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"Environmental Pollution and Challenges of Environmental Sustainability"

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Sirte, October, 14, 2025

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Design of an Eco-Friendly Tandem Solar Cell Based on Lead-Free Perovskite ($MASnI_3$)/Silicon with Enhanced Performance via SCAPS-1D

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Eco-friendly solar cells; layer thickness optimization; Lead-free perovskite; MASnI3; Power conversion efficiency; SCAPS-1D simulation; Silicon sub-cell; Tandem solar cell; Tin-based perovskite.

Abstract: The development of high-efficiency and eco-friendly solar cells is a pivotal issue in solar energy research, as they provide sustainable solutions to reduce dependence on fossil fuels and limit environmental pollution. Perovskite solar cells are among the most promising options for renewable energy technologies, due to their ability to achieve high efficiencies, especially when combined with silicon in tandem configurations. This study aims to design and simulate a lead-free tandem solar cell made of tin-based perovskite ($MASnI_3$) and silicon, using SCAPS-1D simulation software. The efficiency was optimized by simulating the thickness of the active and passive layers and selecting the materials to achieve optimal performance. Simulation results showed that the proposed design (ITO/ZnO/$MASnI_3$/C-SiOx (n)/P-Si/P^+-Si) achieved a power conversion efficiency of 27.35%, with an open-circuit voltage of 0.768 V, a high short-circuit current density of 42.06 mA/cm^2, and a fill factor of 84.64%. The effect of temperature rise on the performance of the solar cell was also simulated, and the cell showed very reasonable thermal stability and was in the optimal range for tandem solar cells. These results confirm that lead-free tandem solar cells based on $MASnI_3$ and silicon are a promising option for providing clean and safe energy, enhancing their potential for future fabrication and application.

Introduction

In recent years, perovskite solar cells are receiving significant attention due to their potential for high efficiency and lower production costs. Perovskite was first successfully used in solar cells in 2009 when Japanese researchers, led by Kojima et al., incorporated organic metal halide perovskite into dye-sensitized solar cells, achieving power conversion efficiency (PCE) of 3.8%. This milestone marked the beginning of rapid advancements in perovskite solar cell technology. By 2012, efficiency had improved to 10%, and by 2016, it surpassed 22% (NREL, 2018).

As of 2023, perovskite solar cells have achieved efficiencies exceeding 26%, establishing them as a promising technology in photovoltaic (ScienceDaily, 2023).

This rapid progress in perovskite solar cell technology is driven by several key factors: Material advancements have enhanced perovskites' ability to efficiently absorb light while simplifying the manufacturing process. Additionally, their cost-effectiveness stems from the availability of inexpensive raw materials, making them more affordable than traditional silicon-based cells. Furthermore, simplified fabrication methods, such as spin-coating and printing, provide a low-cost alternative to the complex, high-temperature processes required for silicon solar cell production (Zhang & Park, 2024). The following figure shows the evolution of the efficiency of perovskite solar cells from 2009 to 2024.

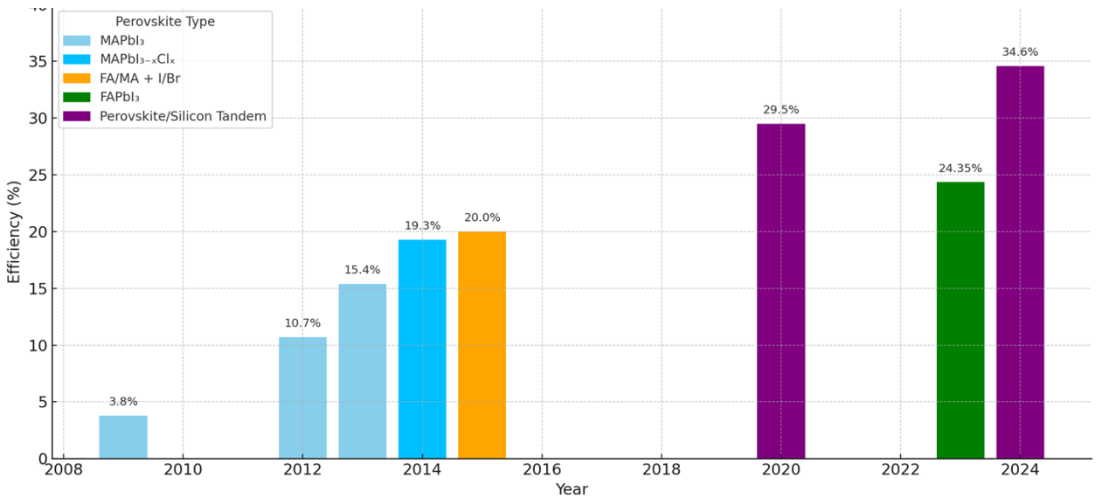

Figure (1): Efficiency Progress of Perovskite Solar Cells (2009-2024)

