

Modeling Efficiency Loss in Sb_2Se_3 Solar Cells

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Abstract—SCAPS simulation is conducted to model effect of defects on performance of Sb_2Se_3 solar cells. Doping concentration slightly impacts short current density and fill factor, however it strongly increases Voc. Donor type traps in Sb_2Se_3 significantly reduce Voc and fill factor and fill factor reduction is more obvious than Voc reduction. Acceptor traps in Sb_2Se_3 slightly influence Voc, but fill factor and photocurrent can be obviously affected. It is acceptor type interface traps that affect photovoltaics parameters. Predicated CdS- Sb_2Se_3 solar cell has efficiency of 25.7%. Predicted Sb_2Se_3 solar cells with decreasing lattice mismatch and band offset demonstrate efficiency of 30.3%.

Keywords— Sb_2Se_3 solar cells, defect, interface states, efficiency

I. INTRODUCTION

Antimony Selenide (Sb_2Se_3) is the one of such absorber materials and has recently emerged as a promising alternative to CdTe solar cells. Except high element abundance, the constituents of Sb_2Se_3 are non-toxic and low in cost [1-2]. Like CdTe, Sb_2Se_3 is a simple binary compound with only one stable phase and stoichiometry, which is different from multivalence CuSe and SnSe binary systems [1-4]. Sb_2Se_3 exhibits a direct bandgap of 1.1–1.3 eV, which approaches the ideal Shockley–Queisser value for single-junction solar cells [7-15]. It demonstrates efficient light harvesting with an absorption coefficient of 10^5 cm^{-1} in the near-IR region up to approximately 1000 nm [4]. Sb_2Se_3 solar cells has theoretical efficiency >30% which is comparable to CIGS or CdTe solar cells [1-8]. These attributes facilitated Sb_2Se_3 solar cell recent rapid development.

In 2009, Nair et al explored the application of Sb_2Se_3 as light-absorber and reported a conversion efficiency of 0.66% [1]. Progress was stalled until 2014, Choi et al and Zhou et al obtained efficiency values of 3.21% and 2.26% respectively [2-3]. One of the greatly attractive features of Sb_2Se_3 was found by Zhou et al in 2015, which is one-dimensional crystal structure [4]. The one-dimensional crystal structure of Sb_2Se_3 decreases the number of dangling bonds at grain boundaries, which can decrease photoexcited charge-

carrier recombination losses [5]. Since then, Sb_2Se_3 thin-film solar cells was reported with a certified device efficiency of 5.6% [6]. In 2018, by improving the crystallinity of Sb_2Se_3 films, the efficiency of Sb_2Se_3 thin-film solar cells were further improved to 6.6% and 7.6% [7,8]. In 2019, the advantage of one-dimensional (1D) crystal structure is used to construct Sb_2Se_3 solar cells with Sb_2Se_3 nanorod arrays absorber, resulting in the efficiency of 9.2% [9], which provided approach to further improve this solar device performance.

Despite such progress, the path to improve Sb_2Se_3 solar cell efficiency requires significant progress on the open circuit voltage from 400mV, short circuit current density from 32.58 mA/cm^2 , fill factor from 70.3 [15]. To date, investigation of these efficiency loss mechanism is in the very preliminary stage and negligible efforts have been made, preventing Sb_2Se_3 as a high efficiency and inexpensive solar cell technology at the terawatt scale.

It is essential to understand the critical factors that cause efficiency loss of Sb_2Se_3 solar cells to improve efficiency. Herein, systematically study device physical and electronic properties of Sb_2Se_3 solar cells are conducted by SCAPS simulation, which provide new insights regarding potential mechanism of efficiency loss. In the numerical models, we analyze effect of traps in Sb_2Se_3 layer and interface states photovoltaic performance. By fitting numerical I-V simulations with I-V curves reported by [9], we established a numerical model of 9.2% CdS- Sb_2Se_3 solar cells. The simulation study explores the physical models of Sb_2Se_3 , which will form insight and a solid foundation for further optimization of the device performance and will provide new knowledge for the investigation of similar materials.

