Device simulation of perovskite/silicon tandem solar cell with antireflective coating

B. Gopal Krishna · Dhriti Sundar Ghosh · Sanjay Tiwari

Abstract
Optical design, photon management, and energy conversion efficiency are investigated through numerical simulation of perovskite/silicon tandem solar cell using the single-diode model. A strong near-infrared reflectance of roughly 60% is present in the perovskite-based top cell. ZnO and Si₃N₄ anti-reflection coating layers are placed on the surface of the perovskite layer and silicon sub-cell of the tandem solar cell respectively for photon management and minimizing the near-infrared reflectance loss. ZnO will act as an electron transport layer as well as an anti-reflection coating layer. The ZnO layer will minimize the near-infrared reflectance loss by the top cell in the device structure and allow the maximum transmittance of near-infrared photon energy to the silicon sub-cell. Intermediate anti-reflection Si₃N₄ layer assists in the maximum localization of the transmitted near-infrared photon energy in the silicon sub-cell. The efficiency of over 32% is achieved by optimizing the parameters of different materials such as perovskite, silicon, and anti-reflection coating layer in the tandem solar cell. The innovative idea of using electron transport material ZnO as an anti-reflection coating layer in the perovskite-based top cell can minimize the reflection loss by nearly 20%. The combination of ZnO and Si₃N₄ anti-reflection coating layers improved the conversion efficiency of the tandem cell by 1%. This result paves the way to realize highly efficient tandem solar cells through photon management.

Keywords Perovskite · Near-infrared · Reflection · Tandem solar cell · Single-diode model · Anti-reflective coating

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1 Introduction

Perovskite/silicon tandem solar cells are next-generation photovoltaic devices that can overcome the theoretical efficiency limit of silicon solar cells. The Shockley–Queisser theory limit refers that the maximum theoretical efficiency limit of silicon solar cells with a 1.12 eV energy bandgap of the light-absorbing layer is 33%. The maximum efficiency of silicon solar cells is limited to 29.4% due to Auger recombination. The Shockley–Queisser theory limit refers that the maximum theoretical efficiency limit of a perovskite/silicon solar cell with a 1.72 eV energy bandgap of the light-absorbing layer is 42–44%. The multiple photoactive absorbers with different energy bandgaps are stacked monolithically to form two-terminal tandem architecture (2T) or electrically decoupled four-terminal tandem architecture (4T) solar cells (Carmona et al. 2014; McGehee 2014). The tandem solar cell can achieve power conversion efficiency above 30%. The highly efficient III–V semiconductors (GaAs and GaInP) based tandem solar cells would not be able to compete with cost-effective silicon solar cells due to their high fabrication cost. Perovskite solar cell has achieved a remarkable efficiency of over 25% in recent years as compared to the 2nd generation thin-film solar cells (Krishna et al. 2021). Perovskite has an energy bandgap of 1.65 eV, which allows it to absorb photons with a wavelength less than 800 nm, whereas silicon has an energy bandgap of 1.12 eV, which allows it to absorb photons with a wavelength greater than 800 nm in the solar spectrum. The efficiency of the tandem cell will be improved when the bandgap of the top cell (short wavelength absorber) is increasing while the bandgap of the bottom cell (long wavelength absorber) is decreasing. Therefore, perovskite and silicon materials can be used in top and bottom sub-cells to create tandem solar cell whose matching absorption spectra considerably enhance solar spectrum utilization and cut down on preparation costs (Eperon et al. 2014; Eperon et al. 2015; Krishna et al. 2021; Askari et al. 2017).

