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Original Article

Simulation of Solar Cell using SCAPS 1-D and Effect of Defect Density on Lead-Free Solar Cell Performance

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Abstract *- Perovskite Solar Cells (PSCs), recognized as third-generation photovoltaic devices, offer significant commercialization potential due to their impressive Power Conversion Efficiencies (PCE). Challenges such as limited stability and performance degradation over time persist. Numerical modelling, performed using SCAPS1-D, identified the defect tolerance levels in the absorber and other layers present in a solar cell. Increasing the defect density directed to a substantial decline in PCE from 29.04% to 25.94%. Simulations estimated the impacts of metal type, material, and its acceptor or donor densities in the electron transport layer, providing deeper insights into the correlation between defect mechanisms and PSC performance along with free charges of the active layer. During simulation, the total defect density of the CH3NH3SnI3/FTO interface increases, and efficiency falls to 25.94% from 29.04%. and fill factor reduced to 75.5% from 84.42%. The thickness of the absorber layer used is 0.450 um. The less defect density, the more efficient the solar cell will be.*

Keywords *- Simulation, Defect density, Charge carrier, Efficiency, Fill factor, PCE.*

1. Introduction

All types of defects can act as recombination centres, negatively impacting performance by increasing charge carrier losses. Bulk Defects also Include vacancies, interstitial atoms, and dislocations in the crystal structure. It is very common in polycrystalline silicon due to grain boundaries. Surface defects arise due to unsaturated bonds and lead to high surface recombination rates, affecting efficiency. Interface Defects are found at junctions between different materials (e.g., silicon and passivation layers) and are responsible for charge trapping and increased recombination rates. Another is impurity-related defects caused by contamination from metals (e.g., iron) during the manufacturing process. Maintaining low defect densities and appropriate absorber thicknesses are essential strategies for enhancing the stability and performance of perovskite solar cells.

2. Literature Review

Numerical simulations using tools like the Solar Cell Capacitance Simulator (SCAPS-1D) are developed at the University of GENT (ELIS), Belgium. It has provided insights into optimizing PSC performance by examining various parameters [1]. Simulations of this tool include tunnelling, optics, recombination, heat flow, voltage control, defect density, thickness of absorber layer, etc. For electrons and holes, it provides results by solving the Poisons equation and continuity equation [2]. This type of advanced tool is required to promote energy independence to control greenhouse gases and environmental pollution [3]. Green energy helps us reduce acid rain and ozone layer depletion [4], along with limitless and renewable energy sources [5]. At present, China, the US, and Japan are the countries that use solar energy on a very large scale. Only China contributes up to 37% of it [6]. Installation increment will improve the energy sector as well as employment worldwide and help in sufficient development [7]. Recently, foremost efforts are introduced to progress the efficiency of solar cells by various changes [8]. These parameters include defect density, temperature, recombination of charge carriers, thickness, etc. [9]. Various required changes result in more eco-friendly solar cells of greater efficiency [10]. Doping density is a major parameter that affects performance [11]. Defect density- in solar cells refers to the number of structural or electronic defects present per unit area or volume of the semiconductor material. Temperature also influences efficiency [12]. But here, doping, defect density, and recombination are discussed in detail. Doping density controls changing electric field intensity and, thus, efficiency also [13]. By increasing total defect density, all types of defects present in the layer contribute to the fill factor, and PCE decreases [14]. It can be considered that techniques recently developed for better morphological and compositional properties are helpful in solar energy progression [15]. According to a study, phosphorus can improve conversion efficiency by up to 0.19% [16]. But above all, it is required that a solar cell has low VOC and better PCE and is non-hazardous and non-toxic in nature. It must be safe ecologically [17]. Lead-free solar cells are

safe, non-toxic, and easy to install. Interface recombination should be eliminated. Because interface defects and recombination results in misaligned energy, this energy reduces PCE [18]. As defect density shows a pronounced decrement in PCE [19]. However, there are 4 layers Electron transport layer is TiO_2, the Hole transport layer is nickel oxide, NiO_3. The absorber layer is methyl ammonium tin tetra bromide $CH_3NH_3SnI_3$. Defect density and recombination of charge carriers are responsible for lowering the efficiency of solar cells. This mechanism becomes more significant at high carrier concentrations [20].

