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Numerical Simulation of Tin Based Perovskite Solar Cell: Effects of Absorber Parameters and Hole Transport Materials

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The organometal perovskite solar cells have shown stupendous development and have reached a power conversion efficiency (PCE) of 22.1%. However, the toxicity of lead in perovskite solar cells is a major challenge towards their incorporation into photovoltaic devices and thus needs to be addressed. Tin perovskite ($CH_3NH_3SnI_3$) have attracted a lot of attention recently and could be a viable alternative material to replace lead perovskite in thin film solar cells. A detail understanding of effects of each component of a solar cell on its output performance is needed to further develop the technology. In this work, we performed a numerical simulation of a planar heterojunction tin based perovskite solar cell using SCAPS (Solar Cell Capacitance Simulator). Results revealed that thickness and defect density of the absorber material strongly influence the PCE of the device. Various types of hole transporting material (HTM) were compared and analysed to improve the performance of the solar cell. Parameters such as hole mobility and acceptor density of HTM also signified dependence on PCE of the device. These results indicate the possibility to design, fabricate and enhance the performance of tin based perovskite solar cells.

Keywords: Tin perovskite Solar Cell, Simulation, HTM, SCAPS.

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1. INTRODUCTION

Organic-inorganic metal halide perovskites have gained tremendous attention for their application in high-performance solar cells because of its peculiar features like high conversion efficiency and low-cost processing. The PCEs of such devices have increased from 3.8% [1] in 2009 to 22.1% [2] in early 2016. However, one of the major challenges towards their application on a major scale is their relative stability and toxicity induced by lead. The most viable substitution for lead is tin which is also a member of the group 14 elements in the periodic table. Research for alternative absorber materials for synthesis of low-cost and highly efficient solar cells are in great demand recently. Methyl ammonium tin iodide ($CH_3NH_3SnI_3$) perovskite [3, 4] are highly desirable as photovoltaic material because of its excellent characteristics like direct-bandgap (1.3 eV), a high absorption coefficient and long diffusion length. In addition of being an environmentally benign material, it is low-cost, non-toxic and abundantly available on earth. The researchers have developed solar cell based on tin perovskite and reported a PCE exceeding 6% [3]. However, there are few issues that need to be addressed before their widespread use in photovoltaic industry: resistance to degradation and replacement of expensive hole transport material (HTM). HTM plays an essential role in a photovoltaic device for determining its stability and PCE. An HTM needs high carrier mobility and should form a defect free interface with the absorbing layer to minimize carrier recombination. So far, there has been no report on the numerical simulation of the tin based perovskite solar cells. Numerical simulation is the best approach to address and understand effects of absorber layer and HTM on the performance of a solar cell. It is an important tool which can provide significant information towards the development of the solar device. The simulations were carried out using SCAPS software [5] developed at the Department of Electronics and Information, University of Gent.

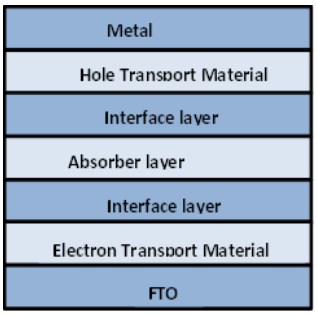

Fig. 1 – Schematic diagram of the $CH_3NH_3SnI_3$ solar cell

2. SIMULATION PROCEDURE

Here, we have controllably designed a tin based perovskite solar cell model and investigated the effects of thickness and defect density of absorber layer and different HTM on the device behaviour. A planar heterojunction architecture (Fig. 1) with layer configuration of FTO/TiO_2 Electron transport material (ETM)/Interface layer 1/absorber layer $CH_3NH_3SnI_3$/Interface layer 2/(HTM)/Metal contact has been adopted for the simulation. 2, 2', 7, 7' – tetrakis (*N*, *N* – di-p-methoxyphenyl amine)-9,9'-spirobifluorene (spiro MeOTAD), Cu_2O, copper thiocyanate (CuSCN) and Poly (3-hexylthiophene-2,5-diyl) (P3HT) are used as different HTM for the simulation.

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The parameters for different layers in the simulation are chosen on the basis of theoretical considerations, experimental data and existing literature or in some cases, reasonable estimation [3, 4, 6-12]. Thermal velocities of the electron and hole are both set to be equal to 10^7 cm/s. The tin perovskite shows a *p*-type conducting behaviour caused by self-doping process of Sn^{2+}'s easy oxidation into Sn^{4+}, so the absorber is a *p*-type semiconductor doped with a carrier density of $1 \cdot 10^{19}$ cm^{-3}. The defects in the absorption layer are set to be in the neutral Gaussian distribution with a characteristic energy of 0.1 eV, with a defect density of 10^{13} cm^{-3}. The work function of the FTO and metal contact are considered to be 4.4 eV and 5.10 eV respectively.

