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PERFORMANCE ANALYSIS OF LEAD-FREE SOLAR CELL IN DIFFERENT THERMAL CONDITIONS USING SCAPS 1-D

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ABSTRACT
This simulation is performed with SCAPS-1D (Solar Cell Capacitance Simulator-one-dimensional) and discusses the major parameters affecting solar cell performance. The SCAPS-1D solves equations for charge transport, recombination, and electrostatics, allowing optimization of photovoltaic device structures. Important factors such as temperature, defect density, doping concentration, series and shunt resistance, and layer thickness influence short-circuit current density (J_{sc}), open-circuit voltage (V_{oc}), fill factor (FF), and efficiency are discussed. Solar cells encounter various challenges such as limited stability and toxicity, still they offer several advantages. To mitigate the toxicity associated with lead (Pb), some alternatives which are less harmful like tin (Sn) are being explored. In this study, effective electron transport layers (ETLs) and hole transport layers (HTLs) are being studies that can be used to develop efficient Sn-based PSCs and improve their performance. The devices operational stability and its efficiency are heavily influenced by thermally activated mechanisms. Therefore, investigating the thermal properties of halide perovskites has become a critical aspect. Thermal conductivity, thermal diffusivity and heat capacity parameters are important to understand the real-time operation of these materials. The simulation results indicate that temperature and related parameters affect solar cell efficiency. At favourable temperatures a good efficiency can be achieved, but beyond these limits, if the temperature is further raised, the efficiency decreases, followed by dropped performance.

KEYWORDS: Numerical Analysis, Heterojunction, Photovoltaic, Recombination, Photovoltaic Simulation

INTRODUCTION

In recent years, the growing global demand for energy, along with rising environmental concerns, has increased the focus on clean and sustainable energy technology option. Among the emerging photovoltaic technologies, perovskite solar cells (PSCs) have attained most of the attention because of their high-power conversion efficiency, low fabrication cost, and simple manufacturing process. More than these advantages, conventional PSCs are primarily based on lead-containing materials, which cause serious environmental and health risks due to their toxic nature. As a result, considerable research efforts have been directed toward developing safer and more environmentally friendly lead-free alternatives.

Among the various lead-free materials, tin (Sn)-based perovskites have emerged as one of the most promising options because tin has properties similar to lead and exhibits excellent light-absorbing characteristics. These advantages make tin-based perovskite solar cells suitable candidates for next-generation photovoltaic applications. In this study, the thermal behaviour of lead-free tin-based perovskite solar cells has been investigated using the SCAPS1-D simulation software. The effects of different transport layers and varying temperature conditions on device performance have been systematically analysed and describes.