However, perovskite is not without its drawbacks, as most compositions contain lead, which is highly sensitive to moisture, water, heat, and oxygen. Exposure to moisture can lead to hydrolysis and degradation, breaking down the perovskite structure, while water damages the crystal. Heat accelerates these degradation processes, and oxygen especially under light exposure induces phase transformations and further deterioration of the material (Khan et al., 2024).

In addition, lead is a heavy and toxic element, and its leakage poses a risk to the environment if solar modules are damaged by factors such as fires or natural disasters, exposed to moisture without adequate protection, or have reached the end of their lifespan and are not properly handled. This is especially true in the absence of proper policies for handling lead-containing module waste, which exposes the environment to the risk of long-term pollution. (Li et al., 2023)

Due to these challenges, researchers are actively investigating new lead-free perovskite materials offer a promising pathway to improving the stability and sustainability of perovskite solar cells while addressing environmental concerns.

One of the most promising applications of lead-free perovskites is in tandem solar cells (TSCs), where a perovskite layer is stacked on top of a silicon cell or another stabilizing material. This tandem architecture enhances light absorption and energy conversion efficiency, offering a pathway to surpass the efficiency limits of conventional silicon solar cells without entirely replacing them. (Bush et al., 2017)

Before discussing the design of tandem cells, it is important to define perovskite and briefly explain its chemical structure.

Perovskite is a calcium titanium oxide mineral with the chemical formula $CaTiO_3$. It was discovered in the Ural Mountains of Russia by Gustav Rose in 1839 and is named after the Russian mineralogist Lev Perovski (1792–1856) (Perovskite.info, 2023).

While true perovskite is composed of calcium, titanium, and oxygen, the term "perovskite" is now used to describe any compound with the ABX_3 structure, which is derived from the structure of $CaTiO_3$. Where:

- **A** is a large cation, typically an organic methyl ammonium ($CH_3NH_3^+$, MA^+) or formamidinium ($CH_3CH_2NH_3^+$, FA^+).
- **B** is an inorganic medium-sized metal cation, typically lead (Pb^{2+}) or tin (Sn^{2+}).
- **X** is a halide anion, such as iodide (I^-), bromide (Br^-), or chloride (Cl^-)

In the ideal cubic structure, A cations occupy the corners of the cube, B cations are positioned at the centres, and X anions are located at the face centres. This arrangement gives perovskites unique properties, making them valuable in various applications such as solar cells and sensors (Perovskite, 2023; Noman et al., 2024).

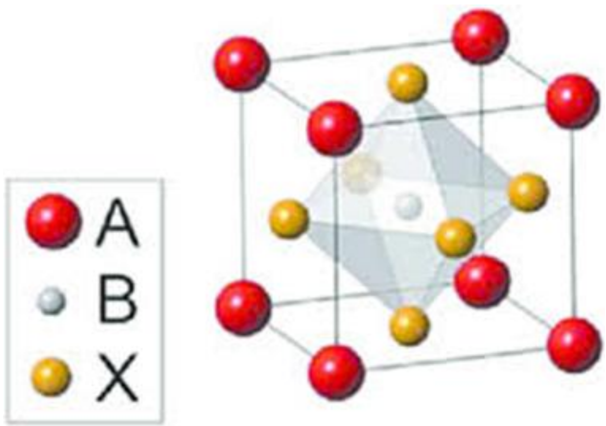

Figure (2): The Crystal Structure ABX_3 of Perovskite materials

The most commonly used perovskite for solar cells is methyl ammonium lead iodide ($CH_3NH_3PbI_3$), but Tin-based perovskite materials such as methyl ammonium tin iodide ($MASnI_3$) or ($CH_3NH_3SnI_3$) have attracted attention as promising alternatives for ($MAPbI_3$) methyl ammonium lead iodide perovskite in perovskite solar cells; due to their similar structural and electronic properties, while being more environmentally friendly (Lee et al., 2014).