Infrared photons are transmitted from the perovskite layer to the silicon sub-cell which leads to the photogeneration of charges. Light or photon management and optical design are important for developing highly efficient solar cells. There is an influence of light management on the parameters of the perovskite/silicon tandem solar cell. The perovskite layer exhibits properties such as a high absorption coefficient and low transmittance at photon energy above its band gap. The transmittance of a perovskite-based solar cell is 67% for the wavelength in the 800–1200 nm region because there is parasitic absorption from the perovskite and charge transport layers. The transmittance of the silver-coated perovskite solar cell is 53% in the near IR region. The reflection loss from the front of the perovskite solar cell is 10% in the 400–800 nm region. Therefore, a strong near-infrared reflectance of roughly 60% is present in the perovskite-based top cell (Li et al. 2017). The tandem solar cell’s efficiency will be affected by this reflectance. A single or multilayer anti-reflection coating layer can be placed on the surface of the top or bottom cell to minimize reflection loss. Herein, a numerical simulation of a perovskite/silicon tandem solar cell is performed using a Matlab analytical program. The single-diode model for a solar cell is used for simulation with ideal working conditions. ZnO and Si₃N₄ are used as an anti-reflection coating layer for photon management in the perovskite/silicon tandem cell. The ZnO layer is placed on the surface of the perovskite layer in the top cell. ZnO will act as an electron transport layer as well as an anti-reflection coating layer. The intermediate Si₃N₄ anti-reflection coating layer is introduced between the high energy gap (top cell) and the lower energy gap (bottom cell) to assist the localization of photon energy in a bottom cell. The perovskite and silicon sub-cells are connected in a series configuration. The combination of top and
bottom anti-reflection coating layers will improve the conversion efficiency of the tandem solar cell because the optical properties of the solar cell will be enhanced. The efficiency of the tandem device is found to be over 32%. The simulated efficiency values based on this model are compared with the theoretical and experimental results for other types of tandem cells described in the literature (Davidson 2017; Mitroi et al. 2017; Lehr et al. 2018; Altazin et al. 2018). This work provides a pathway for enhancing the power conversion efficiency of perovskite/Si tandem cells through photon management.

2 Device structure

The energy band gap of the top cell is required to be higher than the bottom cell for optimal operation of the perovskite/silicon tandem solar cell. The bandgap of perovskite material is between 1.5 to 2.2 eV which is higher than the bandgap of silicon (1.12 eV). Therefore, the perovskite solar cell and silicon solar cell are chosen as the top and bottom cells respectively in tandem architecture. The simulation of series-connected tandem cell configuration is carried out using the single-diode model. In a series-connected tandem cell, the photocurrent of the bottom cell must match the top cell’s photocurrent. The efficiency of the tandem device is optimized by varying parameters of different materials under illumination (AM1.5) over the wavelength ranging from 300 to 1200 nm. The design of a tandem solar cell consists of a perovskite absorber layer CH$_3$NH$_3$PbI$_3$ with a direct energy band gap of 1.65 eV. The perovskite sub-cell has p-i-n architecture in which electron transport material and hole transport material are ZnO and Cu$_2$O respectively. ZnO will also act as an anti-reflection coating layer. Cu$_2$O has high hole mobility, better stability, and transparency. The device structure of the bottom sub-cell is n+ Si emitter/p-type Si/p+ Si/BSF having n−p−p+ solar cell structure. The highly doped n+ Si emitter layer acts as a hole transport layer in the tandem architecture w.r.t. perovskite sub-cell. The p-type Si acts as a light-absorbing layer with a high light-absorption coefficient (Hasan et al. 2017). The intermediate Si$_3$N$_4$ anti-reflection coating layer is placed on the surface of the bottom cell to assist

Fig. 1 3D schematic view of perovskite/Si tandem cell
localization of photon energy in a bottom cell (Li et al. 2017). The different parameters of the perovskite/silicon tandem solar cell are given in Table 1. The tandem device architecture is shown in Fig. 1.

