EFFICIENCY ENHANCEMENT OF WSe_2 BASED SOLAR CELL WITH Sb_2S_3 AS A HOLE TRANSPORT LAYER

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Abstract—In recent years, researchers have increasingly focused their attention on tungsten diselenide (WSe_2) as a potential material for solar cell technology. This is primarily due to its exceptional properties, which make it a highly promising candidate for efficient light absorption in solar cell applications. Improving the efficiency of a novel solar cell constructed from ITO/TiO_2/WSe_2/Sb_2S_3 is the primary focus of this research. Power conversion efficiency (PCE), fill factor (FF), short circuit current (J_{sc}) and open circuit voltage (V_{oc}) are just few of the performance parameters that this research hopes to shed light on as a result of the Sb_2S_3 HTL layer. The possible impact of defect density at the Sb_2Se_3/WSe_2 and WSe_2/TiO_2 interfaces has also been investigated. At the optimal thickness of 1.0 µm for WSe_2 with a doping density of 1×10^{16} cm^{-2}, the values for V_{oc}, J_{sc}, FF and η were calculated to be 1.27 V, 24.08 mA/cm^2, 86.26% and 26.11%. this study's findings provide light on how a Sb_2Se_3 HTL can be used to boost solar cell's efficiency.

Keywords— Back suaface field, transition metal dichalcogenides, solar cell and efficiency.

I. INTRODUCTION

Semiconductor absorber materials [1-6] have made thin-film solar cells an attractive option for numerous photovoltaic device uses. The low cost of raw materials, the reliability of vacuum deposition methods, the adaptability to large-scale manufacturing processes, and the effectiveness of power conversion are just a few of the reasons for this trend. However, there are considerable obstacles to developing extremely efficient solar cells utilizing particular materials due to the scarcity of rare earth elements and worries about their toxicity [7,8]. Many important efforts have been made to improve thin-film solar cell (TFSC) photovoltaic (PV) efficiency by employing innovative absorber materials found in nature [9-11].

Transition metal dichalcogenides (TMDs) have piqued the interest of scientists due to their novel properties [12-14]. Nano-electronics, optoelectronics, and photovoltaics [15,16] are just a few of the technologies that could benefit greatly from thin films made of transition metal dichalcogenides (TMDs). Tungsten diselenide (WSe_2) has gained a lot of attention in recent years due to its potential asa light absorbing material. Thin-film solar cells can take advantage of its high carrier mobility, non-toxicity and optical absorption coefficient over 10^5 cm^{-1} [17-19], as well as its abundance in the Earth's crust. Recent years have seen a surge in atudy into WSe_2 possible use as an absorber layer in thin-film heterojunction solar cells. Tungsten diselenide (WSe_2) based thin-film solar cells (TFSCs) have had a number of different photovoltaic (PV) device architectures created and evaluated, both experimentally and numerically, in an effort to improve performance [20-23].

It has been observed that the theoretical maximum efficiencies of optimized WSSe/WS_2 and WSSe/WSe_2 solar cells are at 17.73% and 18.87%, respectively [24]. The researchers conducted a measurement to determined the PCE of ZnO/Wse_2/Au based solar cell, with ZnO serving as the buffer layer and efficiency was found to be 16.29% [25]. Solar cells with an ITO/WS_2/WSe_2 structure and a thickness of 1 m have been measured to have an efficiency of 21.20% using a different numerical methodology [26]. The conversion efficiency of the WSe_2-based photovoltaic device was shown to increase from 14.3% to 35.4% throughout a broad range of absorber thicknesses (0.1-100.0 m) [27]. It has been shown experimentally that the efficiency of WSe_2/WS_2 van der Waals heterojunction solar cell is only 2.4% [28]. The solar cell utilizing WSe_2 as the active material and SeCl as the charfe carrier achieved a efficiency of 17.1% [29].

Thin-film solar cells (TFSCs) have significantly higher photovoltaic conversion efficiencies than conventional solar cells based on WSe_2. Photo-

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generated carrier recombination at the back contact may be to blame for the poor power conversion efficiency. An interlayer between the WSe_2 material and the back contact is offered as a practical solution to these problems. Using a highly doped p-type semiconductor as the HTL is beneficial because it allows for proper band alignment and reduces carrier recombination loss at the interface between the HTL and the absorber layer [30, 31]. Another advantage of this setup is that the minority carrier is blocked from reaching the rear metallic contact by the strong electric field created at the p+-p junction. The incorporation of a p-type hole transport layer (HTL), as stated by Haider et al. [32], allows for more effective transportation of holes from the absorber layer to the metallic contact at the rear of the device. This is because to a little offset between the valence and conduction bands. Consequently, Antimony selenide (Sb_2Se_3) semiconducting materials are employed as HTL materials due to their requisite physical and electrical properties, which encompass a band gap of 1.7 eV, commendable chemical stability carrier mobility, and low toxicity [33, 34].