So, with this understanding of what perovskites are, how do we achieve high-performance tandem solar cells? This is what this paper aims to discuss.

Research Methodology

Tandem solar cell is a subtype of multijunction solar cells, which can convert a broader range of solar spectrum into electricity by stacking multiple layers with different bandgaps. And this can achieve higher power conversion efficiencies (PCE) than conventional single-junction cells.

Tandem cell architecture:

- The top cell is made of a wide bandgap material, absorbs high-energy light.
- The bottom cell is made of a narrower bandgap material, and absorbs lower-energy light.

Combining perovskite and silicon layers in tandem solar cells offers several key benefits, including: Higher efficiency, lower cost, and compatibility with existing silicon technology (Ossila, 2024).

To achieve competitive power conversion efficiency while eliminating toxic lead, thereby reducing the environmental footprint of perovskite solar technology, we will design perovskite/silicon tandem cell, and focus on optimizing the layer structure to maximize light absorption using SCAPS-1D simulation.

SCAPS-1D (*Solar Cell Capacitance Simulator, 1-Dimensional*) is a solar cell simulation program developed by the Department of Electronics and Information Systems (ELIS) at the University of Gent, Belgium. The program is freely available for download and runs on Windows operating systems. (Burgelman, Decock *et al*., 2023)

Our designed structure of a perovskite/silicon tandem cell consists of these layers:

- **Perovskite Top Cell**
  - **Transparent conductive oxide (TCO)** as front electrode: It enhances light absorption while facilitating efficient charge transport. Indium Tin Oxide (ITO) is typically used to improve efficiency and performance, due to its excellent optical transparency and electrical conductivity address stability issues in perovskite cells (Srinivasachari, 2023).
  - **Electron transport layer (ETL):** It facilitates efficient electron extraction and transfer from perovskite to TCO. ZnO has an energy-band structure and physical properties such as high mobility and compatibility with perovskite materials, which makes it an ideal n-type ETL material (Hoque et al., 2019).
  - **Top absorbing layer (Perovskite)**: It is used to enhance overall efficiency by capturing higher-energy photons that the silicon doesn't absorb. The organic-inorganic lead-free tin-based perovskite, methyl ammonium tin iodide perovskite ($CH_3NH_3SnI_3$, or $MASnI_3$) offer

high efficiency, lightweight properties, and cost-effectiveness. It acts as the absorber layer, and its bandgap is 1.35 eV, which is tunable and thus compatible to be paired with a silicon (Si) solar cell with a bandgap of 1.124 eV, thus forming a tandem cell (Das & Paul, 2020).

- **Silicon Bottom Cell**
  - **The emitter layer:** The n-type emitter layer acts as the electron transport layer (ETL) in bottom sub-cell. Recent studies have shown that using crystalline silicon oxide C-SiOx as emitter layer enhances efficiency by optimizing light management and reducing reflection losses (Moinuddin et al., 2024).
  - **Bottom absorbing layer (Silicon):** P-type crystalline silicon (doped with elements like boron, which introduces holes or positive charge carriers) with band gap Energy (approximately 1.124ev), which is optimal for absorbing sunlight in the visible spectrum near-infrared ranges. It achieves exceptional integration with perovskite layer in the top cell, allowing for improved light absorption and reduced spectral loss, thus enhancing overall efficiency (Phulara, 2022).
  - **Back surface field (BSF):** It is an electric field created by placing a heavily doped p-type Crystalline-Si behind the main absorbing silicon layer. It acts as HTL, and reflects electrons that arrive backward and prevent them from recombining reducing charge loss and improving efficiency.
  - **Metal back contact:** It is usually made of metals such as aluminum or silver. Its primary role is simple mechanical and electrical (collecting charges only) and does not contribute to efficiency calculations in SCAPS-1D setups.

This structure maximizes light absorption and minimizes recombination losses, leading to improved efficiency in solar energy conversion.