LITERATURE REVIEW

The increasing demand of efficient and environmentally sustainable photovoltaic devices has led to a shift towards sustainability, including solar power. The effect of temperature on the performance and stability of the solar cell in SCAPS-1D can be easily observed and recorded [1]. The efficiency of the solar cell decreases with an increase in temperature from 300 K to 400 K due to energy loss caused by electron escape due to carrier recombination and heating [2]. It was also observed that temperature had a negative effect on Voc and FF, causing low efficiency of solar cells. Recombination losses and defects are caused by high temperature in thin-film solar cells [3], [4]. It was also concluded that the temperature is one of the factors causing instability in perovskite solar cells, where efficiency deterioration occurs due to the thermal effects. Despite the scholars highlighting the negative influences of temperature on the performance of solar cells, they also proposed ways to select appropriate materials and the required thickness of layers to mitigate the problem of heat management. [5] local heating and open circuit voltage decreases, reducing efficiency, while current slightly increases and can accelerate degradation and reduce lifetime efficiency [6]. Thermal effect on the semiconductor band gap, while Burgelman et al. (2003) demonstrate it through modeling of thin-film devices, and described the major impact of temperature on charge transport and recombination. Efficient thermal management and material optimization are essential for maintaining solar cell performance and stability [6-7]. Solar energy systems offer significant environmental benefits compared to conventional fuels but still cause certain ecological challenges such as land-use change and material-related impacts but all these effects can be minimized through proper site selection [8], lifecycle assessment, and sustainable design. It is most sustainable alternatives when implemented with strategic environmental planning [9-10]. Sharma et al. (2015) highlighted research trends and diverse applications of solar cells [11]. For large-scale solar adoption Continuous innovation, efficiency improvement, and supportive strategies are essential as it is a key solution to meet future energy demands [12] and achieving sustainable development through clean and renewable power generation [13]. Through SCAPS-1D simulation, in (2013), Khoshsirat and Yunus recommended that in CIGS thin-film solar cells structure and material parameters also defines device performance and efficient energy solutions [14]. Through careful selection of absorber and transport layers Lead-free perovskite materials can achieve equally improved photovoltaic performance. The non-ideal factors such as defect density, interface quality, and recombination strongly influence efficiency and stability of $CH_3NH_3PbI_3$-based planar solar cells. [15] These findings indicate that material engineering and interface improvement play an important role in improving device output and reliability for high performance and environmentally safe perovskite solar cells [16]. Variation in absorber layer thickness directly influences optical absorption depth, charge carrier diffusion length, and the electric field distribution, thus affecting the short-circuit current density (J_{sc}) and power conversion efficiency (PCE) [17]. Shockley–Read–Hall (SRH) recombination paths present due to increased defect density trap-assisted, which to which charge carrier lifetime get deteriorated and reduce open-circuit voltage (Voc). Improving film thickness and reducing defect-mediated recombination are essential for achieving efficient, stable, and environmentally safe lead-free perovskite solar cells [18]. The recent studies highlight that the advancement of solar energy systems largely depends on optimizing energy conversion efficiency [19] and abating recombination losses. [20]. Concentrated photovoltaic thermal configurations improve overall output by simultaneously utilizing both electrical and thermal fractions of incident solar radiations [21]. As already explained recombination is strongly influenced by defect states and interfacial charge trapping, As a result, it reduces carrier lifetime and efficiency. Controlling these recombination pathways is essential for improving device stability and power conversion performance [22]. Enhanced structural design, controlled carrier dynamics, and progressive modelling approaches are important strategies for developing next-generation high-efficiency solar technologies. Minimizing the recombination losses at the bulk and interfaces enhances both the open-circuit voltage and the fill factor [23]. Recent studies show that carrier recombination—whether radiative, Auger [24], or Shockley–Read–Hall (SRH)—effects the photovoltaic conversion efficiency [25]. Simulation studies using SCAPS-1D show that device performance strongly depends on structural parameters such as layer thickness, band alignment, and defect density, particularly in lead-free compositions [26].

Defect passivation and interface should be used mindfully to improve carrier mobility, suppress recombination losses, and achieve stable high performance perovskite devices [27]. For improving charge carrier lifetime and power conversion efficiency in solar cells, the suppression of non-radiative recombination pathways and precising defect management are important. More efficient cell architectures have demonstrated that interface trap states and ion migration-induced hysteresis in perovskite devices are critical limiting factors [28]. Similarly, Vishnoi et al. (2025) showed through SCAPS-1D simulations that optimizing absorber thickness and reducing defect density in lead-free perovskites substantially increase conversion efficiency without compromising device stability. [29]

Solar cells performance is considerably affected by temperature as temperature increases above the standard test condition (25°C), several physical and electrical mechanisms—such as bandgap narrowing, increased recombination, and resistive losses takes place and lead to decreased efficiency and fill factor (FF) [30]. The table below summarizes how temperature variations influence key parameters such as open-circuit voltage (Voc) and short-circuit current [31]. (Isc), FF, and efficiency (η), based on recent studies and simulation data [32]. Research using simulation tools such as SCAPS-1D allows detailed understanding of charge transport and recombination dynamics in thin-film solar cells. [33]. Burgelman et al. (2000, 2003) first developed the SCAPS-1D software at the University of Ghent to simulate polycrystalline and thin-film solar cells, provides us base for modern device-level modelling. Consequent works have applied this simulation platform to study defect densities, temperature effects [34, 35], and interface recombination in both lead-based and leadfree perovskite architectures. Temperature rise leads to a reduction in voltage and overall efficiency [36].