### Table 1 Input parameters for perovskite/Si tandem solar cell

| Parameters/materials                      | ZnO | CH$_3$NH$_3$PbI$_3$ | Cu$_2$O | n$^+$Si Emitter | p-type Si | p$^+$Si BSF |
|-------------------------------------------|-----|---------------------|---------|-----------------|-----------|-------------|
| Thickness                                 | 200 nm | 150 nm | 50 nm | 50 nm | 280 μm | 30 nm |
| Bandgap (eV)                              | 3.37 (Hasan et al. 2017) | 1.65 (Hasan et al. 2017) | 2.1 (Hasan et al. 2017) | 1.124 (Hasan et al. 2017) | 1.124 (Hasan et al. 2017) | 1.124 (Hasan et al. 2017) |
| Electron affinity (eV)                    | 4.35 (Hasan et al. 2017) | 3.93 (Hasan et al. 2017) | 3.6 (Hasan et al. 2017) | 3.9 (Hasan et al. 2017) | 4.05 (Hasan et al. 2017) | 3.9 (Hasan et al. 2017) |
| Dielectric Permittivity (relative)        | 10 (Hasan et al. 2017) | 30 (Hasan et al. 2017) | 10 (Hasan et al. 2017) | 11.9 (Hasan et al. 2017) | 11.9 (Hasan et al. 2017) | 11.9 (Hasan et al. 2017) |
| CB effective density of states (cm$^{-3}$) | $2 \times 10^{18}$ | $2.5 \times 10^{20}$ | $1 \times 10^{19}$ | $2.8 \times 10^{19}$ | $2.8 \times 10^{19}$ | $2.84 \times 10^{19}$ |
| VB effective density of states (cm$^{-3}$) | $1.78 \times 10^{19}$ | $2.5 \times 10^{20}$ | $1 \times 10^{19}$ | $2.6 \times 10^{19}$ | $2.6 \times 10^{19}$ | $2.64 \times 10^{19}$ |
| Electron mobility (cm$^2$/Vs)             | 100 | 50 | 30 | 1250 | 1010 | 1212 |
| Hole mobility (cm$^2$/Vs)                 | 25 | 50 | 30 | 443 | 443 | 421 |
| Donor Concentration (cm$^{-3}$)           | $1 \times 10^{20}$ | 10$^{13}$ | 0 | $8 \times 10^{20}$ | 0 | 0 |
| Acceptor Concentration (cm$^{-3}$)        | 0 | 0 | $2.5 \times 10^{16}$ | 0 | $5 \times 10^{18}$ | $9.5 \times 10^{20}$ |

### 3 Optical and electrical modeling

The maximum theoretical efficiencies are evaluated as a function of the energy bandgap and thickness of the light-absorbing layer (perovskite and silicon layer) for tandem architecture. The energy band gap of the absorber layer in the top cell is equivalent to 1.65 eV. Therefore, the absorber layer will absorb approximately all the incident light which has energy higher than 1.65 eV or wavelengths smaller than 750 nm. The structure of the top cell will act as a window for the bottom cell for the wavelength ranging between 750 and 1100 nm (Sayed et al. 2022).

The following assumptions are taken into account in the current study which includes sub-cell materials, adsorption process, and illumination conditions. The assumptions considered to derive the JV characteristics of the tandem solar cell are:

a. Standard AM 1.5 spectrum profile (solar radiation = 1000 Wm$^{-2}$);
b. There are negligible recombination losses or resistive losses for each sub-cell;
c. The temperature of the tandem cell is maintained at $T = 298$ K;
d. There are no optical losses due to glass (FTO or ITO);
e. The interfaces in the device are flat.

For measuring the JV characteristics of a solar cell under standard testing conditions, the total irradiance on the solar cell should be 1000 W/m² with an air mass of 1.5 (AM1.5) and 25 °C cell temperature. There is an influence of illumination conditions on the tandem solar cell. The direct component of light is assumed to be incident along the surface normal to the solar cell. The diffused component of light isotropically illuminates the solar cells from the upper half of space. The direct component is affected by the angle of incidence of light. When the diffuse portion of solar irradiance is considered, the tandem solar cells are more robust to the angle of incidence. In this study, the direct component of light is assumed to be incident on the surface of the solar cell normally at AM 1.5. The AM 1.5 direct solar spectrum is incident on the surface of the top cell. However, the spectral irradiance of this spectrum is reduced at the top of the silicon layer due to partial perovskite layer absorption (Dutta Gupta et al. 2012; Bittka et al. 2018). Therefore, the optimization of the thickness of the layer of perovskite and silicon is necessary. The generation rate for the top cell and bottom cell is computed by the Eqs. (1) and (2) respectively (Gharibshahian et al. 2020).

Generation rate for the bottom cell

\[
G_{\text{bot}} = \int_{0}^{+\infty} \left( \frac{A}{hc} \right) I(\lambda) (1 - \alpha_{\text{top}}) \alpha_{\text{bot}}(\lambda) d\lambda
\]  

(2)

Here \( I(\lambda) \) is the wavelength-dependent AM 1.5 irradiances.

The absorption coefficient for the top cell

\[
\alpha_{\text{top}}(\lambda) = 1 - e^{-\alpha_{\text{perovskite}}(\lambda)L_{\text{top}}}
\]  

(3)

The absorption coefficient for the bottom cell

\[
\alpha_{\text{bot}}(\lambda) = 1 - e^{-\alpha_{\text{Si}}(\lambda)L_{\text{bot}}}
\]  

(4)

Here \( L_{\text{top}} \) and \( L_{\text{bot}} \) is the thickness of the top and bottom cells respectively.

