Design and Performance Analysis of Perovskite Solar Cell

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***Abstract*—Searching for solar-absorbing materials comprising earth-abundant materials with chemical stability is of the critical importance of evolving photovoltaic technologies. The Mott-Hubbard type transition-metal oxides (TMOs) generally contain only earth-abundant elements and intrinsically have long-term chemical stability, which is ideal for constructing low-cost and resilient photovoltaic devices. In this study, different aspects of constituent layer parameters thickness, defect density buffer layers has been considered to identify the device performance of perovskite solar cell. An efficiency of 21.67% (with Voc of 0.93 V, Jsc of 26.65 mA/cm2 and fill factor of 0.87) has been achieved with TiO_2 based buffer layer.**

***Index Terms*—Perovskite, Mott Insulator (MI), Transition metal oxides (TMOs)**

I. Introduction

Inorganic thin film photovoltaics (PV) are mainly based on CdTe, amorphous Si or CIGS. In the newest times, hybrid organo-metal halide perovskites have appeared with noted solar cell conversion efficiencies over 21% [1]. Very lately, adding another aspect to the study of TMO, narrow-band-gap Mott insulators were proposed as encouraging solar-absorbing materials [2], [3]. The Mott- Hubbard-type TMOs usually contain only earth-abundant elements and intrinsically have long-term chemical stability, which is well suited for creating low-cost and durable photovoltaic devices. Furthermore, the Mott and charge-transfer insulators, with different compositions but similar perovskite structures, can offer band gaps which range from near infrared to ultraviolet (UV). The wide-range bandgap tunability and structure compatibility might enable multijunction solar cells to increase the solar absorption.

II. Mott insulators as an absorber

MI are materials that work as insulators while they're just predicted that should be conductors under conventional band theories. However, MI has the ability to become conductive due for instance to defects, strain and oxygen stoichiometry. This phenomenon is known as the Mott transition. Manousakis et al. [2], [3] theoretically predicted that carrier multiplication process get triggered by the the strong Coulomb interaction in Mott insulators; i.e., multiple electron-hole pairs can be efficiently produced by a single photon, thus, increasing the quantum efficiency [2], [3]. Most crucial, such Mott-insulator-based solar-harvesting devices, if realized, will integrate to many other functional TMOs in heterojunction devices and give power for driving other functionalities. For narrow-gap MI, it truly is claimed that high quantum efficiencies of such solar cells could be caused by impact ionization and generation of multiple electron-hole pairs.

Lanthanum Vanadium Oxide (LVO) can be described as a p-type semiconductor in the bulk. Along with the electron configuration of $3d^2$ (t_{2g}^2) within the trivalent vanadium cation, LVO is well referred to as a prototypical Mott insulator .The solid 3d electron-electron interaction divides the V t_{2g} band into a fully occupied lower Hubbard band (LHB) and an empty upper Hubbard band (UHB) [2], [4], within the strongly correlated electron system. The optical band gap obtained from the photoconductivity measurement is around 1.1 eV [5]. In accordance with the Shockley-Queisser limit curve [3] the band gap of LVO is at the optimal value for solar energy conversion.

III. Device Structure

The structure of the perovskite solar cell in the simulation was buffer/interface defect layer(IDL)/absorber. Table I summarizes input parameters for each layer.Here, N_A and N_D denote acceptor and donor densities, ϵ_r is relative permittivity, E_g is band gap energy, μ_n and μ_p are mobilities of electron and hole, χ is electron affinity and N_t is defect density. The presence of surface defect density at the interfaces is a specific feature of cells that must be accounted for in any physics-based model. Precise values of the physics parameters are difficult to acquire, particularly for new materials, and we assumed and collected with our very best knowledge as of this stage.

The following parameters are used in this simulation; Thermal velocity of electron and hole is 10^7 cm/s . Pre-factor A_α is 10^5 to obtain absorption coefficient (a) curve calculated by $\alpha = A_\alpha(hv - E_g)^{1/2}$. For defect analysis, defect present in absorber is double acceptor type with uniform density of $1x10^{15}$. Correlation energy of 0.2eV is used. The energy levels are present at 0.6eV and 0.4eV. Capture cross section of electron and hole are 10^{-17} cm^2 and 10^{-13} cm^2 respectively for first energy level while 10^{-15} cm^2 for the second level. Defect present in interface is same as absorber with defect density of $5x10^{16}$.

IV. Results

A. Optimization of absorber thickness

The thickness of the absorber has been varied upto $2\mu m$ to optimize the performance of the cell module. For the simula-

TABLE I
SIMULATION PARAMETERS OF PEROVSKITE SOLAR CELLS IN THIS STUDY.