Table. 1: (Data from references) Effects Studied Earlier

j	**Voc (V)**	**I_{sc} (A/cm²)**	**Fill Factor (FF, %)**	**Efficiency (η, %)**	**Key Observation / Reference**
25	0.72	0.035	81.0	20.0	Reference condition (STC: 25 °C, 1000 W/m²) – baseline performance. PV Education (2024)
35	0.70	0.0355	79.5	19.1	Small drop in Voc; FF begins to decline. Jeeng et al. (2022)
45	0.68	0.036	78.0	18.2	Voc drops ~40 mV; recombination losses increase.

55	0.66	0.0362	76.2	17.0	Efficiency decreases ~15%
					compared to 25 °C. Springer Open (2024)
65	0.64	0.0364	74.5	16.0	Higher temperature increases recombination; FF degrades.
75	0.62	0.0366	72.8	15.0	Efficiency loss ≈ – 0.35%/°C cumulative.
85	0.60	0.0368	71.0	14.1	Notable power loss; cell near thermal limit.
95	0.58	0.037	69.5	13.3	Severe degradation; risk of hot spots. PMC (2023)

Methods: The SCAPS-1D: Definition SCAPS-1D (Solar Cell Capacitance Simulator) was developed at the University of Gent, Belgium. It is a one-dimensional simulator that simulate different model and multi-layer solar cells by solving Poisson's equation and carrier continuity equations under steady-state illumination. The software allows analysis of current-voltage (I–V), capacitance voltage (C–V), and quantum efficiency (QE) characteristics. It includes parameters such as doping, bandgap, carrier mobility, defect density, and interface states, and accounts for recombination mechanisms like Shockley–Read–Hall, radiative, and Auger recombination. This flow-chart will make it easy to learn,

Open SCAPS-1D
↓
Set Problem (device/layers)
↓
Define Parameters Temperature, Voltage, Frequency, Rs/Rsh, Illumination
↓
Select Simulation I–V, C–V, QE, C-f
↓
Set Scan Range & No. of Points
↓
Calculate (Single Shot/Batch)
↓
View Results I–V Graph, QE Curve, AC/C–V Data
↓
Curve fitting / Script Graphs
↓
Save Simulations & Graph/Data

Flow-chart- Software Scaps1-D

STEP-1

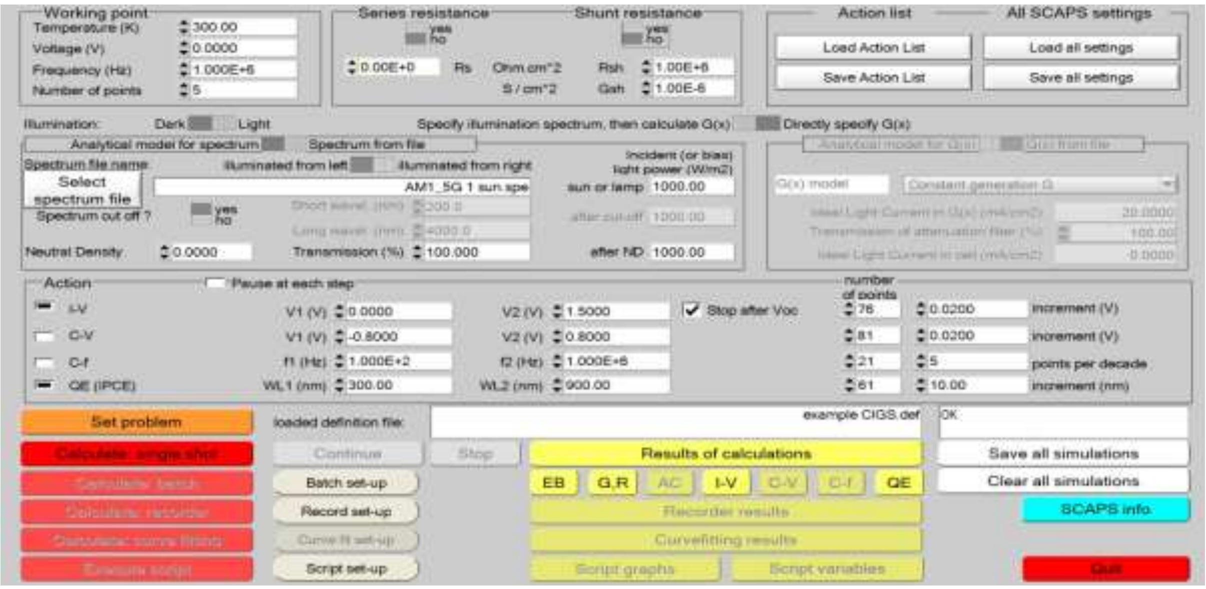

Figure.1: Set-Up Over-View of Software (SCAPS-1D)