3. RESULTS AND DISCUSSION

3.1 Effects of Absorber Thickness

To confirm the optimum absorber thickness, simulation has been carried out in the range of 50 to 1500 nm. Other parameters are kept constant. The simulated result show that with increasing the absorber thickness, J_{sc} of the device increases apparently and reaches the maximum value ~ 24 mA/cm^2 at approximately 400 nm thickness and then decreases as shown in Fig 2a. It is evident from the same figure that Voc rises to an optimal value of 0.682 V at 100-125 nm thickness and then saturates with very slight decay as thickness increases. The relative decrease in Voc is not very significant. Fill factor of the modelled device rises initially upto 200 nm of thickness and further continuously decreases from 45.2% to 36.8% with increasing thickness as shown in Fig. 2b.

The nature of PCE curve appears similar to J_{sc} curve of the device as indicated in Fig 2b. Efficiency reaches to the highest point (6.8%) at ~ 400 nm as similar to J_{sc} and drops down with further increase in thickness. The results suggest that an optimal thickness of 380-500 nm for absorber layer could result in high efficiency tin perovskite solar cells. If the absorber thickness surpasses the optimal value then it results in more excess carriers and more traps which give more opportunity for occurrence of recombination.

3.2 Effects of Defect Density of the Absorber Layer

There are several defects such as vacancies, dislocations and grain boundaries which are always present in the absorber and HTM layer. These defects influence carrier recombination, reduction in lifetime and carrier mobility. The simulation has been carried out to study the effects of defect density ranging from $1 \cdot 10^{10}$ - $1 \cdot 10^{18}$ cm^{-3} on device performance. It is clear from Fig. 2c, d that the performance of the device is constant up to the defect density of $1 \cdot 10^{15}$ cm^{-3} and then reduces with further increase in defect density.

3.3 Effects of Hole Mobility and Acceptor Density of HTM

The HTM layer, Spiro-OMeTAD, is widely used in perovskite solar cells, which has remarkable influence on the device property. To examine the effects of HTM layer characteristics on power conversion efficiency, two typical parameters, hole mobility and acceptor density, are chosen for this study. Fig. 3a shows the results for PCE as a function of hole mobility. It is