II. EXPERIMENTAL METHODS

Simulation of Sb_2Se_3 solar cells was conducted by a SCAPS-1D simulator application. It estimates J-V curves and quantum efficiency. In each layer, shallow donor or acceptor and its density are defined, and they are assumed to completely ionized and does not contribute to recombination. Defect states like donor type defect states and acceptor type defect states are introduced in the SCAPS simulator. Interface defects between

window layer and Sb_2Se_3 are also introduced in the SCAPS simulator. In the simulation, material parameters are chosen based on the reported values [1-9].

III. RESULT AND DISCUSSION

A. Acceptor and Defect States in Sb_2Se_3 Layer

According to the simulation models, shallow acceptor concentration of Sb_2Se_3 contributes doping and affects open circuit voltage, and obviously impacts photocurrent and fill factor. We simulated shallow acceptor concentration from 10^{13} to 10^{18} , shown in the figure 1. As shown, an increase in shallow acceptor density from $1 \times 10^{13}/\text{cm}^3$ to $1 \times 10^{14}/\text{cm}^3$ has negligible impact on Voc and efficiency. At the beginning of shallow acceptor density of $1 \times 10^{15}/\text{cm}^3$, Voc and efficiency are significantly increased. Voc and efficiency are increased to 743mV and 20% when shallow acceptor density is $1 \times 10^{15}/\text{cm}^3$. With shallow acceptor density of $1 \times 10^{16}/\text{cm}^3$, Voc and efficiency reach 805mV and 21.8. Furthermore, Voc and efficiency are increased by 184mV (927mV) and by 23.5% (24.7%) when shallow acceptor density increase from $1 \times 10^{15}/\text{cm}^3$ to $1 \times 10^{18}/\text{cm}^3$. As shown, an increase in shallow acceptor density slightly impacts short current density and fill factor, however it strongly increases Voc and thus efficiency.

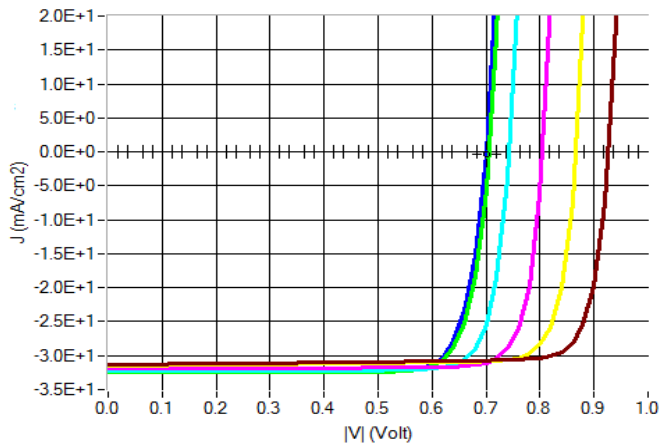


Fig.1. Simulated I-V curves of Sb_2Se_3 solar cells with doping concentration of $10^{13}/\text{cm}^3$ (dark blue curve), $10^{14}/\text{cm}^3$ (green curve), $10^{15}/\text{cm}^3$ (blue curve), $10^{16}/\text{cm}^3$ (purple curve), $10^{17}/\text{cm}^3$ (yellow curve) and $10^{18}/\text{cm}^3$ (dark red curve).

Effect of donor type traps on efficiency of Sb_2Se_3 was conducted, shown in Figure 2. Table 1 shows donor trap parameters [7] which are used to simulate. Donor type traps in Sb_2Se_3 compensate shallow acceptor doping concentration and significantly reduce Voc, fill factor and efficiency. For example, when donor trap density increases from $2.6 \times 10^{14}/\text{cm}^3$ to $1.5 \times 10^{15}/\text{cm}^3$, Voc reduced by 50mV (661mV), fill factor reduced from 76% to 54% and efficiency is reduced from 17% to 11%. Furthermore, when donor trap density beyond $1.5 \times 10^{15}/\text{cm}^3$ for example $2.0 \times 10^{15}/\text{cm}^3$, efficiency is significantly reduced to 7.3%, the major reason is fill factor reduction, where fill factor is reduced to 39% and Voc reduces only 10mV (651mV). It is possible that donor trap have deteriorated junction, demonstrated by purple color cure in figure 2. Fill factor reduction is more obvious than Voc reduction, which is major factor for efficiency reduction.