![Fig. 2](image_url) Equivalent circuit of an ideal solar cell
The simulation of potential differences across the solar cell can be carried out by assuming that the solar cell has an ideal diode current−voltage (IV) characteristic. The equivalent circuit of the ideal solar cell is shown in Fig. 2.

From the circuit, the total current \( I \) and saturation current \( I_s \) of the solar cell is given by the Eqs. (5) and (6) (Sze and Ng 2007)

\[
I = I_s \left[ e^{\frac{qV}{kT}} - 1 \right] - I_L
\]  
\[
I_s = AqN_cN_v \left( \frac{1}{N_A} \sqrt{\frac{D_n}{\tau_n}} + \frac{1}{N_D} \sqrt{\frac{D_p}{\tau_p}} \right) e^{-\frac{E_g}{kT}}
\]  

Here \( I_L, N_c, N_v, k, q, D_p, D_n, \tau_p, \tau_n, N_A, N_D, E_g, T \) are the photocurrent, conduction band carrier density, valence band carrier density, Boltzmann constant, the charge of an electron, hole diffusion coefficient in the emitter, electron diffusion coefficient in base, a hole lifetime in the emitter, an electron lifetime in base, acceptor density, donor density, band gap energy, and absolute temperature respectively.

Open circuit voltage (\( V_{oc} \)) can be found by taking \( I = 0 \). The equation for open-circuit voltage is given by Eq. (7) (Sze and Ng 2007)

\[
V_{OC} = kT \frac{q}{q} \ln \left( \frac{I_L}{I_s} + 1 \right)
\]

Short circuit current (\( I_{sc} \)) can be found by taking \( V = 0 \). The equation for short-circuit current is given by Eq. (8) (Sze and Ng 2007).

\[
I_{sc} = q \int [1 - R(\lambda)] \phi(\lambda) \text{IQE}(\lambda) d(\lambda)
\]

Here, IQE(\( \lambda \)), R(\( \lambda \)), and \( \phi(\lambda) \) are the internal quantum efficiency of the solar cell for a particular wavelength, the fraction of these photons reflected from the surface, and the number of incident photons per area per time per unit bandwidth respectively.

The equation of 1D steady-state continuity equation for low-injection condition and doping profiles \( N_D >> N_A \) are given by the Eqs. (9) and (10) (Sze and Ng 2007).

For electrons in the p-type layer

\[
G_n - \left( \frac{n_p - n_{p0}}{\tau_n} \right) + \frac{1}{q} \frac{dJ_n}{dx} = 0
\]  

For holes in the n-type layer

\[
G_p - \left( \frac{p_n - p_{n0}}{\tau_p} \right) + \frac{1}{q} \frac{dJ_p}{dx} = 0
\]

Here \( G_n \) and \( G_p \), \( J_n \) and \( J_p \) are the electron and hole generation rate, and the electron and hole current densities respectively. \( n_p, n_{p0}, p_n, \) and \( p_{n0} \) are the total and thermal equilibrium carrier concentrations.

The spectral response of the cell is dependent on the wavelength of radiation, which can be evaluated by external quantum efficiency and internal quantum efficiency. The EQE and IQE can be calculated by the Eqs. (11) and (12) (Sze and Ng 2007)
Here $J_{ph}$ is the photocurrent density.

A tandem perovskite/silicon solar cell is modeled in Matlab using the above equations. The parameters such as doping concentrations, diffusion coefficients, thickness, and band-gap energy are optimized for analytical modeling to calculate the voltage, current density, and quantum efficiency of the tandem solar cell. Reflective index (n), extinction coefficient (k), absorption coefficient, and reflectivity values of silicon, perovskite, ZnO, and Si$_3$N$_4$ materials are also taken into consideration to evaluate the external quantum efficiency (EQE) and reflectivity of light-absorbing materials. The current is the same and voltages are added in the series connected tandem solar cell. The simulation model gives the values of open-circuit voltage, short-circuit current, fill factor, maximum power, and efficiency of both sub-cell and tandem cell respectively for photon flux at AM 1.5 solar spectrum. The parameters are optimized to achieve a theoretical efficiency of the tandem solar cell of over 32%.

