Numerical Simulation of Copper Bismuth Oxide Based Solar Cells Using SCAPS-1D with WO_3 as Electron Transport Layer: Nonideal Conditions

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There are simulation studies on copper bismuth oxide (CBO) based solar cells (SCs) using SCAPS-1D. However, all are in ideal conditions which are far away from realistic values. In this work, simulation studies have been performed for thin film SCs with CBO and WO_3 as a light harvesting layer (LHL) and electron transport layer (ETL) using SCAPS 1D in nonideal conditions such as parasitic resistance, reflection losses, and recombination.

Keywords—Copper Bismuth Oxide, SCAPS-1D, nonideal conditions

I. INTRODUCTION

The renewal of energy is crucial to tackle the issues of global warming and environmental pollution. Harvesting and conversion of solar energy to electrical energy is the best choice for the renewable energy sector. Nonetheless, the industrial-level production in mono-crystalline silicon SCs still has an efficiency of limited to 22-23 % [1]. The researchers are looking for several alternative and efficient materials to replace silicon based SCs.

CBO is one of the best choices for SC application due to its band gap of 1.5 eV, good absorption coefficient, and wide range of absorption. However, low hole mobility and recombination due to a shorter lifetime are inherent problems of CBO [2]. There are few numerical studies reported to check the feasibility of CBO-based SCs and the experimental realizations have not been reported yet. The simulation is in ideal conditions are predicted a photo conversion efficiency (PCE) of 20-30% with various configurations [3,4].

Among these reports, there is a highly efficient cell with WO_3 as an ETL and CBO as an LHL [4]. In this work, explored the performance of glass/FTO/WO_3/CBO/Au SCs by applying all nonideal conditions and identified the optimized parameters to get the better performance of SCs.

II. DEVICE STRUCTURE AND SIMULATIONS

The proposed device structure is glass/FTO/WO_3/CBO/Au, and performance is analyzed using SCAPS-1D. The FTO is a window layer and Au acts as the back contact. The materials parameters are used for ideal conditions as given in Table I, and additional parameters for nonideal conditions are provided in Table II.

TABLE I. MATERIAL PARAMETERS FOR IDEAL CONDITION

Parameters	Materials		
	FTO [4]	**WO_3 [4]**	**CBO [4]**
Thickness (nm)	50	50	1000
Band gap (eV)	3.6	2.7	1.5
Electron affinity (eV)	4.0	3.8	3.72
Dielectric permittivity	9.0	4.8	34
CB effective density of states (cm^{-3})	2.2 x 10^{18}	2.2 x 10^{21}	1.2 x 10^{19}
VB effective density of states (cm^{-3})	1.8 x 10^{19}	2.2 x 10^{21}	5.0 x 10^{19}
Electron thermal velocity (cm/s)	1.0 x 10^7	1.0 x 10^7	1.0 x 10^7
Hole thermal velocity (cm/s)	1.0 x 10^7	1.0 x 10^7	1.0 x 10^7
Electron mobility (cm^2/Vs)	100	100	1.1x 10^{-3}
Hole mobility (cm^2/Vs)	25	25	1.2 x 10^{-3}
Uniform donor density N_D (cm^{-3})	1 x 10^{18}	6.35 x 10^{18}	-
Uniform acceptor density N_A (cm^{-3})	-	-	3.7 x 10^{18}
Defect type	-	Single Acceptor	Single Donor
Bulk Defect density (cm^{-3})	-	1 x 10^{12}	1 x 10^{12}

III. RESULT AND DISCUSSION

A. Ideal Condition

The performance of SCs under ideal conditions were performed by fixing the LHL thickness of 1000 nm from the previous studies [4] and the initial thickness of FTO and WO_3 fixed at 50 nm. The obtained photovoltaic (PV) parameters in ideal conditions are open circuit voltage (V_{oc}), short circuit current (J_{sc}), fill factor (FF) and PCE are 1.35V, 23.23 mA/cm^2, 89.13 %, and 27.95 % respectively. The thickness of FTO varied from 50 nm to 500 nm, and PCE decreased slightly (from 27.95 % to 27.86 %), may be due to the slight reduction of transmission in the window layer. The increase in ETL thickness from 50 nm to 450 nm improves the PCE from 27.95 % to 28.15 % due to better charge collection. Considering the material cost and fabrication process, the thickness of ETL and window layer is fixed to be 50 nm throughout this discussion.

B. Nonideal conditions

The three main losses are considered here as a nonideal condition such as the losses from parasitic resistances, reflectance, and recombination.