The figure shows the working interface of the SCAPS-1D software used for analysing the performance of solar cells. It provides different sections to adjust simulation parameters such as illumination condition, voltage range, frequency, and resistance values according to the required set-up. The interface also includes analysis options like I–V, C–V, C– f, and QE for studying the electrical behaviour of the device. For improving charge carrier lifetime and power conversion efficiency, user can easily modify before running the simulation program. Various control options are provided for performing calculations, saving data, and generating graphical results.
Due to its flexible simulation environment and easy operation, SCAPS-1D is widely used for modelling and optimization of thin-film and perovskite solar cells. It provides compatible input conditions and environment, during the simulation.

STEP-2

Figure.2: Set-Up Over-View of Layer-Added (SCAPS-1D)

The layer setup window of the SCAPS-1D software used for modelling and analysing solar cell structures is represented in the figure. Different layers of the device such as FTO, TiO_2, $CH_3NH_3SnBr_3$, and NiO_3 are arranged in sequence to form the complete perovskite solar cell structure. The interfaces formed between adjacent layers are also shown in the software. On the right side of the panel, a schematic representation of the multilayer device structure is displayed to provide a clear view of the layer arrangement inside the solar cell. Different layers and material parameters can be added, modified, or removed according to the required simulation conditions. Numerical settings and device-related information are also provided to control the simulation process. The influence of different material layers and interface properties on the overall performance of the solar cell device can be studied using this layer configuration setup.