The anti-reflective ZnO-coated perovskite layer and intermediate anti-reflective Si$_3$N$_4$ coated silicon bottom cell is analyzed in series-connected tandem configuration and compared with the non-coated intermediate anti-reflective coated tandem solar cell. The single anti-reflection (SAR) and double anti-reflection (DAR) models are used to get the optimum thickness of AR coating and to minimize the reflection from the top and bottom sub-cells (Hu et al. 2019; Green et al. 2014; Ashwith et al. 2015; Jošt et al. 2020; Sahouane and Zerga 2014; Du et al. 2015).

4 Results and discussion

The tandem solar cell is analyzed under illumination at AM 1.5 over wavelengths ranging from 300 to 1200 nm. The efficiencies of with and without intermediate anti-reflective Si$_3$N$_4$ coated perovskite/silicon tandem solar cell are recorded and compared.
4.1 Absorption coefficient and bandgap of perovskite and silicon material

The comparison between the absorption coefficient of the perovskite and crystalline silicon materials is shown in Fig. 3. The values of the extinction coefficient ‘k’ of the two materials are used to calculate the absorption coefficient (Green and Keevers 1995; Green 2008; Phillips et al. 2015). Perovskite is a direct bandgap semiconductor with a high absorption coefficient and a low penetration depth. The diffusion length of perovskite is larger than the penetration depth. Therefore, there is no requirement for light trapping in the top cell to increase short-circuit current and quantum efficiency. However, silicon is an indirect bandgap material with a low absorption coefficient close to the bandgap. The penetration depth of silicon close to the bandgap is larger than the thickness of the typical solar cell. Therefore, there is a requirement for light trapping in the bottom cell to increase short-circuit current and quantum efficiency. The light trapping in the bottom cell can be achieved by texturing the silicon’s surface or placing an anti-reflective coating layer. The textured surface or ARC layer will support the refraction of light to improve the optical path length in the bottom cell. Therefore, photon or light management in the bottom cell is more difficult than in the top cell. The efficient coupling of the incident light, designing a light-trapping structure with small parasitic optical losses, and confinement of light by trapping structure will improve the performance of the bottom cell. The reflection and parasitic losses must be minimized to improve the performance of the top cell. The band gap of the perovskite can be controlled by changing the halide or organic molecule composition in the ABX$_3$ structure. The best-studied material is CH$_3$NH$_3$PbI$_3$ with a bandgap of ~ 1.65 eV. The optimization of the optical properties of the perovskite-based top cell will allow for obtaining a high extinction coefficient and large diffusion length for realizing solar cells with high short-circuit current densities and energy conversion efficiencies. The improvement in the light incoupling and minimization of optical losses will enhance the optics of the solar cell (Hossain et al. 2019). Therefore, anti-reflective layers are placed in the tandem solar cell to minimize optical losses.

Fig. 4 The variation in the overall efficiency of the tandem cell due to the change in the bandgap of the perovskite material
4.2 Optimization of the bandgap and thickness of the perovskite layer

There is an influence of perovskite’s bandgap and its thickness on the efficiency of the top cell. There is a decrease in short-circuit current $J_{sc}$ and an increase in open-circuit voltage $V_{oc}$ with increasing values of bandgap because of the reduction in the photo-generated charge carriers (Nagel et al. 1999; Minemoto and Murata 2015). The perovskite bandgap varied from 1.65 to 1.70 eV during the numerical simulation of the tandem solar cell. The maximum efficiency of over 32% is achieved by optimizing the bandgap and thickness of the perovskite layer. The optimized values of the bandgap and thickness for the perovskite layer are 1.65 eV and 150 nm respectively. The variation in the overall efficiency of the tandem cell due to the change in the bandgap and thickness of the perovskite is shown in Figs. 4 and 5.