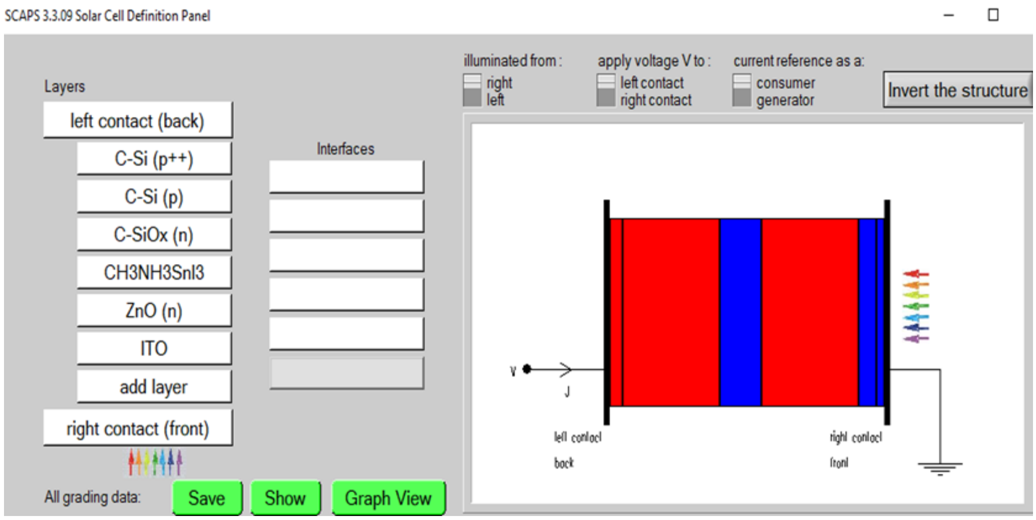

Figure (3): Design $MASnI_3$/Si tandem cell on SCAPS

Parameters of layers are taken from literature reviews (Das & Paul, 2020), (Moinuddin et al., 2024). The thickness of the active and passive layers was simulated to achieve the optimal thickness for this design, resulting in high efficiency.

The primary variables analyzed and optimized were the thickness of the active and passive layers. Many simulations were performed for this model, varying the thicknesses each time, until the optimal thicknesses for the highest efficiency was reached. The final optimal values of these thicknesses were included in the input parameters table and were not derived from previous studies, but were derived through the self-simulation methodology of this study.

Table (1): Parameters of ITO/ZnO/$MASnI_3$/C-SiOx/p-Si tandem cell

	ITO	ZnO	$MASnI_3$	C-SiOx (n)	C-Si (p)	C-Si(p+)
Thickness (µm)	0.045	0.100	0.575	0.245	0.565	0.080
Bandgap (ev)	3.500	3.370	1.350	1.124	1.124	1.124
Electron Affinity (ev)	4.600	4.350	4.170	3.900	4.050	3.900
Relative permittivity	8.900	10.00	6.500	11.90	11.90	11.90
CB effective density (cm^{-3})	2.20E+19	2.2E+18	1.00E+18	2.80E+19	2.8E+19	2.84E+19
VB effective density (cm^{-3})	1.80E+19	1.78E+19	1.00E+19	2.60E+19	2.6E+19	2.68E+19
Electron mobility (cm^2/vs)	1.00E+1	1.00E+2	1.60E+0	1.25E+3	1.04E+3	1.212E+3
Hole mobility (cm^2/vs)	1.00E+1	2.50E+1	1.60E+0	4.43E+2	4.21E+2	4.21E+2
Donor density (cm^{-3})	1.00E+19	1.00E+20	0	2.00E+20	0	0
Acceptor density (cm^{-3})	0	0	3.20E+15	0	1.00E+17	9.00E+20
Defect density (cm^{-3})	1.00E+16	1.00E+16	-	1.00E+14	1.00E+14	1.00E+14

Set up the simulation environment by define illumination, which is typically (AM 1.5G spectrum) for solar radiation and calculate.

Results and discussion

Simulation results gave significant progress in efficiency and performance. The cell efficiency exceeded 27.35%, as seen in Figure (4):