Simulation demonstrates that donor traps slightly reduce short current density Jsc. Jsc will be increased by 12% when donor traps reduce from $2.0 \times 10^{15}/\text{cm}^3$ to $2.6 \times 10^{14}/\text{cm}^3$. It emphasizes donor traps are important parameters to impact efficiency. In order to improve Voc and fill factor, it is important to reduce donor traps in Sb_2Se_3 .

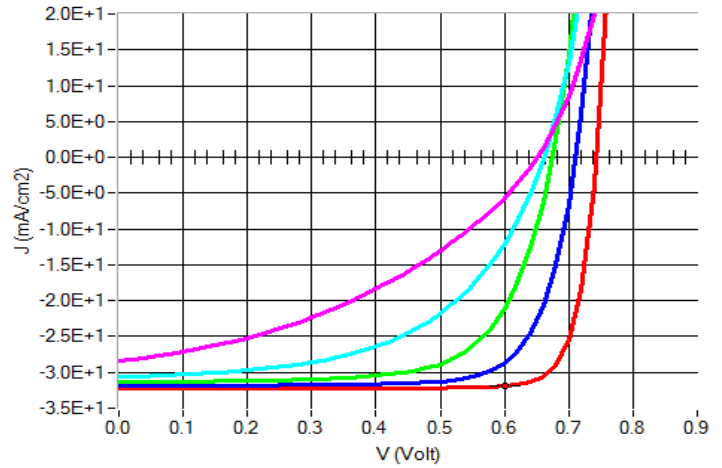


Fig.2. Simulated I-V curves of Sb_2Se_3 solar cells with donor traps of zero (red curve), $2.6 \times 10^{14}/\text{cm}^3$ (dark blue curve), $1.0 \times 10^{15}/\text{cm}^3$ (green curve), $1.5 \times 10^{15}/\text{cm}^3$ (blue curve) and $2.0 \times 10^{15}/\text{cm}^3$ (purple curve).

Table 1 Traps in Sb_2Se_3 layer

Defect type	Donor	Acceptor
Capture cross section Electrons (cm^2)	4.0×10^{-13}	1.00×10^{-15}
Capture cross section Holes (cm^2)	1.00×10^{-15}	4.90×10^{-13}
Energy distribution	Single	Single
Energy level (eV)	$\text{Ec}-0.61$	$\text{Ev}+0.71$
Nt density ($1/\text{cm}^3$)	$2.6 \times 10^{14} \sim 2.0 \times 10^{15}$	$1.1 \times 10^{14} \sim 1.0 \times 10^{15}$

Acceptor type traps were introduced to investigate their impact on efficiency. Two type acceptor traps were reported [7] and they are located with $\text{Ev}+0.71\text{eV}$ and $\text{Ev}+0.48\text{eV}$ [7]. Acceptor traps with $\text{Ev}+0.48\text{eV}$ has slightly impact efficiency when capture cross section is $1.5 \times 10^{-17}\text{cm}^2$ [7]. Simulation also shows when capture cross section is increased, the efficiency is obviously reduced even acceptor trap maintain same density. Herein we refer the result from [7] for acceptor trap cross section, and influence of cross section on efficiency is not demonstrated here. Therefore, acceptor traps with $\text{Ev}+0.71\text{eV}$

are studied and simulated curves are shown in Figure 3. Table 1 shows acceptor trap parameters [7] which are used to simulate. Acceptor traps has less impact on efficiency when compared with donor traps. Efficiency is reduced by 40% (from 18.4% to 11%), where fill factor, Jsc and Voc are reduced by 25% (from 79% to 59%), 14% (from 31mA/cm² to 27mA/cm²) and 6% (from 737mV to 691mV) respectively when acceptor traps increase from 1.1*10¹⁴/cm³ to 1.0*10¹⁵/cm³. Acceptor trap density has slight influence Voc, but fill factor and photocurrent can be obviously affected.