4.3 Current matching issue in the perovskite/silicon tandem solar cell

A good current matching is required between the perovskite sub-cell and silicon sub-cell to achieve maximum efficiency for the tandem configuration. The variation of the bandgap and thickness of the light-absorbing material can be carried out to match the current...
density between the top and bottom sub-cells. The VI curve for the perovskite/silicon solar cell is shown in Fig. 6. The highest value of open-circuit voltage $V_{oc}$ and short-circuit current $J_{sc}$ are found to be 1.2 V and 25.4 mA cm$^{-2}$ for the top cell respectively. The highest value of open-circuit voltage $V_{oc}$ and short-circuit current $J_{sc}$ are found to be 0.66 V and 53 mA cm$^{-2}$ for the bottom cell respectively. The open-circuit voltage $V_{oc}$ for a tandem solar cell is found to be 1.64 V which is nearly the sum of the open-circuit voltage of both sub-cells. The maximum short-circuit current $J_{sc}$ of tandem solar cell is similar to that of the top sub-cell which means the value of current density depends upon the perovskite sub-cell. This could lead to non-ideal current matching between both sub-cells as shown in Fig. 6. The energy bandgap and the thickness of the perovskite layer in the top sub-cell need to be varied to achieve a good current matching between the two sub-cells. The perovskite layer acts nearly like an intrinsic layer due to low residual doping concentration.

4.4 Silicon tunnel junction

Silicon tunnel junction connects both perovskite and silicon sub-cells which act as a short circuit during tandem solar cell operation. The doping concentration of the n++ and p++ regions of this junction plays an important part in the efficient band-to-band tunneling effect. The perovskite’s bandgap and its thickness are optimized. Now, the tunnel junction doping concentration is also optimized to get a minimum doping concentration of around $10^{19}–10^{20}$ cm$^{-3}$. This minimum doping concentration will lead to a good interconnection between both sub-cells for an efficient tunneling effect. This value is the degeneracy limit of silicon below which there would be weak overlapping of conduction and valence bands and weak band-to-band tunneling (Rolland et al. 2014; Baudrit and Algora 2008).

5 Photon management in perovskite/silicon tandem cell

The reflectivity of the single and double anti-reflective layers is obtained by Eqs. (13) and (14) respectively (Kaddouri et al. 2015)

$$R_{SAR} = \left| r_{SAR}^2 \right| = \frac{r_{s1}^2 + r_{s2}^2 + 2r_{s1}r_{s2}\cos(2\theta_s)}{1 + r_{s1}^2 r_{s2}^2 + 2r_{s1} r_{s2} \cos(2\theta_s)}$$

(13)

$$R_{DAR} = \left| r_{DAR}^2 \right| = \frac{r_1^2 + r_2^2 + r_3^2 + r_4^2 r_5^2 + 2r_4 r_5 (1 + r_3^2) \cos(2\theta_1) + 2r_4 r_5 (1 + r_1^2) \cos(2\theta_2) + 2r_1 r_5 \cos(2(\theta_1+\theta_2)) + 2r_1 r_5 \cos(2(\theta_1-\theta_2))}{1 + r_1^2 r_2^2 + r_3^2 r_4^2 + r_2^2 r_5^2 + 2r_1 r_2 (1 + r_3^2) \cos(2\theta_1) + 2r_1 r_2 (1 + r_4^2) \cos(2\theta_2) + 2r_1 r_2 \cos(2(\theta_1+\theta_2)) + 2r_1 r_2 \cos(2(\theta_1-\theta_2))}$$

(14)

The parameters in Eqs. (15) and (16) are dependent on the refractive index and thickness of the anti-refractive coating layer and silicon. Therefore, $R_{SAR}$ and $R_{DAR}$ can be calculated from the optimal refractive index and thickness of the silicon and anti-reflective material.
5.1 ZnO antireflective layer