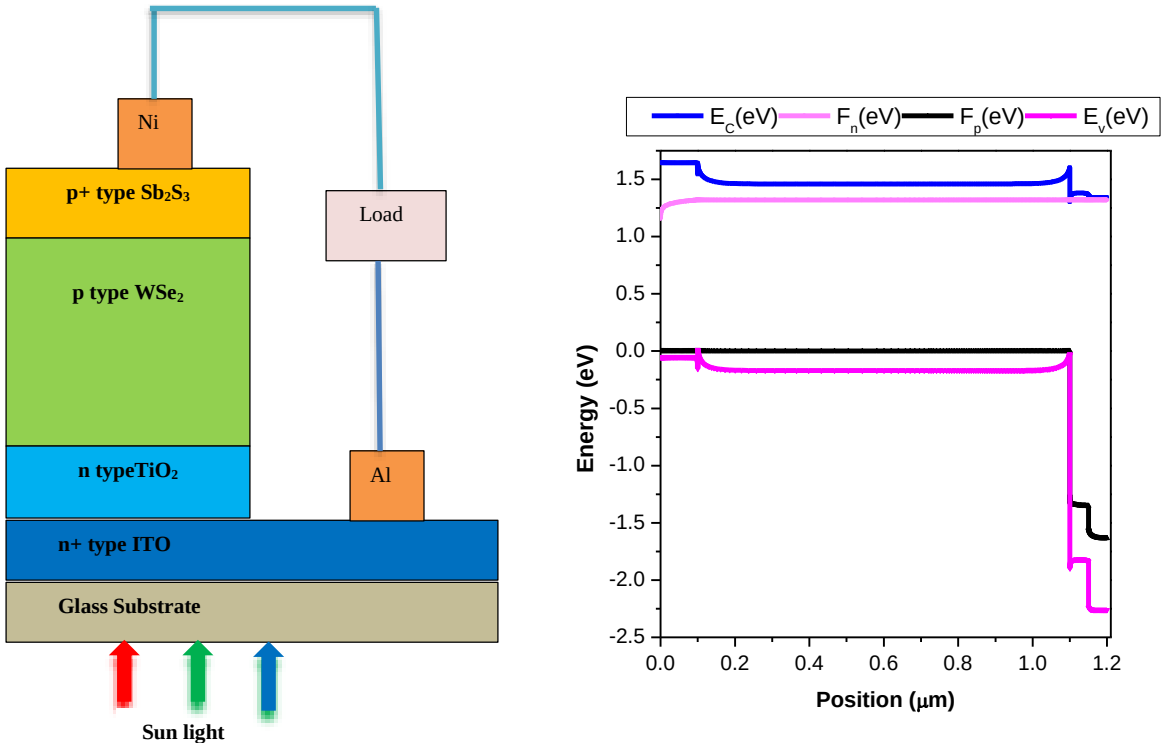
The performance parameters of photovoltaic (PV) systems, such as V_{oc}, J_{sc}, and FF, have been examined and optimised in this work to boost efficiency. In order to improve the SC's output parameters, we examine how changing the layer thickness, doping concentration, defect concentration affect the device's performance.

II. Device Structure and Simulation

SCAPS-1D software was used to investigate performance characteristics for the newly constructed ITO/TiO_2/WSe_2/Sb_2Se_3 solar cell. Desiging and simulating the gadget construction. The University of Ghent's Department of Electronics and Information Syatems' revised SCAPS-1D can simulate and analyze solar cell architectures' optoelectrical properties [35].

Band alignment and the fundamental structure of a TFSC with an Al/ITO/TiO_2/WSe_2/Sb_2S_3/Ni heterojunction are shown in Fig. 1. Here, the n- TiO_2, p- WSe_2, and p+- Sb_2S_3 layers that make up the dual heterojunction are contacted at their edges by Ni and at their faces by ITO.

The layer-specific physical properties are listed in Table 1. Table 2 shows the interface parameters for Al/ ITO/TiO_2/WSe_2/Sb_2S_3/Ni solar cell device study. With an assumen global air mass AM 1.5G solar spectrum and an operating temperature of 300K, the PV output characteristics have been determined.



