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Simulation of Lead-free Solar Cell with SCAPS 1-D software and Effect of Charge Recombination Solar Cell Performance

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Abstract- Recombination in solar cells leads to the forfeiture of charge carriers (electrons and holes) before they engender electricity, reducing efficiency. It decreases the open-circuit voltage (Voc), increases leakage currents, and causes non-ideal diode behaviour, ultimately lowering power output and overall performance. Minimizing recombination is crucial for improving solar cell efficiency. In thin-film solar cells like CdTe, simulating a nonuniform distribution of defects shows that the effect can be approximated by using a uniform average defect density. Solar cells and their efficiency are highly sensitive to surface recombination velocity (SRV) at both the front and back surfaces, impacting critical parameters such as Isc, Voc, efficiency, and fill factor. SCAPS-1D simulation emphases on a lead-free perovskite solar cell ($CH_3NH_3SnBr_3$), integrating a layer of NiO_3 it is a hole transport layer called (HTL). Simulation Data determine the PCE Power conversion efficiency, 31.97%, and fill factor (FF) of 81.44%, with a short-circuit current density (Jsc) of 52.65mA/cm². Final finding has Voc of 0.7454V. This simulation explains that more the recombination more free charge carriers will combine in very few nanosecond, less free charges will available, to proceed solar cell out-puts. It effects concluding efficiency of solar cell device. Each type of real-life condition and parameters were simulated and noticed.

Indexterms-*Simulation, recombination, efficiency, conversion, interfaces.*

1.Introduction-

A finite difference numerical model is used in this study to examine recombination behaviour within the absorber layer of solar cells, focusing on a comparison between the constant lifetime approximation and the full ShockleyRead-Hall (SRH) model. The findings indicate that the constant lifetime assumption holds true under high defect density conditions but loses accuracy when photon flux is elevated SRV causes increased carrier recombination and the development of a dead layer, leading to significant drops in quantum efficiency, while efficiency improvements from reducing back SRV are more evident in thin cells with shallow junctions

Bulk Recombination -It occurs within a semiconductor material. Electron and holes re-join through impurities or defect. It reduces over all life-time of charge carriers.

Interface Recombination- It occurs at boundary of two materials. It leads to carrier loss and reduced device efficiency and over-all performance

1.1 **Radiative Recombination:** An electron recombines with a hole, emitting a photon. This process is significant in materials like gallium arsenide but less so in silicon-based solar cells.

1.2 **Shockley-Read-Hall (SRH):** Occurs via defect levels within the bandgap, where impurities or crystal defects trap carriers, leading to recombination and energy dissipation as heat.

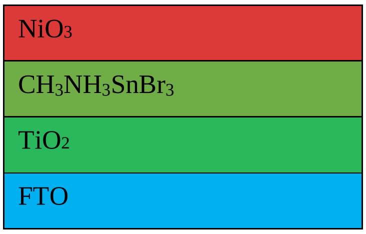
1.3 **Auger Recombination:** A non-radiative process where the recombination energy is transferred to a third carrier, which is then excited to a higher energy state.

Including recombination centres, reduces carrier lifetime. increased Recombination will cause more charge carriers lost before generating electricity. Reduces time for electrons to reach the circuit and effects power output of solar cell. Fewer charge carriers contribute to current thus decreased Efficiency is noted. Recombination in solar cells leads to the loss of charge carriers (electrons and holes) before they generate electricity, reducing efficiency. It decreases the open-circuit voltage (**Voc**), increases leakage currents, and causes non-ideal diode behaviour, ultimately lowering power output and overall performance. Minimizing recombination is crucial for improving solar cell efficiency.