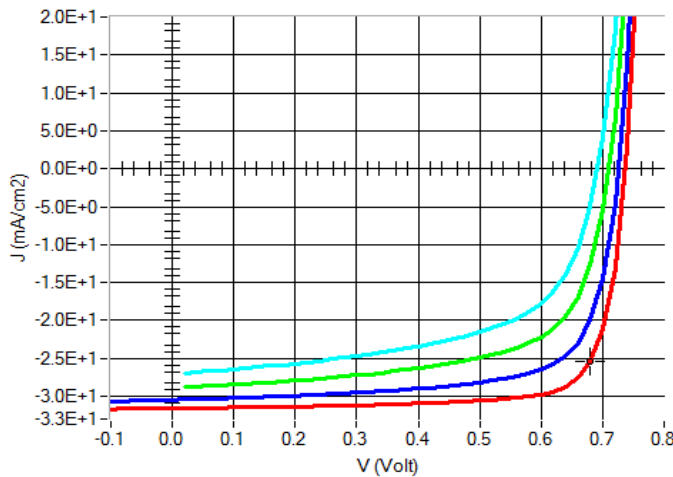


Fig.3. Simulated I-V curves of Sb₂Se₃ solar cells with acceptor traps of 1.1*10¹⁴/cm³ (red curve), 3.0*10¹⁴/cm³ (dark blue curve), 6.0*10¹⁴/cm³ (green curve) and 1.0*10¹⁵/cm³ (blue curve).

B. Interface States of CdS and Sb₂Se₃ Layer

Interface states are a key parameter which significantly impact solar cell performance. Simulation shows there is no noticeable impact of donor type interface states on efficiency. However, acceptor type interface states strongly affect solar cell efficiency. Table 2 shows acceptor type interface traps in the Sb₂Se₃ solar cells.

Table 2 Acceptor Trap in the CdS-Sb₂Se₃ interface

Defect type	Acceptor
Capture cross section Electrons (cm ²)	1.0*10 ⁻¹³
Capture cross section Holes (cm ²)	1.0*10 ⁻¹³
Energy distribution	single
Energy level (eV)	Ei+0
Total density (1/cm ²)	2.8*10 ¹⁰ ~ 6.0*10 ¹²

Figure 4 shows I-V curves of Sb₂Se₃ solar cells with acceptor type interface state traps from 2.8*10¹⁰/cm² to 6.0*10¹²/cm². When acceptor type interface traps are below 1.0*10¹²/cm², Voc and fill factor can be significantly impacted and reduction of photocurrent is insignificant. As an example, when acceptor type interface state density is reduced from 1.0*10¹²/cm² to 2.8*10¹⁰/cm², Voc is remarkably increased by 144mV (from 596mv to 740mV), fill factor is obviously increased from 68% to 82%, and thus efficiency changes from 11% to 19%.

Observed from simulation, influence of interface states on photocurrent is negligible until acceptor type interface traps are above 1.0*10¹²/cm². Under the circumstances, recombination rate via interface states is comparable with photogeneration rate, resulting in that photocurrent is greatly reduced. For example, when interface state density reaches 6*10¹²/cm², photocurrent is reduced from 31mA/cm² to 2.59mA/cm², indicating that junction has been severely deteriorated. In this case, Voc is reduced to 410mV and fill factor is decreased to 55%. Due to very low photocurrent and decreased Voc and FF, efficiency is close to 0.59%, demonstrating that Sb₂Se₃ solar cells have been exacerbated.

Hence, it is crucial to reduce interface states in order to increase all of photovoltaic parameters.

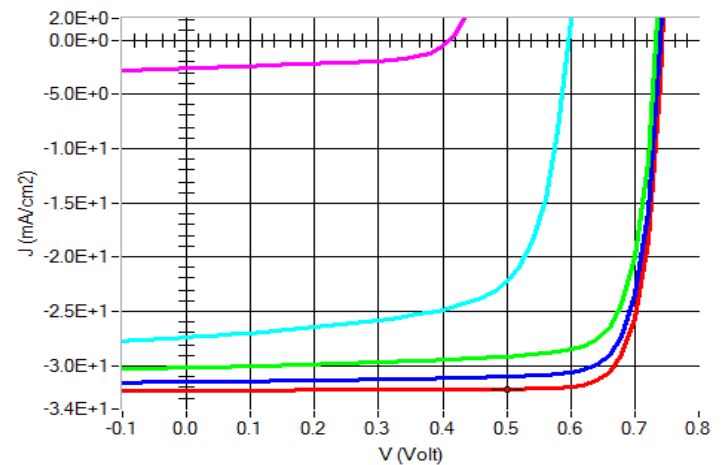


Fig.4. Simulated I-V curves of Sb₂Se₃ solar cells with acceptor type interface state traps of 2.8*10¹⁰/cm² (red curve), 1.0*10¹¹/cm² (dark blue curve), 1.0*10¹²/cm² (green curve) and 6.0*10¹²/cm² (blue curve).