(a) (b)

Fig. 1: (a) Al/ ITO/TiO_2/WSe_2/Sb_2S_3/Ni solar cell, and (b) Corresponding energy band diagram.

TABLE 1

Parameters Of Window TiO_2, Absorber WSe_2, HTL Sb_2S_3 Layers Of Proposed Solar Cell [36-38]

Layer parameters	ITO	*n*-TiO_2	*p*-WSe_2	p^+-Sb_2S_3
W (μm)	0.05	0.05	1.00	0.10
E_g (eV)	3.60	3.20	1.63	1.70
χ (eV)	4.00	4.00	3.70	3.80
ε (relative)	9.00	9.00	22.50	7.00
N_C (cm^{-3})	2.2×10^{18}	1.0×10^{19}	2.8×10^{18}	2.5×10^{19}
N_V (cm^{-3})	1.8×10^{19}	1.0×10^{19}	1.6×10^{19}	3.5×10^{19}
μ_n (cm^2 /V. s)	1×10^{2}	2.0×10^{-2}	1×10^{2}	7.00×10^{-2}
μ_p (cm^2 /V. s)	2.5×10^{1}	2.0×10^{0}	5×10^{2}	2.00×10^{-2}
N_D (cm^{-3})	1×10^{18}	1×10^{18}	0.00	0.00
N_A (cm^{-3})	0.00	0.00	1×10^{16}	1.00×10^{19}
N_t (cm^{-3})	1×10^{14}	1×10^{14}	1×10^{13}	1×10^{14}

TABLE 2

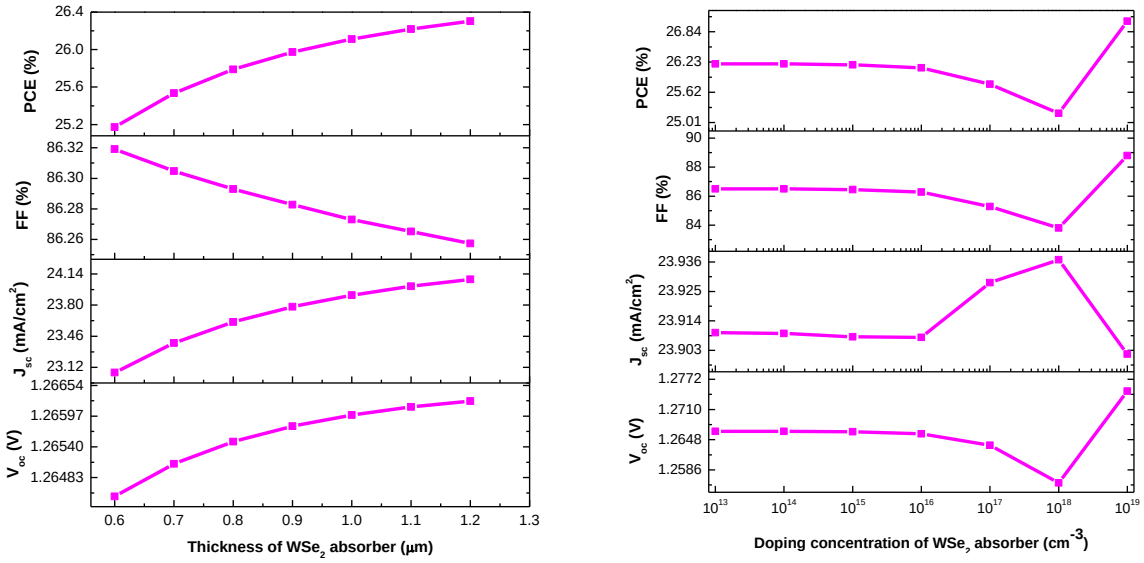
Interface Defect Parameters Of Proposed Solar Cells [38]

Interface parameters	Sb_2S_3/WSe_2 interface	WSe_2/TiO_2 interface
Defect type	Neutral	Neutral
Electrons capture cross-section (cm^{-2})	1×10^{-19}	1×10^{-19}
holes capture cross-section (cm^{-2})	1×10^{-19}	1×10^{-19}
Reference for defect energy level E_t	above the highest E_v	above the highest E_v
Energy w. r. t. reference (eV)	0.60	0.60
Total density (cm^{-2})	1×10^{11}	1×10^{11}

III. RESULTS AND DISCUSSION

A. Impact of WSe_2 thickness and carrier concentration

Fig. 2 displays the outcomes of a study into the effect of carrier concentration and WSe_2 width on PV perfoemance. The WSe_2 absorber layer's thickness was increased from 0.6 μm to 1.2 μm and its doping density from 10^{13} cm^{-3} to 10^{19} cm^{-3}. FF will decrease as the thickness of the WSe_2 absorber layer increases, while V_{oc}, J_{sc}, and η will increase as shown in Fig. 1(a). According to the results presented in Fig. 2(b), the efficiency was constant up to an acceptor concentration of 10^{16} cm^{-3} after which it dropped sharply to 25% before rising again.