The reflection loss in the top cell is mainly because of the back contact and charge transport layers. In the tandem cell structure, ZnO with refractive index \( n = 2 \) and band gap 3.37 eV is placed over the perovskite layer of the top cell to minimize this reflection loss (Hasan et al. 2017; Bond 1965). The optical reflectance spectrum for the ZnO layer on perovskite for different thicknesses is shown in Fig. 7. The thickness of the ZnO is varied from 100 to 300 nm. There is a decrease in the reflection loss from the ZnO layer with an increase in its thickness up to 200 nm. However, there is an increase in the reflection loss from the ZnO layer after increasing the thickness above 200 nm. The reflectivity of ZnO with 200 nm thickness is 15% in the visible range for the ZnO/perovskite layer. It decreases with an increase in the wavelength from 500 to 1200 nm as shown in Fig. 8. The optical spectrum between 200 and 800 nm will influence the perovskite solar cell. When the thickness of the ZnO layer is increased beyond 200 nm and is greater than the wavelength of the incoming light wave, then this will prevent incoming light from entering the top cell. Therefore, the optimal thickness of the ZnO anti-reflection layer is 200 nm at which near-infrared reflection loss by the perovskite-based top cell in the device structure can be minimized and the maximum transmittance of near-infrared energy to the silicon sub-cell can
be possible. When the light enters the top cell, the refractive index of the air is less than the refractive index of the anti-reflective ZnO layer. When light is present inside the top cell and intends to leave the cell, the refractive index of the first layer of the anti-reflection layer is higher than the second medium which is the air. Therefore, there is a reflection of light back into the first environment to prevent the escape of light. Therefore, the anti-reflective ZnO layer behaves like a light trap. The anti-reflection layer typically consists of one or more dielectric layers (non-conductive). The reflection of incident light on the surface of the cell can be minimized because the presence of an anti-reflection layer can reduce the dielectric contrast between the air and the first layer of the cell (Shahverdi et al. 2019). The optical reflectance spectrum of the perovskite-based top cell with and without the ZnO layer is shown in Fig. 9. The reflectivity of the perovskite-based top cell without the ZnO layer is 77% for the 750 to 1200 nm wavelength region because of the presence of back contact and the Cu2O layer. The reflectivity of the perovskite-based top cell with the ZnO layer is 57%. Therefore, the innovative idea of using electron transport material ZnO as an anti-reflection layer in the perovskite-based top cell has reduced the reflection loss by nearly 20%. In this study, it is assumed that there are no losses from glass (FTO or ITO).

5.2 Intermediate Si3N4 anti-reflective layer

The intermediate anti-reflective layer of Si3N4 is placed between the high energy gap (top cell) and the lower energy gap (bottom cell). The intermediate anti-reflective layer is responsible for the localization of photon energy in the bottom cell. The short-circuit current and quantum efficiency of the bottom cell will increase because the intermediate anti-reflective layer reduces reflection and increases the absorption of photons from incoming light. A single anti-reflective (SAR) and double anti-reflective (DAR) Si3N4 reflection model is developed for optimizing the refractive index and thickness of the anti-reflective coating layer over the top and bottom sub-cell of tandem configuration. Silicon nitride films can be optimized by varying their refractive indices and layer thickness. The optimized intermediate ARC layer has provided maximum photon flux and the lowest reflectivity for wavelength ranging between 300 and 1200 nm. The maximum photon flux has increased the current density and efficiency of the cell. The surface reflection is reduced by 30% due to the introduction of the Si3N4 layer over the bottom sub-cell as compared to the tandem configuration without an intermediate ARC layer. The optimized refractive
The index of the intermediate ARC Si$_3$N$_4$ layer is found to be 1.85 which is evaluated by Eq. 15 (Davidson 2017; Philipp 1973).

\[ n_{\text{SAR}} = \sqrt{n_0 n_{\text{si}}} \]  

(15)

Here \( n_0 = 1 \) and \( n_{\text{si}} = 3.42 \) are the refractive indices of air and silicon respectively.

There is a strong dependence on ARC layer thickness, its refractive index, and light wavelength for minimizing reflectivity. The maximum photon flux and low reflectivity can be obtained by setting the wavelength at 600 nm for an intermediate single ARC layer. The optimal thickness can be obtained at wavelength 600 nm and refractive index \( n_{\text{SAR}} = 1.85 \) which is evaluated by Eq. 16 (Davidson 2017):

![Optical reflectance spectrum for an intermediate single antireflective layer of Si$_3$N$_4$](image1)

![Contour plot of reflectivity as a function of film thicknesses for given refractive indices for intermediate double anti-reflection coating](image2)
The optical reflectance spectrum for an intermediate single anti-reflective layer of Si₃N₄ is shown in Fig. 10. The minimum reflection from the intermediate single ARC layer is possible only at a specific range of wavelength, generally at the middle of the visible spectrum (500–600 nm), whereas intermediate double ARC is effective over the whole visible spectrum (Duttagupta et al. 2012).