3. Material and Method

An organic solar cell is being simulated here. This is free of lead impressions.

NiO_3
$CH_3NH_3SnI_3$
TiO_2
FTO

NiO_3– (Nickle oxide)- Hole Transport Layer blocks electron mobility and transports holes. It has a firm crystal assembly and upright chemical stability. For p-type dopant TiO_2- (Titanium oxide)-Electron Transport Layer-it has low electron mobility and high density of holes or vacant sites.

Efficient and stable. It is doped at the top of the solar cell and works as a stable ETL. $CH_3NH_3SnI_3$- (Methyl ammonium tin tetra bromide)-Layer to be fabricated. With different CH_3NH_3**XI**$_3$ quite high and stable efficiency were calculated in earlier research data.

Software SCAPS1-D, a simulation tool, developed at the University of Gent, Electronics and Information System (ELIS), Pietersnieuwstraat, GENT, Belgium. SCAPS stands 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.

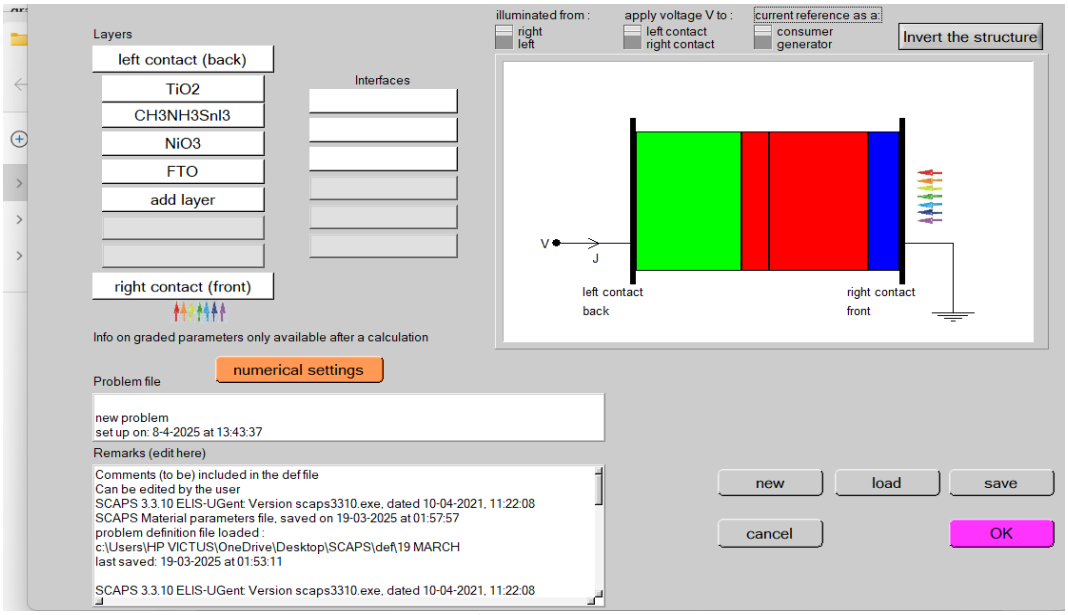

Fig. 1 Software setup overview

Table 1. Key material properties of NiO_3, $CH_3NH_3SnI_3$, TiO_2, and FTO

Properties	NiO_3	$CH_3NH_3SnI_3$	TiO_2	FTO
Thickness (um)	1.350	0.450	1.650	0.450
Bandgap (eV)	1.160	1.000	1.000	1.600
Electric Affinity	4.600	4.600	4.500	4.500
Dielectric Permittivity	9.000	9.000	9.000	10.000
CB Effective DOS	1.000E+19	1.000E+19	1.000E+19	1.000E+19
VB Effective DOS	1.000E+19	1.000E+18	1.000E+19	1.000E+19
ETL (Electron Thermal Velocity)	1.000E+7	1.000E+7	1.000E+7	1.000E+7
HTL (Hole Thermal Velocity)	1.000E+7	1.000E+7	1.000E+6	1.000E+7
Electron Mobility	5.001+1	5.002+1	5.000+1	5.001+1
Hole Mobility	5.000+1	5.001+1	5.001+1	5.000+1
ND (Donor Density)	1.000+14	1.000+15	1.000+15	1.000+17
NA (Acceptor Density)	1.000+17	1.000+16	1.000+15	1.000+14