C. Simulation of Reported CdS - Sb₂Se₃ Solar Cells

According to study above, I-V curves of 7.6 and 9.2% CdS-Sb₂Se₃ solar cells [7, 9] are simulated, shown in Figure 5 and 6 respectively. Donor traps, acceptor traps and interface traps are adjusted to obtain 7.6 % and 9.2% efficiency of Sb₂Se₃ solar cells.

Table 3 shows compared results of simulated and reported CdS-Sb₂Se₃ solar cells. Table 4 and 5 demonstrates parameters used to simulate the reported I-V curve of 7.6% and 9.2% CdS-Sb₂Se₃ solar cells at baseline. In order to obtain fitted curves, the donor traps, acceptor traps and interface states are adjusted to 2.6*10¹⁴/cm³, 3.0*10¹⁴/cm³ and 2*10¹⁰/cm² for 7.6% CdS-Sb₂Se₃ solar cells. Compared simulated parameter of 7.6% and

9.2% solar cells, when donor traps and acceptor traps are decreased and interface states are increased, simulated result is close to reported 9.2% solar cells. Simulated I-V curves are shown in Figure 5 and 6.

Table 3 Compared simulated and experimental CdS-Sb₂Se₃ solar cells [7, 9]

Data	Voc (mV)	Jsc (mA/c m ²)	FF (%)	Efficiency (%)
Simulation	449	27.6	62.6	7.79
Reported Experimental Data[7]	420	29.9	60.4	7.6
Simulation	414	32.5	69.1	9.32
Reported Experimental Data[9]	400	32.58	70.3	9.2

Table 4 Parameters used to simulate the reported I-V curves of 7.6% and 9.2% CdS-Sb₂Se₃ solar cell [7, 9] at baseline

Solar Cell	Layer	Trap Type	Trap Level	Trap Density
7.6%	Sb ₂ Se ₃	Donor	Ec-0.61eV	2.6*10 ¹⁴ /cm ³
	Sb ₂ Se ₃	Acceptor	Ev+0.71eV	3.0*10 ¹⁴ /cm ³
	Interface	Acceptor	Ei+0	2*10 ¹⁰ /cm ²
9.2%	Sb ₂ Se ₃	Donor	Ec-0.61eV	1.0*10 ¹³ /cm ³
	Sb ₂ Se ₃	Acceptor	Ev+0.71eV	1.0*10 ¹⁴ /cm ³
	Interface	Acceptor	Ei+0	6*10 ¹⁰ /cm ²

