances are being reported resulting from the continuous development of better dyes (Duvva et al., 2017; Liess et al., 2017), mesoporous dielectric structures (Liu et al., 2015) and hole transporting materials (Maciejczyk et al., 2016); a power conversion efficiency (PCE) of 13% has recently been published (Mathew et al., 2014). These colourful DSSCs show considerable stability, have low cost, and have been integrated to building materials (Kroon et al., 2007).

A significant reason for the better indoor performance of DSSCs may be their ability to harvest light from both sides (Wenger et al., 2011). Diffuse radiation can also be a high percentage of total radiation in outdoor working conditions. Outdoor field testing of solar cells in Japan and Spain found bifacial solar cells yielding outputs ~1.4–1.6 times that of monofacial solar cells (Cuevas et al., 1982; Joge et al., 2002). Additionally, these field tests also showed lesser hourly variation in output. Japan and Spain have a relatively high fraction of direct radiation ("Annual Solar Irradiance,"; Sanchez-Lorenzo et al., 2013). In more cloudy regions with higher fraction of diffuse radiation, even more gain in output is probable. Bifacial cells also have lower operating temperature which can result in better yield (Raga et al., 2013), and probably stability. Furthermore, bifacial panels can be used as shades and windows to provide glare free diffuse sun light (Hezel, 2003).

A key consideration in design of DSSCs is that light harvesting can be limited by low photoanode thicknesses which cannot easily be increased without introducing fabrication and charge transport problems (Ni et al., 2008), as well as pore filling issues for solid state hole transporting materials (Ding et al., 2009). To overcome these concerns, most high efficiency DSSCs reported in literature use either submicron mesoporous dielectric structures, plasmonic metal nanoparticles, (Ding et al., 2011) or a diffuse backscattering layer (Ito et al., 2008a) to scatter light and enhance path length of light in the device. DSSCs with backscattering layers have very high reflectance for light incident from CE side, rendering them useless for bifacial applications (Miranda-Muñoz et al., 2016). Metal nanoparticles and mesoporous dielectric structures can be used in bifacial solar cells but they have their drawbacks. Elaborate and lengthy methods needed for fabrication of mesoporous structures increases the complexity of device fabrication. Metal

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nanoparticles are often rather expensive and add to cost. Owing to the benefits of bifacial DSSCs there has been considerable research in the field of bifacial DSSCs, but most has been aimed improving the CE performance (Cai et al., 2014; Li et al., 2017; Wu et al., 2015) and electrolytes(Li et al., 2012). Ito el al. improved back efficiency of DSSC with photoanode thickness of 16 µm by including a SiO_2 layer between the electrodes to 5.96% while the front efficiency also improved to 6.54% (Ito et al., 2008b). There have also been an initial effort to improve light harvesting structure in bifacial DSSCs. Miranda–Munoz et al. enhanced the light harvesting in the bifacial DSSCs by embedding large scattering particles uniformly in the nanostructured (NS) TiO_2 photoanode (Miranda-Muñoz et al., 2016). A high back to front efficiency ratio was achieved by this approach. But short circuit J_{sc} yielded by such photoanode ($< 14\,mA\,cm^{-2}$) is considerably less than reported values ($> 18\,mA\,cm^{-2}$) obtained with same dye in other devices (Liu et al., 2015), this suggests a need for better light harvesting and improvement in photoanode structure.

If light is incident on a film with uniformly embedded scattering particles (as used by Miranda–Munoz et al.) a considerable fraction of incident light will be reflected away from the surface of the film following multiple scattering even though backscattering by an individual particle is negligible. Sandwiching such film between two mesoporous nanostructured (NS) TiO_2 layers will result in lesser diffuse reflectance (R_d) from the either side of photoanodes. Devices up to 7.9% efficiency have been reported in literature having scattering layer of submicron TiO_2 mesoporous structures sandwiched between NS TiO_2 (Bakhshayesh, 2015; Dissanayake et al., 2016). These submicron mesoporous structures offer effective light scattering and large surface areas for dye adsorption. Combined, these properties yield good photo conversion efficiency. These qualities can also be achieved in a single sandwiched layer by mixing larger scattering particles with small NS TiO_2 particles. The smaller particles of NS TiO_2 provide large surface area for dye adsorption, whereas the larger particles provide effective scattering. Such mixed layers have been found to be more effective as backscattering layer compared to conventional backscattering layer by Wang et al. and Sun et al. (Bakhshayesh, 2015; Dissanayake et al., 2016) Such layers have high scattering coefficient as solid TiO_2 spheres scatter light more strongly compared to mesoporous TiO_2 structures as a result of greater contrast in refractive index with surrounding (Shital and Dutta, 2016). Such mixed scattering layer, can also be used as light harvesting layer, in which embedded scattering particles will randomise the incident light. But a photoanode with scattering particles in the middle needs to be properly optimized, as too much light scattering will increase reflection losses whereas too little will result in insufficient randomization of light. Monte Carlo simulations are the most commonly used method to optimize light harvesting in DSSCs. Monte Carlo simulation was first used for optical simulation of DSSC by A. Usami. He used this method to suggest the optimum size of scattering particles (Usami, 1997) for best light absorption, and pointed out that total internal reflection plays more important role in improving light harvesting compared to path length enhancement (Usami, 2000). This method was then used to estimate electrical performance parameters of DSSCs employing different kind of nanostructures using well established relations between the performance parameters and electron hole pair generation in photoanodes (Gálvez et al., 2012). In an improvement over that this Monte Carlo simulation was used in conjugation with numerical solution of charge transport equation in DSSC photoanodes, to simulate for short circuit current (J_{sc}), open circuit voltage (V_{oc}) and fill factor (FF) of DSSCs (Gálvez et al., 2014). Guo et al. found the experimental results to be in good agreement with Monte Carlo simulations (Guo and Shen, 2013). For optimization of bifacial solar cells with embedding scattering particles, Monte Carlo simulation was used by Miranda-Muñoz et al. (2016).

