Simulation of multi-valent defects in Perovskite solar cell using SnO_2 as buffer layer

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Abstract— **Recombination of electron in conduction band with hole in valence band through traps result in major deterioration of solar cell parameters. SRH (Shockley-read-hall) or trap assisted recombination is dominant in perovskite based solar cells. The influence of defect density on solar cell parameters is compared between TiO_2 and SnO_2 buffer layers of the proposed Ag/$CH_3NH_3SnI_3$/SnO_2/ZnO solar cell structure. The device with SnO_2 buffer layer has shown improvement of close to 10% in efficiency for the defect range considered (IE13 to 1E17 cm^{-3})**

Keywords— perovskites, defects, efficiency, buffer layer

I. INTRODUCTION

In the thin film solar cell category, perovskite based solar cells has grabbed extensive attention due to better efficiency and low cost. It is also considered as an alternative or successor to the Si based solar cells. The typical structure includes the main absorber perovskite layer with buffer and window layer on top of it [1]. In [2], lead free buffer layer is considered for low toxicity of the solar cell. In our design, lead free Ag/$CH_3NH_3SnI_3$/SnO_2/ZnO is being considered for analysis using SCAPS-1D software. $CH_3NH_3SnI_3$ perovskite solar cell with TiO_2 as buffer layer is published in [1]. However, there is no study on the influence of multi-valent defects on solar cell parameters. In this paper, we propose SnO_2 as the buffer layer or electron transport material instead of TiO_2. Further, we compare the influence of multi-valent defects between TiO_2 and SnO_2, and study the effect on solar cell device parameters such as fill factor and efficiency. We used double acceptor defects for absorber layer, double donor defects for buffer layer with a uniform density of 1E15 cm^{-3}. We also introduced interface defects at two interfaces (absorber/buffer and buffer/window) with a capture cross section of 1E-15 cm^2 and total defect density (integrated over all energies) of 1E16 cm^{-2}.

II. SIMULATION METHOD

The influence of multi-valent defects is done using solar cell capacitance simulator (SCAPS). Basically, the defect with different charge states is considered under thermal equilibrium. In this paper, double acceptor is being considered. The software solves drift-diffusion, Poisson and current continuity equations for each discrete point created in the mesh region.

III. SIMULATION RESULTS

Figure 1 shows the cross-sectional view of perovskite solar cell under consideration. The J-V characteristics obtained under AM 1.5G spectrum at 300k is shown in Fig.2. A comparison of J-V between SnO_2 and TiO_2 is done to see the influence of buffer layer on device parameters. There has been an improvement in fill factor with SnO_2 resulting in better efficiency. For the same thickness and doping, the efficiency obtained is 21.6% for SnO_2 in comparison to 19.8 % for TiO_2. Figure 3 shows the variation of fill factor with increase in thickness of absorber layer. For the thickness values below 0.7 µm, clearly the device with SnO_2 buffer layer showed superiority in fill factor as compared to TiO_2. At 0.7 µm, the fill factor values converged to be almost same for both the buffer layers. Similarly, efficiency values are plotted in Fig.4 with variation in thickness of the absorber layer. There is almost 10% improvement in efficiency at each thickness value considered. Finally, we have tabulated (Table 1) all the values for varying defect concentration with TiO_2 and SnO_2. For the defect concentration range 1E+13 to 1E+17 cm^{-3} considered, SnO_2 showed superior values of device parameters (FF, V_{oc}, J_{sc}, η) compared to TiO_2.

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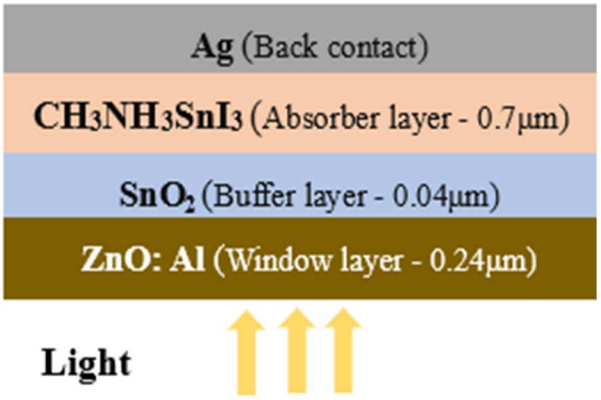