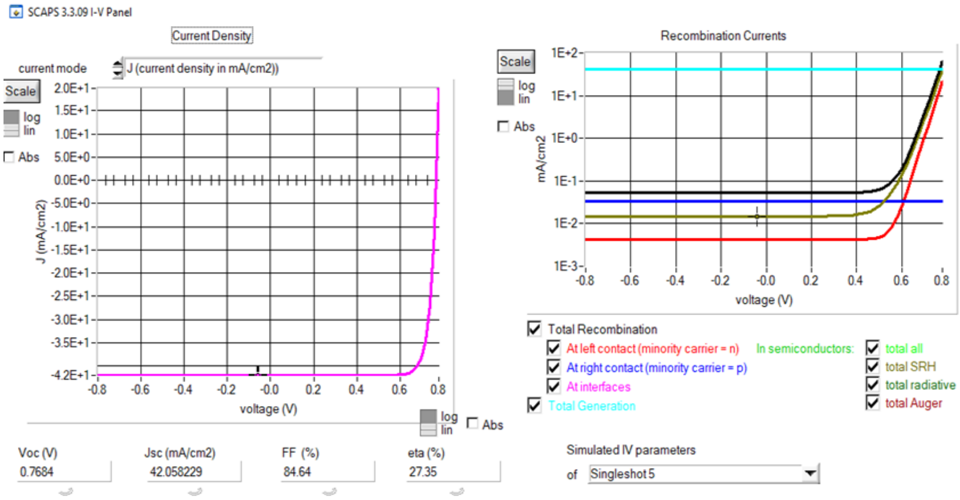

Figure (4): Results of simulation $MASnI_3$/Si tandem cell on SCAPS

The curve exhibits a characteristic shape for a solar cell. The current gradually decreases with increasing voltage due to series resistance and recombination effects. The rise in the high-current region reflects good efficiency in reducing power loss. However, there is a relative decrease in the curve at high voltage, indicating the effect of recombination currents and minor defects. The performance of this cell is determined by:

- The open-circuit voltage (Voc) is 0.768V, indicating strong performance for the perovskite/silicon tandem cell, suggesting better efficiency and promising potential for application in solar energy generation.
- The maximum current density (Jsc) is 42.06 mA/cm², signifying robust current generation capability, indicating better performance and high efficiency.

- The fill factor is 84.64%. A high FF suggests low series resistance and minimal non-ideal losses in the device. Generally, fill factors for high-performance solar cells range from 70% to 85%. Values above 80% usually indicate efficient performance, with anything around or above 84% being particularly strong. An 84.64% fill factor suggests that the cell is efficiently utilizing its output (Green, 1982).

- The power conversion efficiency is 27.35%, placing the cell among the highest-performing solar cells available. Achieving such efficiency is critical for commercial viability. If this performance can be consistently reproduced and scaled, it positions lead-free perovskite/Silicon tandem cells as a competitive alternative in the solar market.

- It is essential to consider that efficiency measured under standard test conditions may differ from real-world performance. Factors such as thermal stability, degradation rates, and performance under varying light conditions will influence the practical deployment of these cells (Bailey & Emery, 1992).

- In summary, an efficiency of 27.35% is an outstanding achievement, indicating excellent performance and potential for commercial applications.

The current recombination plot provides insights into charge carrier losses due to various recombination mechanisms:

- Total recombination (black curve): It represents the total recombination currents, and we notice that at low voltages (0-0.5 V): the current is low (~1E-3 mA/cm²). At medium voltages (~0.5 - 0.7 V): it starts to rise gradually.
- Recombination at contacts (red and blue curves): The minor recombination losses at the left (electron contact) and right (hole contact) electrodes indicate well-matched work functions and efficient charge extraction.
- Shockley-Read-Hall (SRH) recombination (green curve): Moderate level of Shockley-Read-Hall recombination indicates that the effect of defects starts at medium to high voltages, i.e. 0.5V to 0.8V, but does not significantly impair device performance.
- Total generation rate (cyan curve): The high total generation rate, exceeding all recombination currents, confirms that the device maintains a high carrier generation-to-recombination ratio, contributing to its high efficiency.

Simulating the effect of temperature rising on the solar cell performance

As we know, solar cell performance is highly dependent on temperature. High temperatures can actually lead to a loss of efficiency. Therefore, cooling processes are usually performed on modules and collectors to reduce performance degradation. Here, we will study the effect of high temperature on solar cell performance by measuring the temperature coefficient of the solar module. However, we will first discuss the definition of the temperature coefficient of a solar cell.

The temperature coefficient indicates the effect of temperature rising on a solar cell performance, specifically on open-circuit voltage and efficiency. It's giving by:

$$Temperature\ Cofficient\ for\ X = \frac{1}{X_{ref}} \frac{\Delta X}{T - T_{ref}}$$

Where X is the parameter on which we calculate the effect of temperature, X_{ref} is the parameter at a reference temperature, let it be room temperature. ΔX is the change in X at elevated temperature T and reference temperature T_{ref} (Paudyal & Imenes, 2021).

High temperatures can negatively impact solar cell efficiency, due to the resulting voltage drop associated with increased temperature. The temperature coefficient of a solar cell is usually expressed in millivolts per degree Celsius (mV/°C) at case of the voltage or as a percentage (%/°C) in general form (Paudyal & Imenes, 2021).