Parameters	**TiO_2**	**ZnO**	**ITO**	**IDL**	**$LaVO_3$**
Thickness(μm)	0.050	0.050	0.050	0.010	0.350
N_A (cm^{-3})	-	10^5	-	3.85 x 10^{19}	3.85 x 10^{19}
N_D (cm^{-3})	10^{16}	10^{18}	10^{20}	1 x10^{19}	1 x10^1
ϵ_r	9.0	9.0	8.9	30.0	30.0
χ (eV)	3.9	4.1	4.8	4.0	4.0
E_g (eV)	3.2	3.3	3.65	1.1	1.1
μ_n (cm^2/Vs)	20	100	10	1.1 x 10^{-1}	1.1 x 10^{-1}
μ_p (cm^2/Vs)	10	25	10	1.1 x 10^{-3}	1.1 x 10^{-3}
CB density (cm^{-3})	2.2x10^{18}	4x10^{18}	5.2x10^{18}	4 x 10^{18}	4 x 10^{18}
VB density (cm^{-3})	1.8x10^{19}	10^{19}	10^{18}	10^{19}	10^{19}
N_t (cm^{-3})	10^{15}	2 x 10^{17}	10^{19}	10^{14}	5 x 10^{15}

tion, the perovskite with TiO_2 buffer layer has been verified in terms of the absorber thickness. The device modelling has been performed with and without the inclusion of mid gap defect density stress. As seen from Fig. 1 that the efficiency of the solar cell is increasing with the increasing thickness of the absorber layer. Furthermore, the thickness of absorber layer has been found $1\mu m$ optimum. From Fig. 1, at the thickness of $1\mu m$, the recorded efficiency is 29.37% and 21.67% for defect-free and defect respectively which can be seen to be optimum for higher performance in the material.

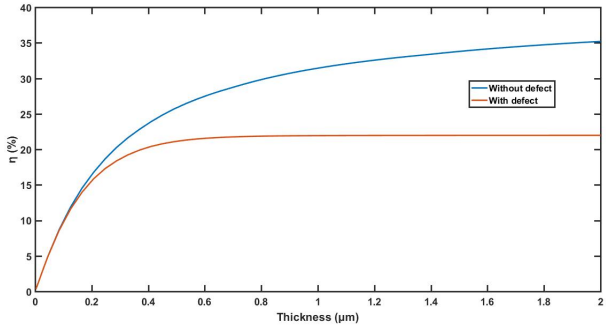

Fig. 1. Solar cell parameters of perovskite solar cells with and without defect as a function of absorber thickness.

B. Performance analysis of different buffer layers

Two buffer layers such as ITO and ZnO have been investigated besides the most frequently used TiO_2. The buffer layer thickness of 50 nm has been used as the base parameter as described in the literature. All the buffers were simulated in presence of defect in the absorber layer. Fig. 2 shows the J-V response for various buffer layers. ZnO buffer layer based cell has achieved high efficiency as 21.25%, suggesting it to be a potential replacement of TiO_2 of efficiency 21.67%. Besides ZnO, ITO buffer layer has achieved efficiencies of 17.03%. As seen from Table II, FF Of ITO is very less compared to other two buffers while having equivalent Voc and Jsc. ZnO and TiO_2 are the very promising buffer for LVO perovskite absorber.

V. CONCLUSION

We have discussed theoretical investigation of perovskite solar cell performance under illuminated behaviour For performance analysis of LVO with different buffer, three different buffers layers were used namely, TiO_2, ZnO and ITO. LVO achieved the efficiency of $\sim$29% with TiO_2 in defect-free condition at optimum thickness. Acceptor density of LVO is 3.85x10^{19} which comparatively higher than other perovskite absorbers. LVO shows band gap of 1.1 eV, and the d-d transitions between lower Hubbard band (LHB) and upper Hubbard band (UHB) and the p-d transitions between the O $2p$ band and the V $3d$ band give rise to wide-range optical absorption in the solar spectrum. TiO_2 and ZnO show the efficiency of 21.67% and 21.52% with comparatively higher results than ITO of 17.09%. These simulations results promote LVO as potential solar light absorber materials.

TABLE II
PERFORMANCE ANALYSIS OF DIFFERENT BUFFERS WITH LVO

	η (%)	Voc (V)	Jsc (mA/cm^2)	FF (%)
TiO_2	21.67	0.9347	26.65	86.97
ZnO	21.52	0.9334	26.47	87.00
ITO	17.03	0.935	26.83	69.56

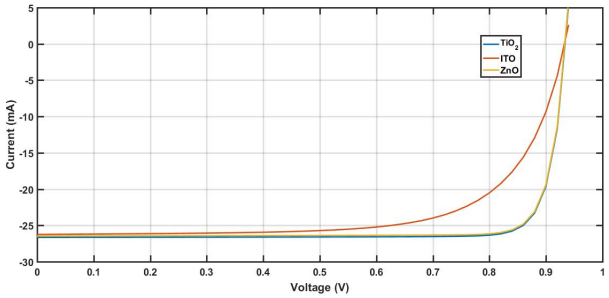

Fig. 2. Simulated J-V characteristic of perovskite solar cell calculated with different buffers.

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