2.**Literature Review-**

Numerical simulations using tools like SCAPS-1D (solar cell capacitance simulator) is developed at University of GENT, (ELIS), Belgium. It provides insights into optimizing PSC performance by investigating numerous parameters [1]. Simulations consist of tunnelling, optics, recombination, heat-flow, voltage control, defect density, thickness of absorber layer etc. It provides results by solving Poisons equation and continuity equation for electrons and holes [2]. This, advanced tool is required to promote energy independence so that green-house gases and environmental pollution can be controlled [3]. Green energy helps us to reduce acid rain and ozone layer depletion [4]. Along with limitless and renewable source of energy [5]. At present China, US, Japan are the countries in solar energy at a very large scale only China contributes up-to 37% of it [6]. Installation increment will improve energy sector as well employment, world-wide and it'll help in sufficient development [7]. In last few decades major dedicated work has been done to progress the solar cell efficiency by various changes. These changes include almost every parameter [8]. These parameters are defect density, temperature, recombination of charge carriers, recombination type, resistance, thickness etc. [9]. Various required changes results into more ecofriendly solar cells of greater efficiency [10]. Doping density is a major parameter which effects performance [11]. These defects can act as recombination centres, negatively impacting the performance of the solar cell by increasing charge carrier losses [12]. Bulk Defects also called Crystal Defects, which Includes vacancies, interstitial atoms, and dislocations in the crystal structure. Recombination in semiconductors occurs at a rate given by $\Delta n/\tau$, where τ is the average lifetime of charge carriers. This lifetime represents the typical duration an electronhole pair exists before recombining. While they are alive, carriers are in motion and can travel a certain distance, referred to as the diffusion length L. This length is determined using the relation L=· Dτ, with D being the diffusion coefficient. The diffusion length plays a vital role in determining how effectively a solar cell can collect and convert charge carriers.[13]. It is very Common in polycrystalline silicon due to grain boundaries. Surface Defects are the defects which arise due to unsaturated bonds and leads to high surface recombination rates, affecting efficiency [14]. Interface Defects is found at junctions between different materials (e.g., silicon and passivation layers) and responsible for charge trapping and increased recombination rates. Another is ImpurityRelated Defects caused by contamination from metals (e.g., iron,) during the process of manufacturing. Maintaining low defect densities and appropriate absorber thicknesses are essential strategies for enhancing the stability and performance of perovskite solar cells [15]. However, here are 4 layers Electron transport layer is TiO_2, with Hole transport layer is nickel oxide, NiO_3. Absorber layer is methyl ammonium tin tetra bromide $CH_3NH_3SnBr_3$. Recombination of charge carrier is responsible for lowering efficiency of solar cell [16]. PSC has hysteresis mainly due to mobile ion and recombination which takes place near interfaces [17]. Interface defect densities are probably higher than bulk junction layers [18] Both the recombination plays role in reducing the final efficiency of solar cell [19]. Non-radiative recombination is called when an electron or hole is trapped in impurity and then recombine with opposite one [20]. Density of trap states, density of mobile ions and degree of hysteresis are directly and closely related to each other [21]. Photos which are freely available, are responsible for the final efficiency [22] but if freely available charges recombine it effects the efficiency. To over come this difficulty, material of solar cell must be carefully selected [23]. Other than these thickness plays an important role in efficiency increment and decrement [24]. It, was also observed during simulation that defects and defect density are equally important in solar cell performance because as defects or defect density increases, traps for charge carriers and recombination rate increases, which leads to a sharp fall in efficiency [25].

3.**Materials –** An organic solar cell is being simulated here. This is free of lead impressions.



3.1 **NiO_3– (Nickle oxide)-** Hole Transport Layer, it transports holes and blocks electron mobility. NiO_3 has a stable crystal structure and good chemical stability. For p-type dopant carbon nano-tubes are also admired but it has some degree of parasitic absorption. It has outstanding electrical and magnetic properties along with optical characteristic. This is also chemically stable.

3.2 **TiO_2- (Titanium oxide)-** Transport Layer-it has low electron mobility and high density of holes or vacant sites. Efficient and stable. It has very important role in solar cell performance. It is doped at the top of solar cell. TiO_2 works as a quite stable ETL for earlier studies as well. TiO_2 is chemically stable with high refractive index. It has no toxicity.

3.3 **$CH_3NH_3SnBr_3$- (Methyl ammonium tin tetra bromide)-** Layer to be fabricated. It works as absorber layer which absorb photons of sunlight and create photocurrent. We can say it is the core part of thin film solar cell. $CH_3NH_3PbBr_3$ a good light harvester. but here we are replacing Pb by Sn to make it toxicity free but with better efficiency. With different $CH_3NH_3\mathbf{X}Br_3$ quite high and stable efficiency were calculated in past researches. Very important and required changes have been done in last some years to achieve good power conversion efficiency and long-life span of solar cells. Activation energy

is very lower than other compared compounds. It has direct bandgap along with high carrier mobility. Long diffusion length of charge carrier is responsible for efficient charge collection in system.