STEP-3

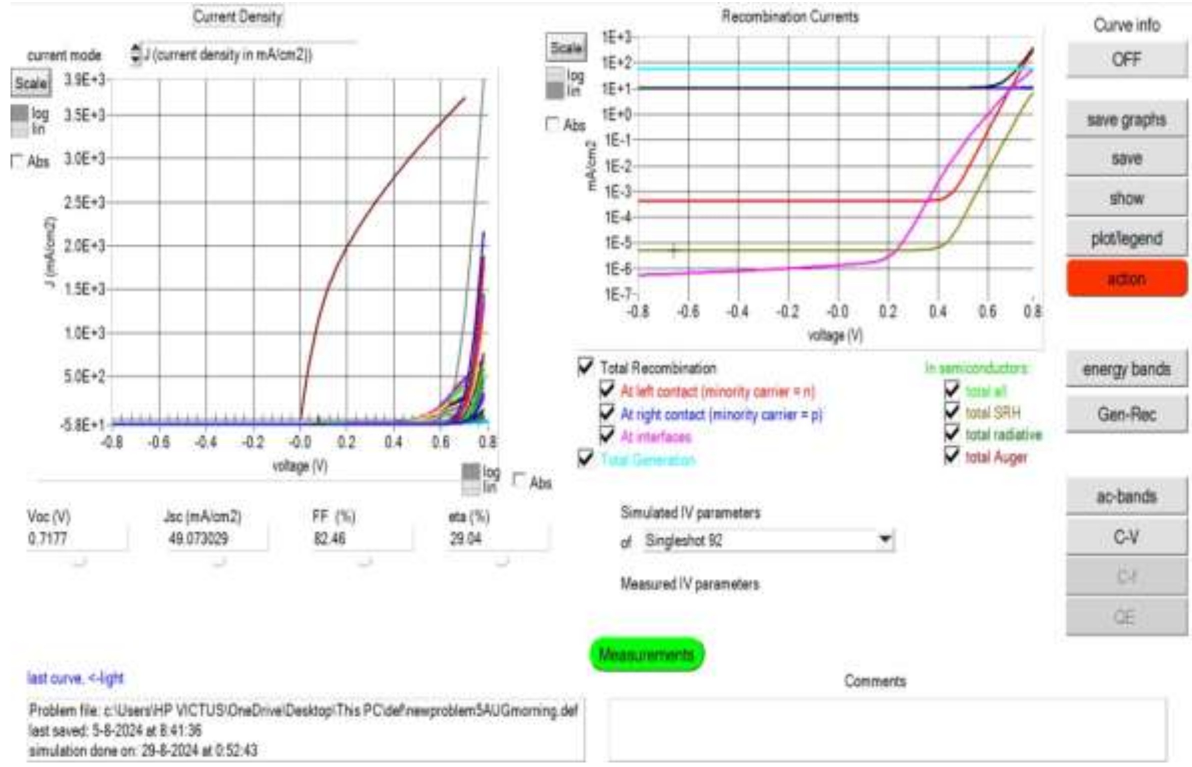

Figure.3: Simulated photovoltaic response obtained using SCAPS-1D

MATERIALS

The diagram illustrates the cross-sectional structure of a perovskite solar cell. Distinct colours and labels are used for each layer, representing its material composition, position, and functional role in the device performance. Each layer performs a specific role in charge generation and transport. The FTO layer acts as a transparent front electrode that allows light to enter and helps collect charge carriers. TiO_2 works as the Electron Transport Layer (ETL), assisting electron movement while reducing charge recombination. The $CH_3NH_3SnBr_3$ perovskite layer serves as the main light absorber due to its direct bandgap and strong absorption properties, generating electron–hole pairs under sunlight. Above this, NiO_3 functions as the Hole Transport Layer (HTL), extracting holes and blocking electrons to improve carrier separation. the layered structure of the proposed lead-free perovskite solar cell used for SCAPS-1D simulation analysis. Different layers including FTO, TiO_2, $CH_3NH_3SnBr_3$, NiO_3, and the metal electrode are arranged in sequence to support charge generation and carrier transport inside the device. The FTO layer works as the transparent front contact that allows light to enter the cell, while TiO_2 helps in electron transport and minimizes recombination losses. The $CH_3NH_3SnBr_3$ layer acts as the main absorber region where electron–hole pairs are generated after light absorption. NiO_3 supports hole transport toward the back contact and improves charge separation within the structure. The metal electrode finally collects the charge carriers and completes the external circuit, helping in improving the overall performance of the solar cell.

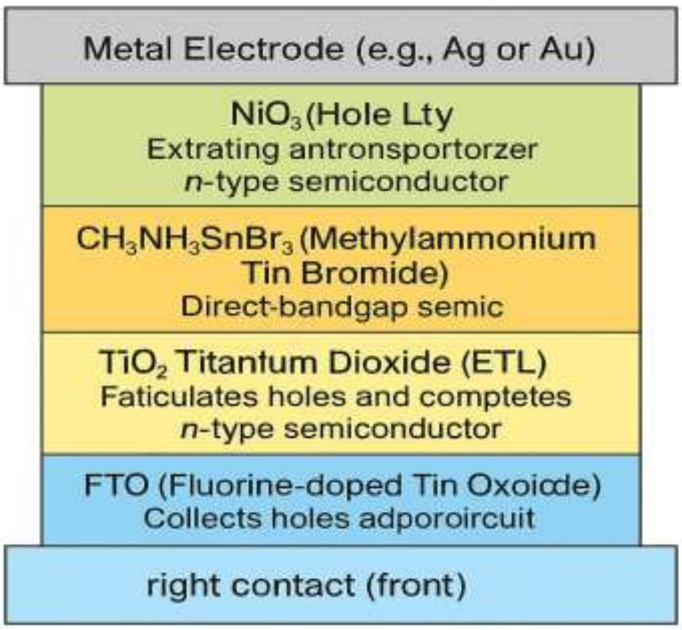

Figure: 5 Schematic representation of the FTO/TiO_2/$CH_3NH_3SnBr_3$/NiO_3/Metal

electrode layered structure of the perovskite solar cell.