Many factors are affected by the rise in temperature. To know the degree of their impact, the simulation performed on the designed solar cell at temperatures (300,310,320,330,340) K. The values obtained for open-circuit voltage, short-circuit current density, fill factor and the overall efficiency were recorded and the following results were obtained:

1. **Effect of temperature rising on open-circuit voltage**

Temperature (K)	300	310	320	330
Open-circuit voltage (V)	0.7581	0.7425	0.7266	0.7108

We notice that the open circuit voltage decreases linearly with increasing temperature. The decrease in open circuit voltage with increasing temperature is an expected behavior for solar cells, as heat affects the bandgap of the absorber material, leading to increased generation and recombination of charge carriers, thus reducing the voltage.

When we plotting these values graphically, we get the following figure:

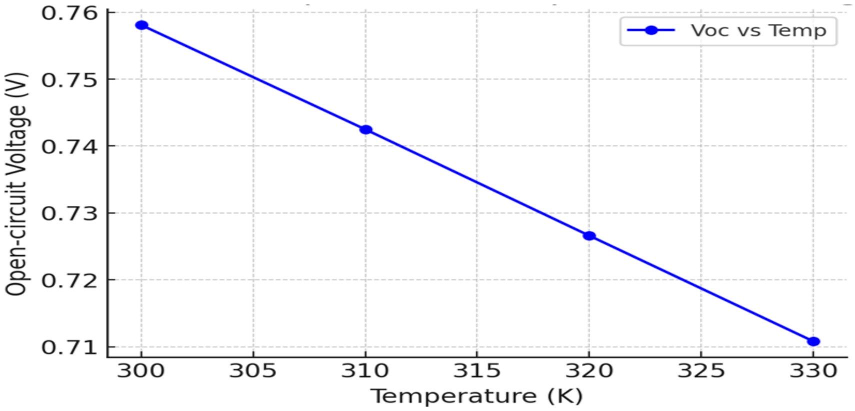

Figure (5): Effect of temperature on open circuit voltage

The temperature coefficient of open-circuit voltage β can be calculated by:

$$\beta = \frac{1}{Voc}\frac{\Delta Voc}{\Delta T}$$

$$\beta = \frac{1}{0.7581}\frac{0.7108 - 0.7581}{330 - 300}$$

$$\beta = -0.002\ V/℃$$

That is, the voltage drops by 0.2 millivolts for every degree Celsius rise in temperature, and can be expressed as (-0.2%/C). This is within the expected valuesfor solar cells made of perovskites and silicon. According to the scientific study (Paudya & Imenes, 2021).

2. Effect of temperature rising on short-circuit current density

Temperature (K)	300	310	320	330
Short-circuit current density (mA/cm^2)	42.0581	42.0593	42.0604	42.0608

The short-circuit current (Isc) of solar cells tends to increase with increasing temperature. This is due to the decrease in the energy band gap of these cells at high temperatures. However, this effect is very small compared to the decrease in open-circuit voltage, so the overall efficiency decreases even with a high short-circuit current. When we plotting these values graphically, we get the following figure:

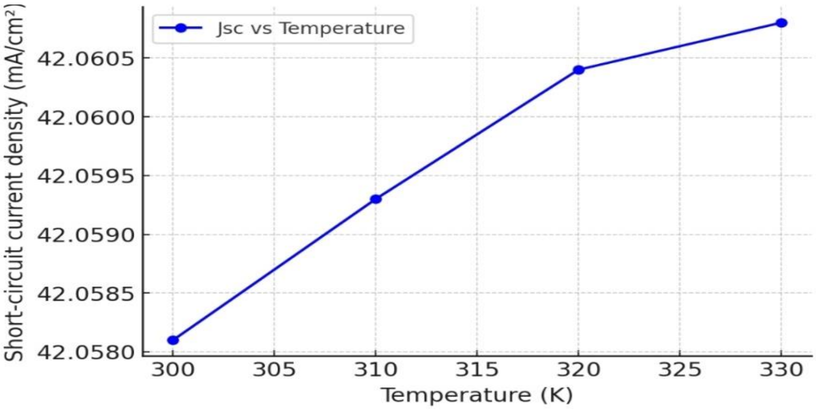

Figure (6): Effect of temperature on short-circuit current

The temperature coefficient is given by:

$$\alpha = \frac{1}{Isc}\frac{\Delta Isc}{\Delta T}$$

$$\alpha = \frac{1}{42.0581}\frac{42.0608 - 42.0581}{330 - 300}$$

$$\alpha = 0.0002\ \%/℃$$

This means that the short circuit current increases very slightly with increasing temperature, which is expected behavior given the physical nature of solar cells.