3.4 **Fluorine-doped tin oxide (FTO)** functions as the transparent conductive substrate in solar cells. It is optically transparent and mechanically robust, playing a crucial role in preventing charge leakage. Organic polymers used in conjunction with FTO typically exhibit intrinsic structural disorder, resulting in broad absorption spectra, which contribute to improved photovoltaic performance. It shows good optical transparency in visible region.

4.Mechanism of recombination-

Recombination mechanisms—processes where electrons and holes annihilate each other. It's a critical factor influencing efficiency. The primary recombination types include. A process where a free electron and hole combine and annihilate each other, and reduces efficiency. It involves electron dropping from the conduction band to valance band, filling the hole and releasing photons. More the free chargers available for more time more will be the recombination and less will be the effect the final efficiency.

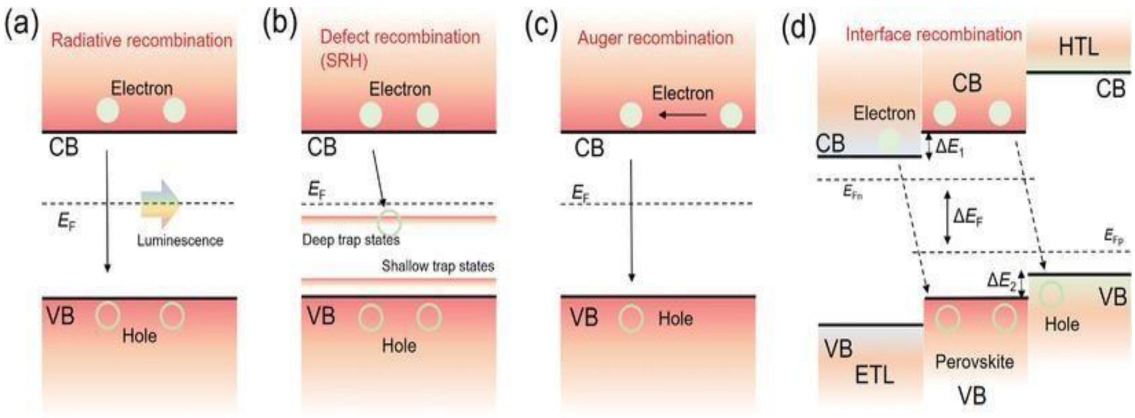


Fig-2 Recombination Mechanism (source-Research Gate)

5.Methods-

Software SCAPS1-D, a simulation tool, developed at University of Gent, Electronics and information System (ELIS), Pietersnieuwstraat, GENT, Belgium. SCAPS stand for Solar cell Capacitance Simulator. SCAPS also include j-v characteristics, spectral response, c-v and c-f defining outputs and graphs for each output.

Fig. 1 Software set-up Over view

Different layers have different thickness according to required results. Temperature was kept 300-310k

6.Results-

Different doping concentration of layers was simulated and result was noted. For efficiency achieved during simulation different parameters were changed multiple times and following are those which

Properties	**NiO_3**	**$CH_3NH_3SnI_3$**	**TiO_2**	**FTO**
Thickness (nm)	1.350	0.450	1.650	0.450
Bandgap (eV)	1.160	1.000	1.000	1.600
Electric Affinity (eV)	4.600	4.600	4.500	4.500
Dielectric Permittivity	9.000	9.000	9.000	10.000
CB Effective DOS (cm^{-3})	10_{19}	10^{19}	10^{19}	10^{19}
VB Effective DOS (cm^{-3})	10^{19}	10^{19}	10^{19}	10^{19}
Thermal Velocity of electron (cm/s)	10^{17}	10^{17}	10^{17}	10^{17}
Thermal Velocity of hole (cm/s)	10^{17}	10^{17}	10^{17}	10^{17}
Electron Mobility (un)	$5 \cdot 10^1$	$5 \cdot 10^1$	$5 \cdot 10^1$	$5 \cdot 10^1$
Hole Mobility (up)	$5 \cdot 10^1$	$5 \cdot 10^1$	$5 \cdot 10^1$	$5 \cdot 10^1$
ND (Donor Density) (cm^{-3})	10^{14}	10^{15}	10^{15}	10^{17}
NA (Acceptor Density) (cm^{-3})	10^{17}	10^{16}	10^{15}	10^{16}