Figure 1: Device Structure

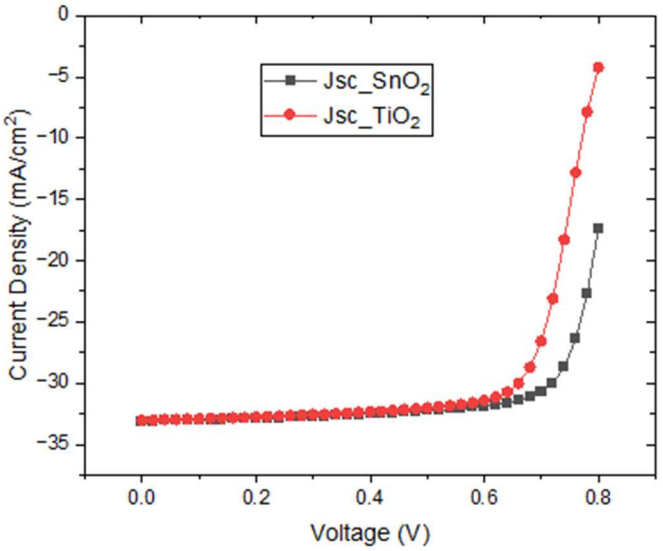

Figure 2: Comparing Current densities of SnO_2 and TiO_2 with double acceptor defects in absorber layer.

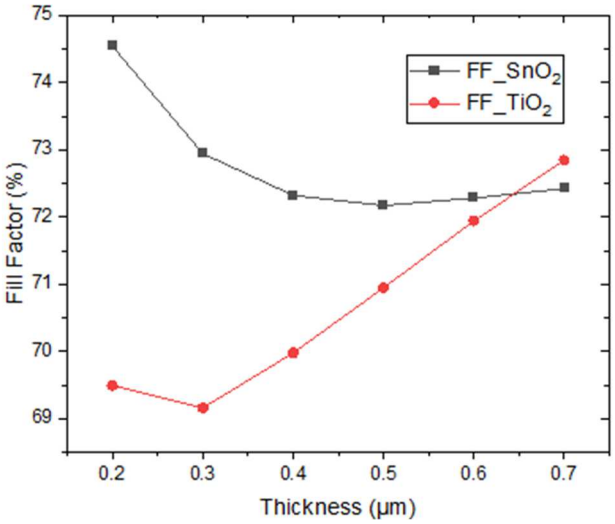

Figure 3: Comparing Fill Factors of SnO_2 and TiO_2 with double acceptor defects in absorber layer.

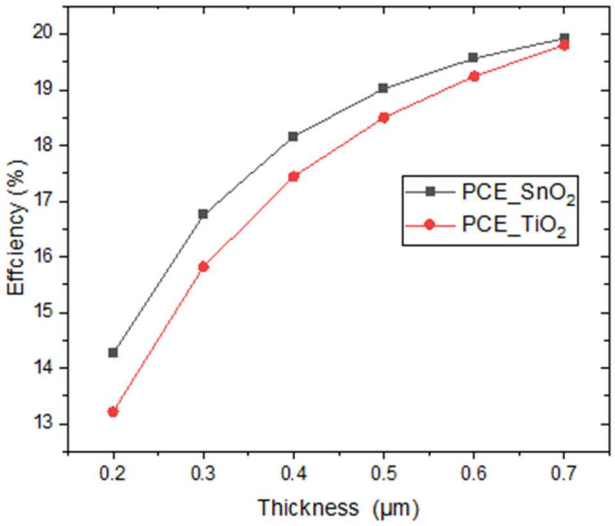

Figure 4: Comparing Efficiencies of SnO_2 and TiO_2 with double acceptor defects in absorber layer.

Uniform density ($1/cm^3$)	Voc_SnO_2 (V)	Voc_TiO_2 (V)	Jsc_SnO_2 (mA/cm^2)	Jsc_TiO_2 (mA/cm^2)	FF_SnO_2 (%)	FF_TiO_2 (%)	PCE_SnO_2 (%)	PCE_TiO_2 (%)
1E13	0.8674	0.8274	33.12	32.72	75.55	73.98	21.71	20.03
1E14	0.8631	0.8265	33.09	32.69	75.19	73.31	21.48	19.81
1E15	0.8388	0.8211	32.78	32.37	72.41	68.91	19.91	18.32
1E16	0.7896	0.7933	29.66	29.26	64.47	59.42	15.1	13.8
1E17	0.7305	0.7322	22.47	22.34	61.67	56.5	10.13	9.25

Table 1: Comparing parameters of SnO_2 and TiO_2 by varying total uniform defect density in absorber layer.

REFERENCES

[1] David Ompong , Michelle Clements 2024,pp.3

[2] Razika Zair Tala-Ighil 2021, pp. 3