(a) (b)

Fig. 2: The effect of PV parameters due to (a) thickness and (b) doping density of absorber lay

B. Effect of defect density of WSe_2 on PV performance

It is crucial to study how defect density affects various device parameters. As the peak defect density increases from 10^{11} cm^{-3} to 10^{15} cm^{-3}, the values of FF, and PCE are observed to decrease from 86.32 to 83.09 V and 26.13 to 22.22%, respectively, at a thickness of 1 µm for WSe_2 as shown in Fig. 3. As the number of defects in the bulk increases, photo-generated carriers undergo Shockley Red Hall (SRH) recombination, degrading WSe2 SC's performance.

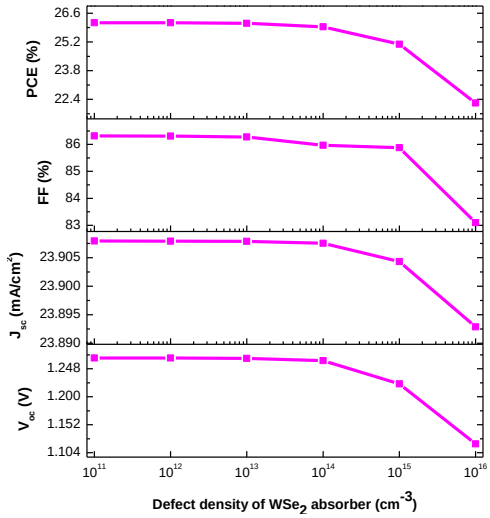


Fig. 3: Impact of defect density of WSe_2 on PV parameters.

C. Impact of Sb_2S_3 doping concentration on PV performance

Fig. 4 shows how PV characteristics change throughout a doping density range of 10^{15}-10^{21} cm^{-3} for Sb_2S_3, with the film thickness held constant at 0.1 µm. Increasing the doping concentration of HTL led to a roughly linear increase in FF and PCE from 70.77 to

86.41% and 18.59 to 26.09%, respectively, but beyond 10^{19} cm^{-3}, both FF and PCE saturate.

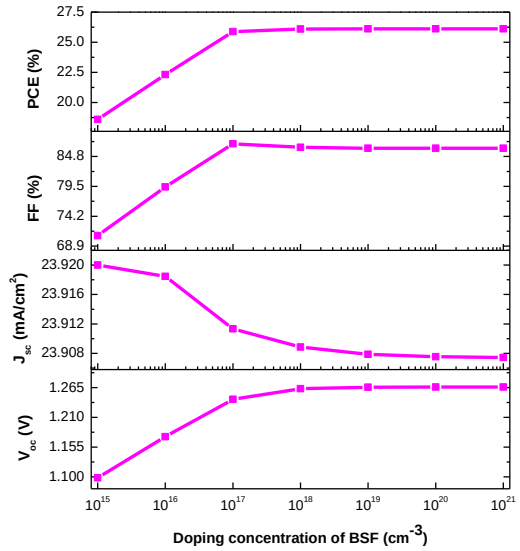
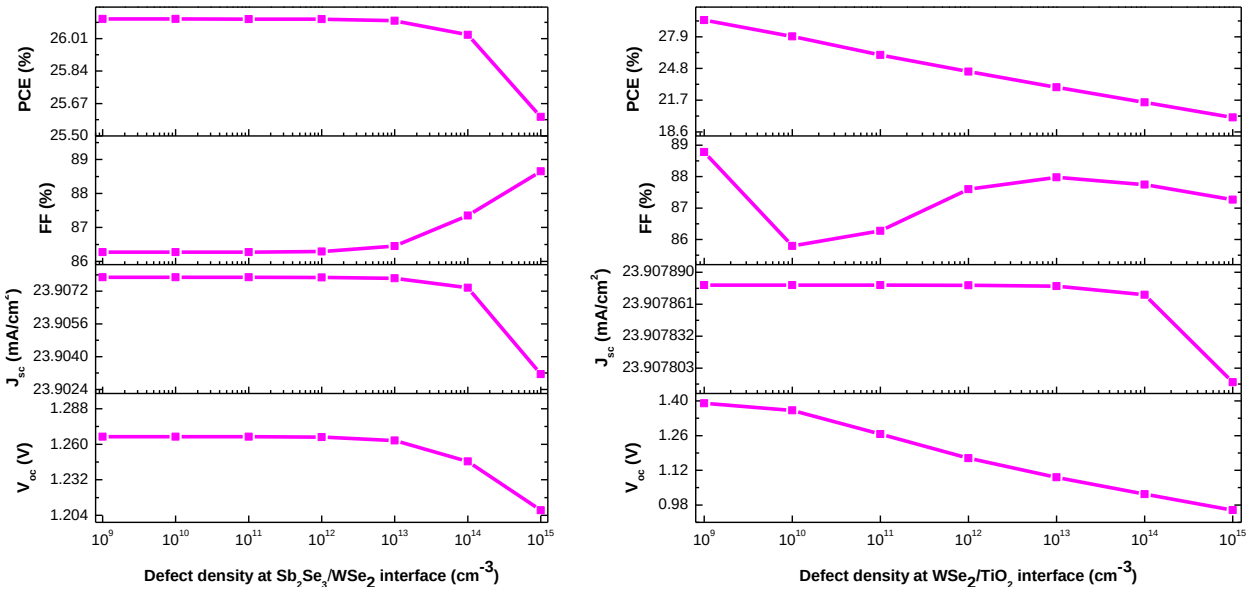