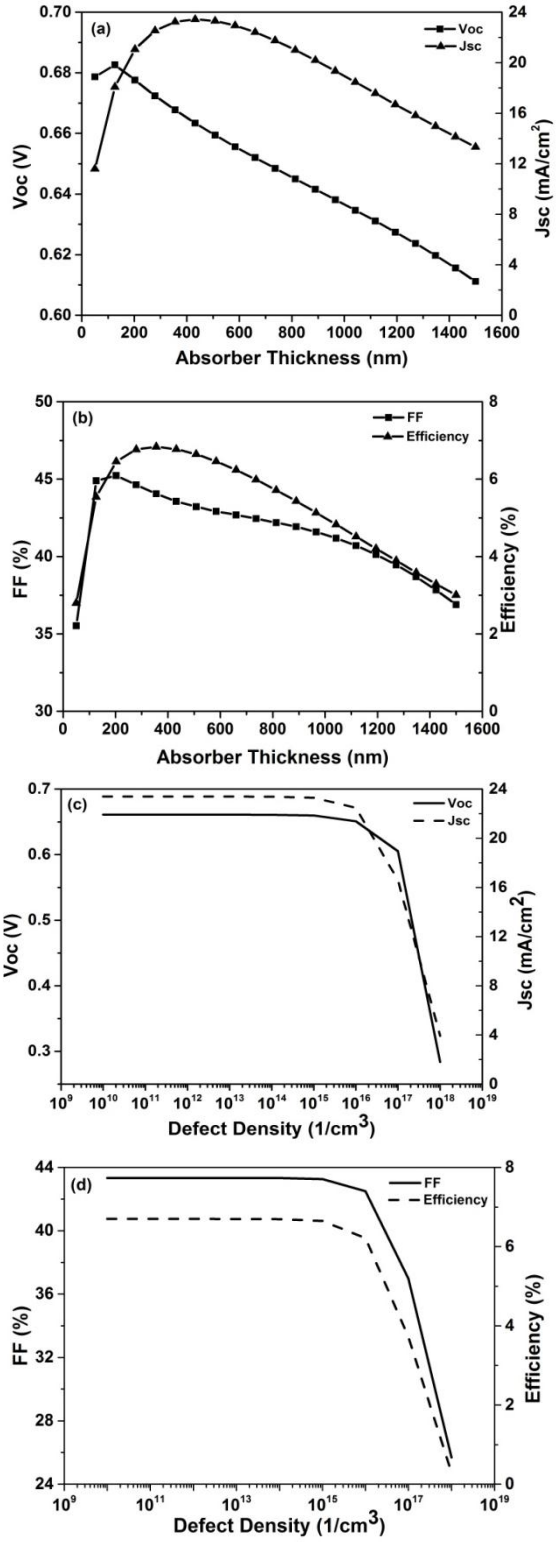

Fig. 2 – Variation of Open-circuit voltage Voc, Short-circuit current density Jsc, Fill factor FF, and Power conversion efficiency (PCE) as functions of absorber thickness (a, b) and defect density of the absorber (c, d)

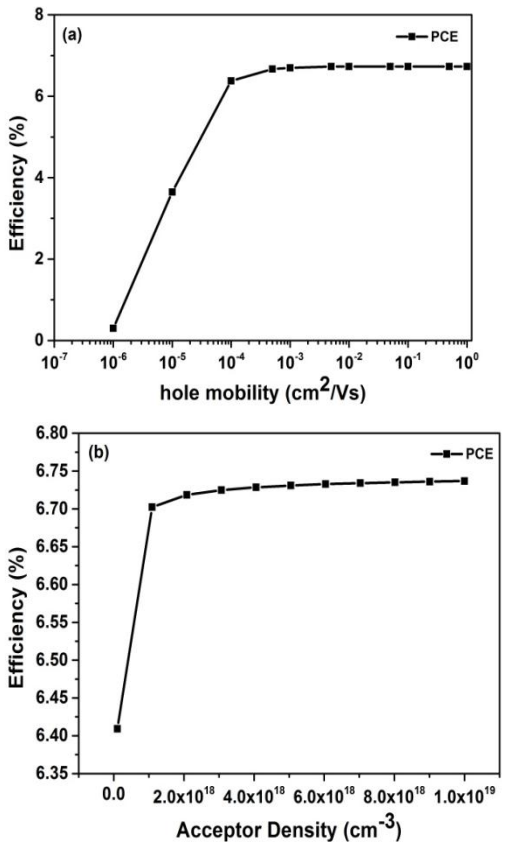

Fig. 3 – Effects of HTM layer characteristics, (a) hole mobility and (b) acceptor density, on PCE of perovskite solar cells

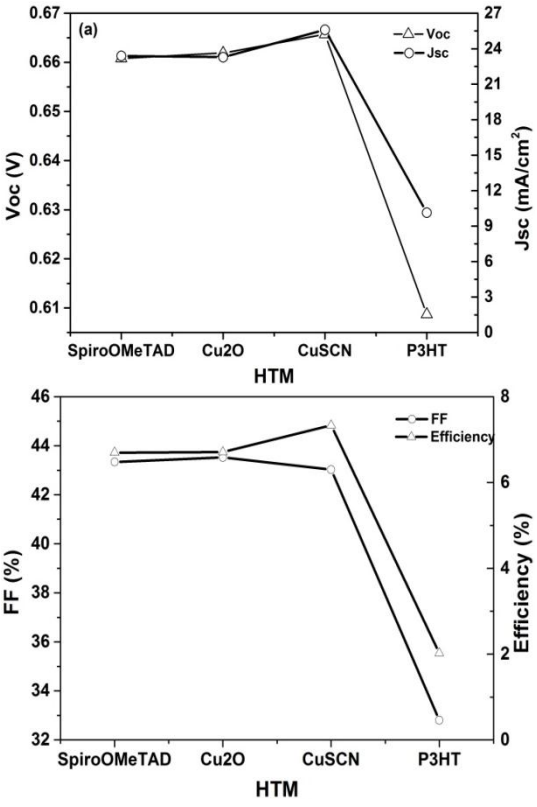

Fig. 4 – Variation of (a) Open-circuit voltage *V*oc and Short-circuit current density *J*sc, (b) Fill factor FF, and PCE as functions of different HTM.

observed that the efficiency shows a maximum saturation point (6.7 %) at hole mobility of $1 \cdot 10^{-3}$ cm²/Vs. The efficiency experienced a rise with increase of acceptor density as depicted in Fig. 3b. It has been already reported that pure Spiro-OMeTAD material has low hole mobility and low acceptor density, which causes a high series resistance and thus restrict the current in the device, leading to an undesirable performance [6]. Therefore, it is a common practice to dope the HTM with additional additives or *p*-type dopants during fabrication.