4. Result

During the simulation, all the parameters were simulated using appropriate approaches. The temperature fluctuated a number of times, but it was observed that 300K was the best for solar cell efficiency. All the parameters are defined in Table 1.

When the simulation is done for the total defect density of the $CH_3NH_3SnI_3$/FTO interface, it is increased from 1.00E+10 to 100E+18, and efficiency falls to 25.94% from 29.04%. and fill factor reduced to 75.5% from 84.42%.

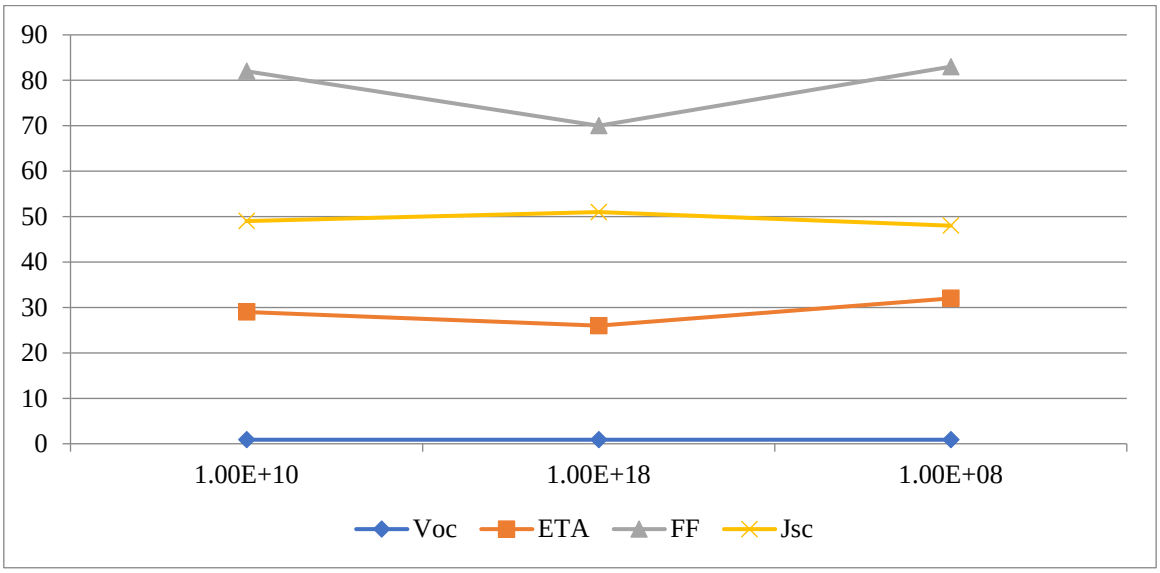

Fig. 2 Defect density graph

5. Conclusion

Optimizing recombination can inadvertently increase losses through other channels. This occurs because reducing recombination at one site raises the overall concentration of free charge carriers, leading to higher absolute losses elsewhere. This interaction underlines the complexity of solar cell optimization. Higher-purity materials can be used to reduce bulk defects for defect density. Passivation of layers can help lower the surface recombination. It is observed that optimized fabrication minimizes impurities and grain boundaries and reduces defect density, which is crucial for improving the efficiency and reliability of solar cells. When the $CH_3NH_3SnI_3$/FTO interface's total defect density increases from 1.00E+10 to 100E+18, efficiency falls to 25.94% from 29.04%. and fill factor reduced to 75.5% from 84.42%. The thickness used for the absorber layer is 0.450 um. Removing defects and defect density is practically impossible, but reducing it can make a solar cell more efficient. Moreover, this simulation is done on lead-free material, so it is safer and less toxic to nature.

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