Finally, the metal electrode (Ag or Au) acts as the back contact, completing the circuit and enabling current flow. Each layer with material and functions along with characteristics has been described in following table-

Table.2: Material and their Characteristics

Layer	Material	Function	Type	Characteristics
Right Contact (Front)	FTO (Fluorine-doped Tin Oxide)	Transparent conducting oxide (TCO) substrate	n-type semiconductor	High optical transparency (>85%), sheet resistance ~10–15
				Ω/sq, work function ≈ 4.4 eV
Electron Transport Layer (ETL)	TiO_2 (Titanium Dioxide)	Facilitates electron extraction and transport from perovskite absorber	n-type semiconductor	Bandgap ≈ 3.2 eV (anatase), high stability, low electron mobility (~0.1 cm²/V·s)
Absorber Layer	$CH_3NH_3SnBr_3$ (Methylammonium Tin Bromide)	Main light-harvesting perovskite material	Direct bandgap semiconductor	Bandgap ≈ 1.9 eV, lead-free, absorbs visible light, sensitive to oxidation
Hole Transport Layer (HTL)	NiO_3 (Nickel Oxide)	Extracts and transports holes towards the back contact	p-type semiconductor	Wide bandgap (≈ 3.6–4.0 eV), high hole mobility, good stability, eco-friendly
Left Contact (Back)	Metal Electrode (e.g., Ag or Au)	Collects holes and completes the circuit	Metallic conductor	High conductivity, reflective, ensures efficient charge collection

Table No. 3 (Used Parameter)

Properties	**NiO3**	**CH3NH3SnI3**	**TiO2**	**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})	1019	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□ 10^{1}	5□ 10^{1}	5□ 10^{1}	5□ 10^{1}
Hole Mobility (up)	5□ 10^{1}	5□ 10^{1}	5□ 10^{1}	5□ 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}

RESULTS AND DISCUSSION

A controlled SCAPS-1D simulation was performed at three different temperatures (300 K, 310 K, and 330 K) to analyse the thermal sensitivity of the device. The results were recorded, and it was concluded that temperature has a significant impact on important photovoltaic result parameters. At 300 K, the cell exhibited an open-circuit voltage (Voc) of 0.7177 V, short-circuit current density (J_{sc}) of 49.07 mA/cm², fill factor (FF) of 82.46%, and power conversion efficiency (PCE) of 29.04%. At the next step, when the temperature increased to 310 K, a slight improvement in J_{sc} (52.66 mA cm^{-2}) and PCE (31.97%) was observed, which may be attributed to enhanced carrier excitation and improved charge transport at moderate thermal levels. However, Voc increased to 0.7454 due to the well-established bandgap narrowing effect with temperature rise. Due to the presence of more free charge carriers at this stage, the efficiency increases.

At 320K-330K, the device experienced a further drop in performance. Voc increased to 0.7593 V and Jsc reduced to 44.51 mA/cm², while PCE considerably declined to 28.34%. This reduction is linked to increased non-radiative recombination and weakened built-in electric field strength at higher temperatures, which limit charge carrier separation efficiency. There are also an effect of free charge carriers and the hindrance caused by them. The variation in FF also reflects changes in series and shunt resistances, influenced by thermal activation of defect states within the absorber and at interfaces. Combining SCAPS-1D with optical and degradation models offers a wide-ranging path to predicting realistic solar cell performance. The simulated temperature-dependent performance analysis of the lead-free thin-film solar cell using SCAPS-1D revealed clear correlations between thermal variation and device parameters. At 300 K, the cell achieved a power-conversion efficiency. The PCE of 29.04%, with Voc = 0.7177 V, J.sc = 49.07 mA cm^{-2}, and FF = 82.46%. Increasing the temperature to 310 K resulted in a transient rise in efficiency (31.97%) resulting primarily from enhanced carrier generation and slightly improved open-circuit voltage (0.7454 V). However, further heating to 330 K produced a performance decline to 28.34%, accompanied by a reduction in Jsc (44.51 mA cm^{-2}) despite a moderate increase in Voc (0.7593 V).

Temperature (K)	Voc (V)	Jsc (mA/cm²)	FF (%)	Efficiency (%)
300	0.7177	49.073	82.46	29.04
310	0.7454	52.658	81.44	31.97
330	0.7593	44.512	83.86	28.34

Table.3: (Summary of SCAPS-1D simulated solar cell parameters at various temperatures)

The parameters include open-circuit voltage (Voc), short-circuit current density (Jsc), fill factor (FF), and power conversion efficiency (η).