3.4 Effects of Different HTM Layer

Apart from Spiro-OMeTAD, there are many solid-state materials which are widely used as hole transport layer in dye-sensitive solar cells. Performance of these materials is also comparable with Spiro-OMeTAD as reported by many groups. In this study, several materials were selected as HTM candidates and the parameters for these materials were chosen from reported literatures introduced in the simulation. Basic cell parameters of the device for different HTM layers are represented in Fig. 4. It is noticeable that PCE of the tin perovskite solar cell with typical spiro-MeOTAD as HTM went up to ~ 6.7% which is very close to the experimentally reported [3] efficiency of $CH_3NH_3SnI_3$ solar cells (6.4%). However, it is noteworthy that CuSCN displays outstanding performance (7.33%) than other HTMs in this study. Cu_2O also exhibits better property and similar results like spiro-MeOTAD and could be considered as a good option for HTM. In addition, it can be noticed that P3HT is not a suitable candidate for tin perovskite solar cells.

It is more evident from Fig. 5 which demonstrates comparison of external quantum efficiency when different HTMs are employed in the designed model. CuSCN shows desirable results throughout the visible and near infrared region as compared to its other counterparts. The variation of efficiency as a function of defect density of absorber layer and interface layers using all HTMs are shown in Fig. 6. In case of CuSCN as HTM, it shows that the efficiency of the device remains almost constant with increase in defect density of the absorber layer whereas a drastic drop in efficiency is observed in case of P3HT as defect density exceeds $1 \cdot 10^{10}$ cm^{-1}.

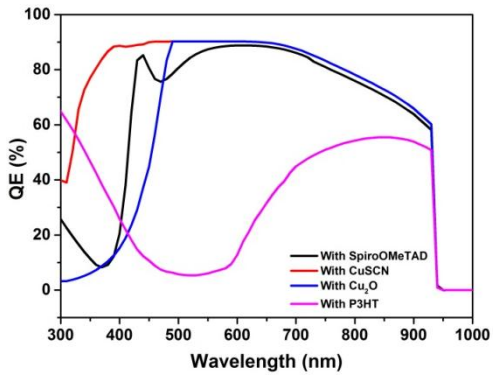

Fig. 5 – Comparison of external quantum efficiency (EQE) for different HTM

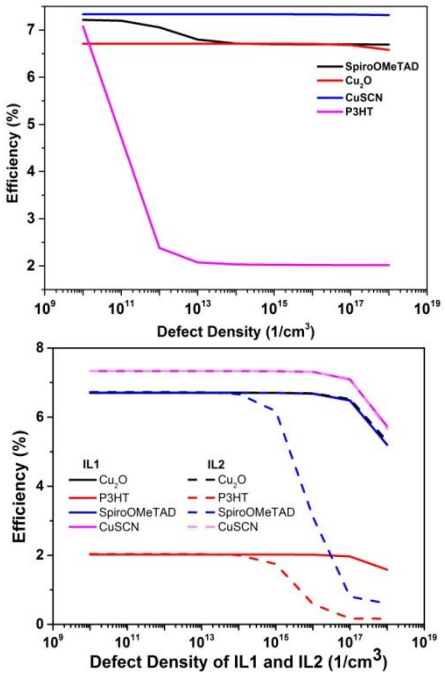

Fig. 6 – Variation of PCE as a function of defect density of HTM and interface layers (IL), IL1 and IL2.

4. CONCLUSION

The $CH_3NH_3SnI_3$ perovskite solar cell was controllably designed and simulated using SCAPS. The model was verified by comparing with solar cell performance parameters reported in literatures. Effect of absorber thickness on device property was studied and it indicated that an optimal thickness range (350-500 nm) is required for preparing efficient solar cells.Different candidates for HTM were employed and basic cell parameters were discussed. The results illuminate that the solar cells with CuSCN as a HTM can achieve relatively higher efficiency which is due to its wide bandgap, high hole mobility, good chemical stability and better chemical interaction with perovskite absorber. Moreover, it is easy to deposit through a solution-processed technique at low temperature which makes it suitable with different substrates.

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