In this paper we report a combination of computational and experimental optimisation of DSSCs photoanode containing a mixed scattering layer sandwiched between two layers of NS TiO_2, as shown in Fig. 1. The dye sensitized mixed scattering layer has low R_d which reduces further by the flanking dye-sensitized NS TiO_2 layers. A step by step approach is used for optimization of DSSCs, beginning with choosing scattering particles suitable for scattering layer on the basis of their scattering parameters: scattering coefficient (S), forward scattering ratio (FSR) and forward path length enhancement (FPLE). These parameters are evaluated by T-Matrix method. The composition of scattering layer in DSSC is optimized by Monte Carlo simulation of interaction of light with full device.

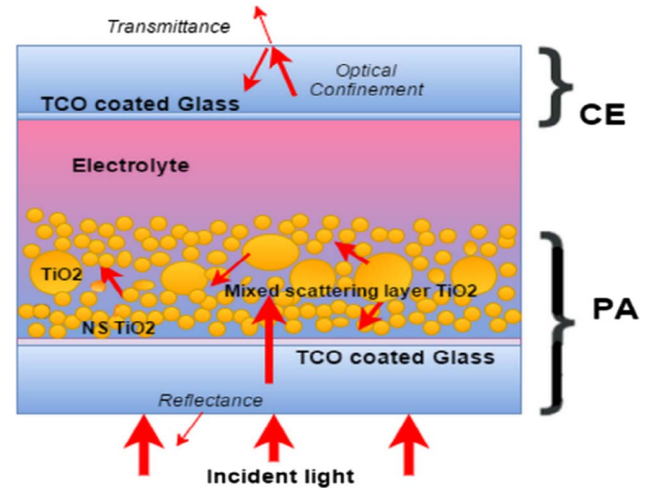

Fig. 1. Schematic of the proposed bifacial dye sensitized solar cell. CE stands for counter electrode consisting of fluorine doped tin oxide (FTO) coated glass with a thin Pt catalytic film. PA stands for Photoanode consisting of dye coated three layered TiO_2 film (A scattering layer in middle, sandwiched between NS TiO_2 layers) deposited on FTO coated glass. The concentration of scattering particles (f_{vsca}) in the scattering layer was varied.

The electron hole pair (EHP) generation profile obtained from it, was then used to approximate J_{sc}. The best front PCE of 8.5% and back PCE 5.3% was measured for DSSC with 12 µm thick photoanode having 6 µm scatting layer in the middle, made by blend of 40% scattering and 60% NS TiO_2 paste (which corresponds to a volume fraction of scattering particles, f_{vsca} ~ 7%).

2. Methods

2.1. Independent scattering properties

Independent scattering properties of scattering particles, evaluated using T-Matrix method were used as inputs for device simulation (Mishchenko and Travis, 1998). T-Matrix method involves expanding incident and scattered field in terms of spherical vector functions. The coefficients for expansion of scattered field (p_{mn},q_{mn}) can be written as product of T-Matrix and coefficients for incident field expansion (a_{mn},b_{mn}).

$$\begin{bmatrix} p_{mn} \\ q_{mn} \end{bmatrix} = \begin{bmatrix} T_{11} & T_{12} \\ T_{21} & T_{22} \end{bmatrix} \begin{bmatrix} a_{mn} \\ b_{mn} \end{bmatrix} \quad (1)$$

Elements of the T-Matrix: T_{11}, T_{12}, T_{21}, and T_{22} are solely dependent on properties of the scattering entities, and can be calculated by extended boundary condition method. T-Matrix calculated for a particular entity, can be used to evaluate scattering parameters for different orientation of that entity with respect to incident light. These parameters were then averaged to find scattering parameters for random orientation.

Simulation of full devices with different types of scattering particles will require a lot of computation. To reduce the number of device simulations, some simple scattering parameters for sorting suitable scattering particles were employed. In the proposed photoanode forward scattering is desirable for our design, in contrast to the