3. Effect of temperature rising on fill factor

Temperature (K)	300	310	320	330
Fill Factor (%)	84.08	83.45	82.81	82.15

When we plotting these values graphically, we get the following figure:

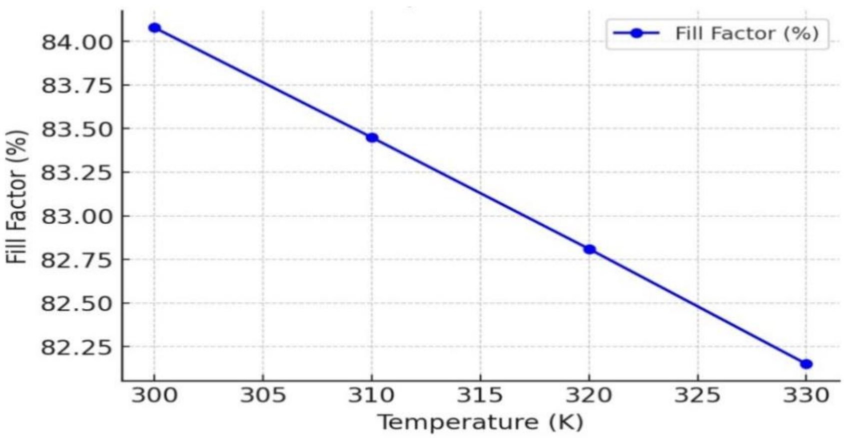

Figure (7): Effect of temperature on fill factor

We note that the fill factor gradually decreases with increasing temperature, indicating the negative impact of temperature on cell performance. To calculate the temperature coefficient of the fill factor (FF), we use the following equation:

$$\kappa = \frac{1}{FF}\frac{\Delta FF}{\Delta T}$$

$$\kappa = \frac{1}{84.08}\frac{82.15 - 84.08}{330 - 300}$$

$$\kappa = -0.076\%/℃$$

According to recent studies, the temperature coefficient of the fill factor for perovskite and silicon cells ranges from approximately -0.05%/C to -0.09%/C, depending on the cell design and material properties. Thus, the obtained value appears to fall within the range of expected values. (Babics et al., 2023)

4. Effect of temperature rising on Efficiency

Temperature (K)	300	310	320	330
Efficiency (%)	26.81	26.06	25.31	24.56

When we plotting these values graphically, we get the following figure:

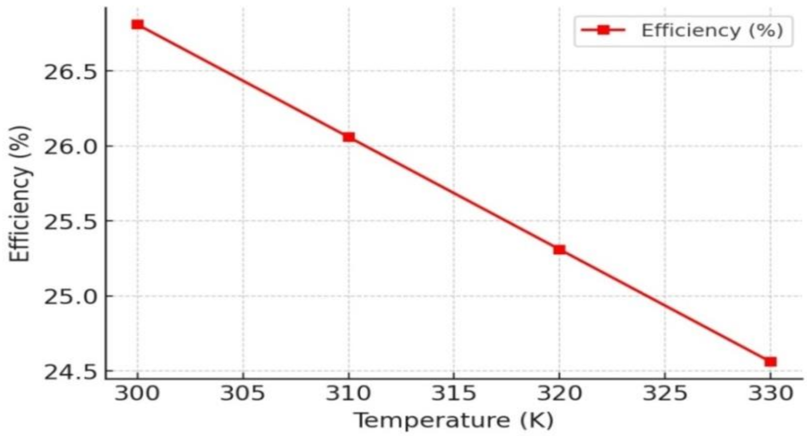

Figure (8): Effect of temperature on Efficiency

The curve illustrates the negative effect of high temperature on the overall efficiency of the solar cell. This is expected behavior given the low open-circuit voltage and fill factor, which negatively impact the efficiency value. To calculate the temperature coefficient of efficiency, we use the equation:

$$\gamma = \frac{1}{\eta}\frac{\Delta\eta}{\Delta T}$$

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$$\gamma = \frac{1}{26.81}\frac{24.56 - 26.81}{330 - 300}$$

$$\gamma = -0.27\%/℃$$

Another way to calculate the temperature coefficient of efficiency is through the relationship:

$$\gamma = \alpha + \beta + \kappa$$

$$\gamma = 0.0002 - 0.2 - 0.076$$

$$\gamma = -0.27\%/℃$$

This means that the efficiency decreases by 0.27% for each degree Celsius increase in temperature. This is an expected value within the range of previously calculated values, which lies between -0.1%/C and -0.3%/C. This demonstrates the validity of the simulation results (Paudya & Imenes, 2021; Babics et al., 2023).