Table-1 (Refence-12)

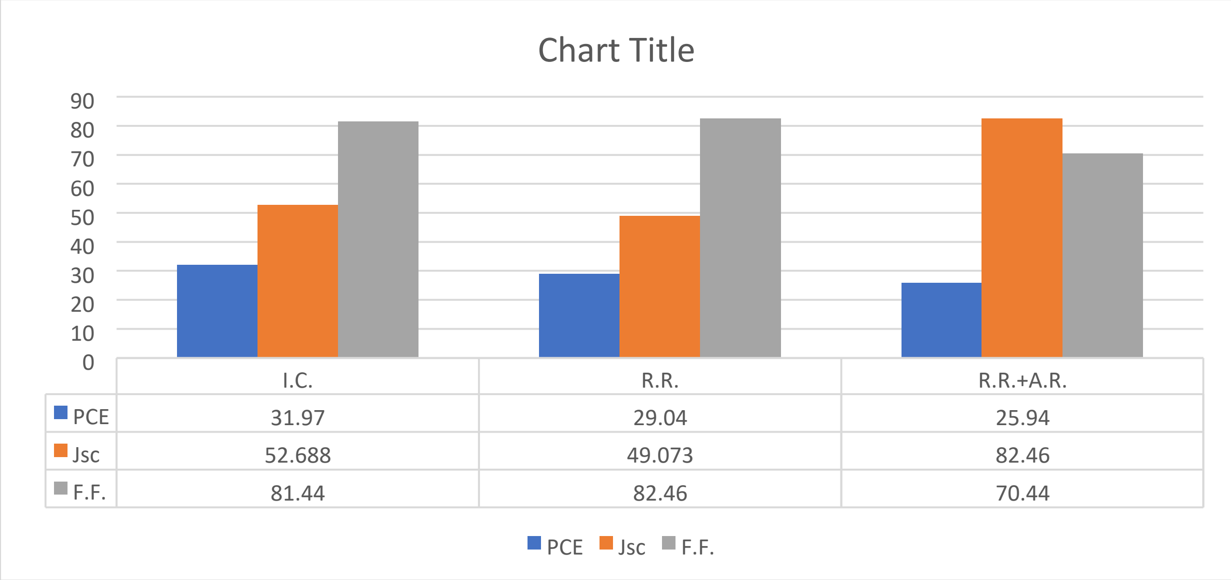
Table -1 shows different parameters like thickness, bandgap, electron and holes velocity, their mobility, along with donor and acceptor density of this simulation. When simulation is performed following results are recorded.

Steps	**Voc (V)**	**Jsc (mA/cm^2)**	**FF %**	**PCE %**
Ideal condition	0.7454	52.658	81.44	31.97
Applying radiative recombination	0.732	49.073	82.46	29.04
Applying auger +radiative recombination	0.727	50.63	70.44	25.94

Table-2

Table 2 shows that in ideal conditions, quite good results of FF, Jsc, PCE and Voc. When radiative recombination is applied all the factors were seen with sharp fall. In this table it is clearly seen when both auger and radiative recombination are applied more decrement was noticed.

Let us understand with graphical presentation.



Here I.C. describes Ideal condition, R.R. is Radiative recombination and R.R.+A.R. is radiative recombination along with auger recombination. Along with ideal condition simulation operated, the results were quite satisfactory, but introducing radiative recombination lowers down the over-all performance. And moving to combined recombination it reduces the performance more as shown in graph.

7.Conclusion- Whether it is interface or bulk recombination, recombination lowers device performance. However, the primary objective of this simulation is interface recombination, that is examined with multiple settings and analysis. Efficiency was 31.97%, fill-factor was 81.44%, and Jsc was 52.65mA/cm2 when recombination was prohibited. However, when both types of recombination were included in layers, the efficiency reduced to 25.94%, fill-factor was 70.44%, and Jsc was 50.63. Which, makes it very evident that recombination or letting free charges combination would ultimately result in lower free charge available within the gadget. The current in the solar cell is caused by these free charges. The major output or current will increase as the free charge exertion increases. Poor material selection, doping errors, contaminants, and numerous other factors can all lead to recombination. Poor efficiencies are recorded due to high recombination loss. Not just recombination always responsible for efficiency but thickness, temperature and defect density also affect the final efficiency.

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