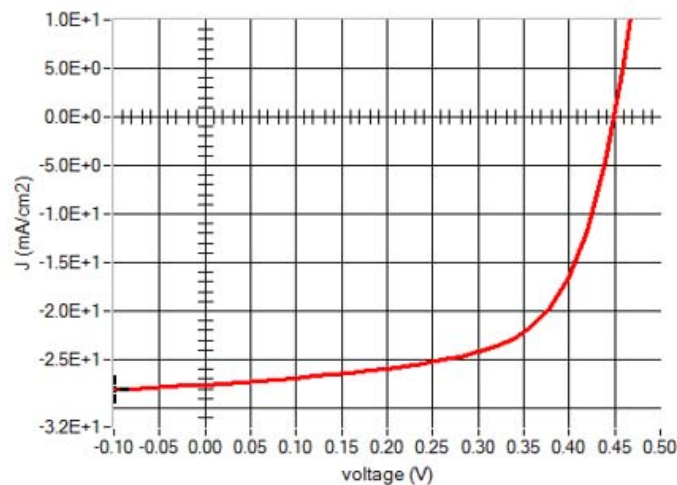


Fig. 5. Simulated I-V curves of 7.6% Sb₂Se₃ solar cells

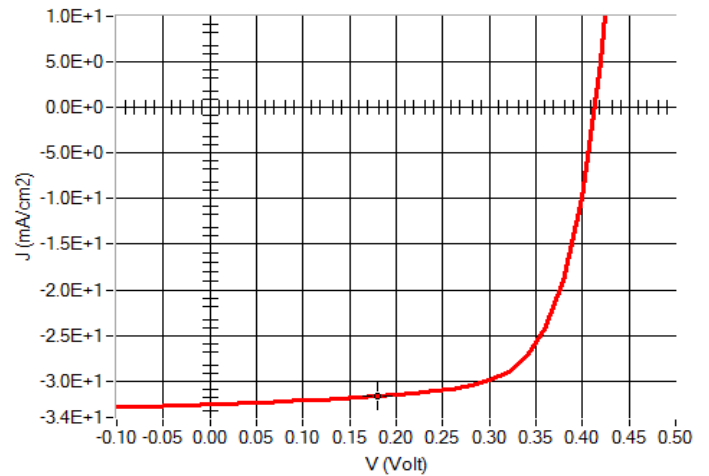


Fig. 6. Simulated I-V curves of 9.2% Sb₂Se₃ solar cells.

D. Predicted Efficiency in Sb₂Se₃ Solar Cells

From simulation model, we have found that donor traps and acceptor traps in Sb₂Se₃ layer, acceptor interface states are important factors which impact photovoltaic parameters. Thus we predicted CdS-Sb₂Se₃ solar cell performance where interface states are 1*10⁹/cm². Figure 5 shows dark and light IV curve for CdS-Sb₂Se₃ solar cell with interface states of 1.0*10⁹/cm². The solar cells generate Voc of 876mV, photocurrent of 37.3 mA/cm², fill factor of 78.6% and power conversion efficiency of 25.7%.

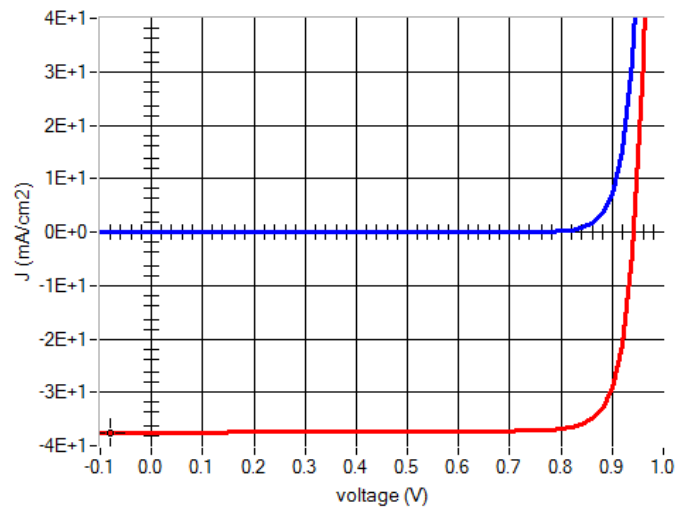


Fig. 7. Predicated dark and light I-V curves of 25.7% CdS- Sb₂Se₃ solar cells.

Thus, in order to achieve high efficiency Sb₂Se₃ solar cells, there are three important parameters which need to be considered. Firstly, CdS is toxic and has energy bandgap of 2.4eV. The window layer with large energy bandgap needs to be developed to provide high quantum efficiency and photocurrent. Lattice mismatch and band offset between window layer and Sb₂Se₃ remarkably contribute to interface

states and interface recombination. Interface recombination is one of the major causes for the loss of Voc, fill factor and efficiency. Therefore, it is important to reduce lattice mismatch and band offset between window layer and Sb₂Se₃. A new window layer (NWL) which is non-toxic, large bandgap, has low lattice mismatch and band offset needs to be searched to enhance Sb₂Se₃ solar cell performance. It could be achieved by insertion of interface layer between window layer and Sb₂Se₃.