TABLE II. MATERIAL PARAMETERS FOR NONIDEAL CONDITION

Parameters	WO_3 [5]	CBO [6]
Carrier lifetime (ns)	0.01	32.0
Radiative Recombination Coefficient (B_r) cm^3/s	1x 10^{-7}	3.15 x 10^{-11}
Electron Auger Recombination Coefficient ($B_{auger,e}$) cm^6/s	1 x 10^{-25}	3.15 x 10^{-29}
Hole Auger Recombination Coefficient ($B_{auger,p}$) cm^6/s	1 x 10^{-25}	3.15 x 10^{-29}

1) Losses from Parasitic Resistances

There are two types of parasitic resistance present in the SCs. The first one is series resistance, which originated from contact between layers and the metal contacts and should be minimum to get better efficiency. The second one arises due to the resistance within the layer which would be the maximum for better performance.

The series resistance varied from 0 to 100 Ω the efficiency reduced drastically from 27.95% to 4.47% (Fig. 1a) mainly due to a reduction in the fill factor (FF) from 89.13% to 24.89% (Fig. 1a). The series resistance mainly affects the fill factor and hence the PCE [7]. The commercially available FTO glass has a sheet resistance of 12-14 Ω with a transparency of about 83.5% [8].

In the case of shunt resistance, which is mainly from the quality of the layer fabricated. Here, the variation of shunt resistance from 10^6 Ω to 100 Ω will reduce the efficiency from 27.95 to 13.20% and also from the FF from 89.12% to 42.84% (Fig. 1b).

The optimized series resistance and shunt resistance kept at 20 Ω from commercially available values of FTO and 10^4 Ω and corresponding to the PCE is 16.69 and 16.63%.

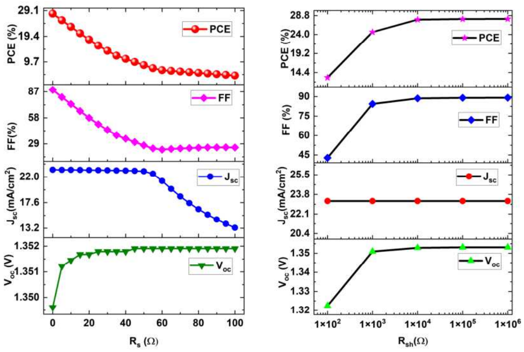

Fig. 1: PV parameters with the variation of series resistance (a) and Sunt resistance (b)

2) Reflection Losses

There are reflections in the cells due to multiple components like glass substrate, FTO coating [9], and other layers. The reflection factor alone varied from 0% to 30% and the efficiency decrement (from 27.91% to 19.37%) is from the reduction of short circuit current density from 23.94 mA/cm^2 to 16.20 mA/cm^2 (Fig. 2a). This is due to a reduction in the amount of light reaching LHL. The average reflection commercially available in FTO-coated glass is around 15% [10], therefore, reflection losses are fixed at 20 % with optimized parasitic resistance and the corresponding PCE obtained a value of 14.4%.

3) Recombination Losses

Radiative recombination and Auger are band-band recombination due to the deexcitation of electrons with the emission of photons and the de-excitation of electrons with the transfer of energy to other electrons, respectively [7]. Insertion of radiative recombination and Auger recombination, the PCE is reduced from 14.40 % to 1.05 % and 0.74 % respectively. This drastic reduction in PCE is due to the slow kinetics of copper bismuth oxide from polaron transport [2].

There is a reduction in all PV parameters with the inclusion of all these losses (Fig. 2b).

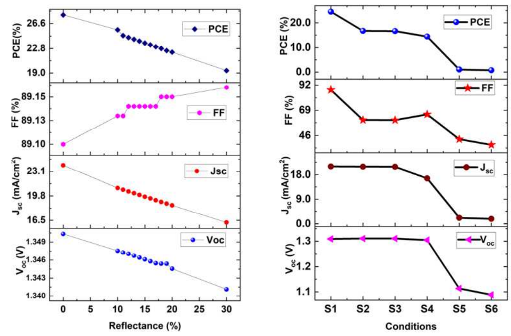

Fig. 2 (a) the PV parameters for variation of reflection and (b) introduction of various conditions S1, S2, S3, S4, S5, and S6 correspond to ideal, series resistance, shunt resistance, with reflection, radiative recombination, and Auger recombinations respectively.

IV. Conclusion

The introduction of nonideal conditions in CBO SCs revealed the actual performance of SCs. The reduction of PV parameters shows that more material modifications would be needed to achieve better efficiency in CBO based SCs.

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