Impact of other environmental factors on the solar cell performance:

1. Light Intensity and Spectrum:
   - Photocurrent (Jsc) Increase: Higher illumination increases Jsc but might also increase temperature, causing efficiency drop due to the temperature effects mentioned above.
   - Spectrum Sensitivity: Our structure has a wide absorption range (MASnI3 for visible and Si for infrared). If the spectrum shifts due to atmospheric conditions (e.g., more infrared in the morning/evening), the efficiency might fluctuate.
2. Humidity Impact:
   - Instability of MASnI3: Tin-based perovskites are highly sensitive to humidity, which can lead to the formation of hydrated phases, reducing charge transport and increasing recombination losses.
   - ZnO Interface Degradation: ZnO is also prone to hydroxylation under humid conditions, potentially affecting electron transport properties at the ZnO/MASnI3 interface.

Optimization Recommendations for designed model:

The curves obtained from the model simulation give an insight into the performance and loss mechanisms of the designed tandem solar. It gave good performance; however, this model needs further optimization. Therefore, we will suggest strategies to improve the efficiency and stability based on the analysis of the curves and recommendations. We also note that the open circuit voltage Voc = 0.768V is reasonable but can be improved for a tandem structure. And the short circuit current density (Jsc = 42.06 mA/cm^2) is very high, which is expected for a perovskite-silicon tandem cell. Also, the fill factor (FF) = 84.64% is excellent, indicating low series resistance and good charge extraction. Hence the efficiency (η) = 27.35% is already close to the upper theoretical limits for lead-free perovskite tandem cells. However, according to the previous environmental factor analysis and recombination current curve, this performance can deteriorate over time and under the influence of environmental factors, so the model may need the following improvements:

- Reducing interface defects and improving energy level alignment: The ZnO/$MASnI_3$ interface should be improved to reduce charge extraction barriers. This is done by replacing ZnO with SnO_2, as the latter has a greater energy alignment with perovskite than ZnO, which leads to improved electron transfer and reduced surface composition. Also, SnO_2 is less susceptible to interacting with perovskite in humidity, which improves stability and reduces performance degradation over time. However, to ensure comprehensive long-term protection, I also recommend encapsulating the entire cell with moisture and oxygen barrier materials, which enhances environmental stability and prolongs cell life.

- Anti-reflection coating (ARC): Applying an additional ARC layer on the ITO such as magnesium fluoride MgF_2 can increase light absorption and thus increase the short-circuit current density and overall efficiency.

Conclusions

This study presents the design of lead-free tandem solar cells composed of tin-based Perovskite as the top sub-cell and silicon as the bottom sub-cell. The tandem structure, (ITO/ZnO/$MASnI_3$/C-SiOx(n)/P-Si/P^+-Si), showed remarkable results, with Voc of 0.768V, Jsc of 42.06 mA/cm², and a fill factor of 84.64%, resulting in a power conversion efficiency of 27.35%. This efficiency is among the highest for lead-free perovskite-based tandem cells. Also, the effect of temperature rise on the performance of designed cell was studied. It showed the highest efficiency and demonstrated good thermal stability, making it suitable as a promising to lead-based tandem solar cells. Recombination current analysis indicated that interface and contact recombination were the primary sources of performance loss over time, so strategies were proposed to improve the long-term performance of the model.

In conclusion, the achieved efficiencies of 27.35% indicate the potential for this cell to compete in the solar energy market, provided that further refinements in material quality, device engineering, and stability are made.

In general, results highlight the role of clean renewable energy as an alternative to polluting fossil fuels. Also, future work should bridge the gap between simulation and experimental fabrication, with a focus on long-term stability, materials used, and efficiency enhancement. By addressing these challenges, lead-free perovskite/silicon tandem cells could become sustainable high-performance alternative to conventional lead-based tandem photovoltaics.

Conflict of Interest: The authors declare that there are no conflicts of interest.

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