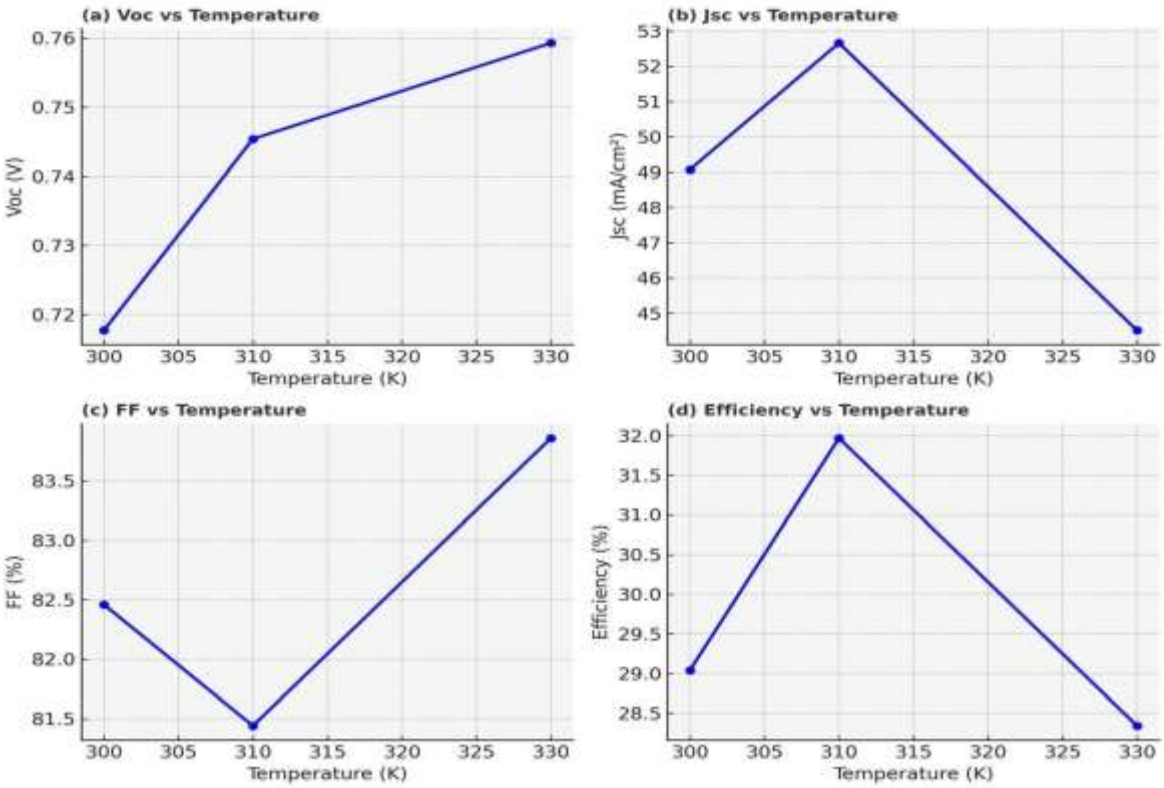

Figure.3: Degradation is dominated by losses in Voc and FF

CONCLUSION

The SCAPS-1D provides insight into how intrinsic material parameters and external conditions influence device behaviour. Importantly, increase in Voc was observed above 300 K from simulation-specific boundary conditions or temperature-dependent material parameters, relatively than purely intrinsic thermal behaviour. The estimated temperature coefficient of efficiency ($C_t \approx -0.08$ % K^{-1}) indicates that the simulated device exhibits strong thermal tolerance compared with conventional Si or CIGS technologies (typically –0.3 to –0.5 % K^{-1}). Collected result data indicate that moderate temperature increase (around 310 K) can briefly improve carrier mobility and Jsc, leading to a short efficiency gain. However, continued temperature rise, increases recombination losses and resistive effects, which cause a deterioration in Voc, FF, and in general efficiency. Along with temperature different other factors also effect the final efficiency of the solar cell performance. However, when temperature rises beyond a certain limit, efficiency decreases because the open-circuit voltage reduces considerably. Recombination of charge carriers and higher diode saturation current cause the voltage drop. Therefore, high operating temperature is one of the main causes of efficiency loss in solar cells. This simulation of lead-free perovskite solar cells may be improved further by controlling defect density and maintaining better interface contact between the device layers. In future studies, different transport materials and thermal operating conditions can be explored to obtain more stable device performance.

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