Fig. 4: Impact of the doping density of Sb_2S_3 HTL layer on PV parameters.

D. Impact of the Sb_2S_3/WSe_2 and WSe_2/TiO_2 interface defect density on PV performance

The SC's efficiency is heavily influenced by the interface states. This paper takes a comprehensive look at how defect density at the Sb_2S_3/WSe_2 and WSe_2/TiO_2 interfaces can affect performance. Nevertheless, as can be seen in the WSe_2/TiO_2 interface, the performance parameters of the SC are substantially impacted from a low value of defects all the way up to a high value of faults as can be shown in Fig. 5(b). This is in contrast to the situation at the Sb_2S_3/WSe_2 interface, where the high concentration of defects at the interface has an effect on the performance characteristics of the SC, as shown in Fig. 5(a). A decrease in cell efficiency is shown when there is a large number of flaws at the interface, as this leads to the creation of many trap centres [41].



(a) (b)

Fig. 5: Impact of defect density on PV parameters; (a) Sb_2S_3/WSe_2 and (b) WSe_2/TiO_2 interface.

TABLE 3

A Comparative Analysis Of The Performance Of WSe_2-Based Solar Cell

Research type/parameters	Device Structure	thickness of absorber layer (μm)	J_{SC} (mA/cm^2)	V_{OC} (V)	*FF* (%)	PCE (%)	Ref.
	ZnO/WSe_2/Au	2	24.75	0.88	-	16.29	[39]
	ITO/WS_2/WSe_2	5	21.77	1.19	89.38	21.20	[40]
Simulation	ITO/CdS/WSe_2/CuSCN	1.2	24.09	1.2	84.07	24.20	[38]
	ITO/TiO_2/WSe_2/Sb_2S_3	1	24.08	1.27	86.26	26.11	This work

Table 3 illustrates the progression of solar cell adchitectures utilizing WSe_2, as observed across various research groups. The current research surpasses earlier estimates of WSe_2 solar cell efficiency, revealing new design guidelines for maximising performance.

IV. CONCLUSION

This study presents a numerical simulation of a dual-heterojunction solar cell, an ITO/TiO_2/WSe_2/Sb_2S_3 structure, utilising the SCAPS-1D software. The simulation incorporates interface defects and explores the effects of varying thickness, doping density, and defects within layer. By introducing a Sb_2S_3 HTL layer into an Al/ ITO/TiO_2/WSe_2/Sb_2S_3/Ni SC, we were able to increase the PCE by 26.11%, acquire a V_{OC} of 1.27 V, a J_{SC} of 24.08 mA/cm^2, and an FF of 86.26%. Based on the results of this study, it appears that Sb_2Se_3 has the potential to improve the performance of WSe_2 based solar cells when combined with an HTL.

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