Table 5 Predicted Photovoltaics Parameter of CdS- Sb₂Se₃ solar cell and TiO₂-Sb₂Se₃ solar cell

Simulation	Voc(mV)	Jsc(mA/cm ²)	FF(%)	Efficiency (%)
CdS-Sb ₂ Se ₃ solar cells	876	37.3	78.6	25.7
	Interface states		1*10 ⁹ /cm ²	
NWL-Sb ₂ Se ₃ solar cells	942	37.5	85.6	30.3
	Interface states		1*10 ⁸ /cm ²	

Furthermore, we predicted dark and light I-V curve of NWL-Sb₂Se₃ solar cell with interface states of 1.0*10⁸/cm². Figure 6 shows dark and light IV curve for TiO₂-Sb₂Se₃ solar cell. The solar cells will generate Voc of 942mV, photocurrent of 37.5 mA/cm², fill factor of 85.6% and power conversion efficiency of 30.3%. Ideally, the performance of Sb₂Se₃ solar cell is enhanced.

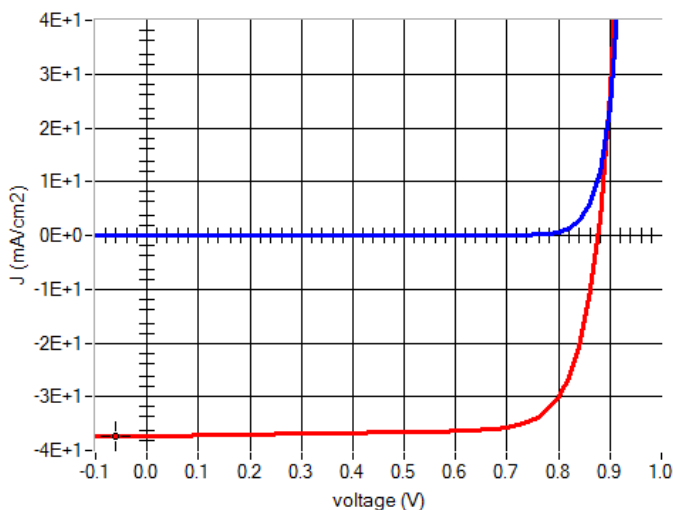


Fig.8. Predicted dark and light I-V curves of 30.3% NWL-Sb₂Se₃ solar cells

IV. CONCLUSION

SCAPS simulation is conducted to establish effect of defects on performance of Sb₂Se₃ solar cells. In the simulation model, doping concentration, donor trap and acceptor trap in Sb₂Se₃ impact Voc, fill factor and efficiency. Shallow acceptor density slightly impacts short current density and fill factor, however it strongly increases Voc and thus efficiency. Voc and efficiency are increased by 184mV and by 23.5% when shallow acceptor density increase from 1*10¹⁵/cm³ to 1*10¹⁸/cm³. Donor type traps in Sb₂Se₃ significantly reduce Voc, fill factor and fill factor reduction is more obvious than Voc reduction, which is major factor for efficiency reduction. Donor traps slightly reduce short current density Jsc. Acceptor traps in Sb₂Se₃ has less impact on efficiency when compared with donor traps. Acceptor trap density in Sb₂Se₃ has slight influence Voc, but fill factor and photocurrent can be obviously affected. It is acceptor type interface traps rather than donor type interface traps that affect efficiency. When acceptor type interface traps are below 1.0*10¹²/cm², Voc and fill factor can be significantly impacted and reduction of photocurrent is insignificant. When acceptor type interface traps are above 1.0*10¹²/cm², photocurrent is greatly reduced, indicating that junction has been severely deteriorated. Furthermore, reported I-V curves of 7.6 and 9.2% CdS- Sb₂Se₃ solar cells are simulated by adjusting donor traps, acceptor traps and interface traps to obtain fitted curves. Moreover, CdS-Sb₂Se₃ solar cell efficiency is predicted with Voc of 876mV, photocurrent of 37.3 mA/cm², fill factor of 78.6% and power conversion efficiency of 25.7%. When interface states between window layer and Sb₂Se₃ is reduced by decreasing lattice mismatch and band offset, efficiency can be enhanced. Predicated new window layer-Sb₂Se₃ solar cells with lower interface states demonstrate Voc of 942mV, photocurrent of 37.5 mA/cm², fill factor of 85.6% and power conversion efficiency of 30.3%.

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