For double anti-reflective coating, the top intermediate anti-reflective layer has a lower refractive index value than the bottom intermediate anti-reflective layer which is attached to the silicon sub-cell (Hossain et al. 2019; Nagel et al. 1999; Minemoto and Murata 2015). The reflectivity for the top and bottom intermediate ARC layers is evaluated for thickness ranging from 20 to 120 nm. The optimized refractive index for the top and bottom intermediate ARC layers is 1.75 and 2.0 respectively. The optimal thickness for the top and bottom intermediate ARC layers is 50 nm and 30 nm respectively. The contour plot of reflectivity as a function of film thicknesses for given refractive indices for the intermediate double antireflection coating layer is shown in Fig. 11. The reflectance is reduced to <25% over a wide range of spectra (i.e., for wavelengths of 300–1200 nm).

6 Optimization of the perovskite/silicon tandem-cell

The efficiency of over 32% is achieved by optimizing the parameters of different materials such as perovskite, silicon, and anti-reflection layers in the tandem solar cell. The maximum value of open-circuit voltage $V_{oc}$ and short-circuit current $J_{sc}$ for tandem configuration are 1.64 V and 25.4 mA cm$^{-2}$ respectively without an intermediate anti-reflective Si₃N₄ coating layer as shown in Fig. 12. The optimization of the efficiency of the perovskite sub-cell is carried out by changing the perovskite’s bandgap and its thickness. Hole transport material (HTM) plays an important role in high photovoltaic performance. Cu₂O possesses high hole mobility, long carrier diffusion length, and matching energy levels with the valence band edge of the perovskite material. Because of the incorporation of Cu₂O, there will be a low series resistance, high shunt resistance, and low ideality factor, which will result in a low recombination loss in the device. There is a reflection loss in the

$$t_1 = \frac{\lambda_0}{4n_{SAR}}$$

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**Fig. 12**  J–V characteristics of the bottom cell, top cell, and tandem cell under AM1.5 illumination without intermediate silicon nitride anti-reflective layer on the bottom cell.
tandem device because there is a reflection of infrared light from the perovskite-based top cell. The contacts in the device can also decrease the transmittance of incident light into both sub-cells due to the absorption and reflection of light, which can decrease the photo-generated current. The reflection and absorption curves of the materials in the top and bottom sub-cells can assist in minimizing reflection losses and improve the efficiency of the device. The optical losses are minimized by introducing an anti-reflective ZnO and Si$_3$N$_4$ layers over the perovskite layer and silicon sub-cell respectively. The open-circuit voltage and short-circuit current are 1.2 V, and 25.4 mAcm$^{-2}$ respectively for the top cell for the optimized thickness of 200 nm for ZnO and 80 nm for Cu$_2$O because there is a lowest reflectance and highest transmittance for incident light on the surface of the top cell. The current mismatch is nearly minimized by optimizing the thickness of the perovskite layer. The optimized thickness is obtained when the current density of the perovskite absorber layer matches the silicon absorber layer. Perovskite material with a band gap of 1.65 eV has to maximize the current density for the top sub-cell. This will help to achieve maximum power conversion efficiency for the tandem device.

The light of a particular wavelength is absorbed by the p-type Si wafer in the bottom cell of the tandem configuration to generate current density ($J$). The free carrier absorption (FCA) in the highly doped emitter and back surface field (BSF) has no contribution to
the current generation in the silicon sub-cell of the tandem configuration. Silicon sub-cell operates at lower injection levels in the tandem configuration as compared to standard irradiance conditions. There would be a variation in the injection level for the silicon sub-cell due to the materials in the top sub-cell and the optical structure of the tandem configuration. The change in photo-generated current leads to variation in open-circuit voltage ($V_{oc}$) and fill factor ($FF$) of the silicon sub-cell. The dependence of injection levels of silicon sub-cell can be evaluated accurately by taking constant diode parameters (Fujiwara and Kondo 2007). The reflection losses can be crucial for achieving high cell efficiency. The reflection losses are taken into consideration in solar cells for evaluating the short-circuit current in which the absorption layer’s thickness is smaller as compared to the collection length of minority carriers. An intermediate single and double antireflection layer of silicon nitride are introduced over the bottom sub-cell to minimize reflection loss in the tandem solar cell. The influence of the intermediate ARC layer on the bottom cell is investigated by optimizing its refractive index over wavelength ranging from 300 to 1200 nm. There is an enhancement in open-circuit voltage $V_{oc}$ and short-circuit current $J_{sc}$ for an intermediate double anti-reflective layer-based bottom cell as compared to an intermediate single anti-reflective layer-based bottom cell as shown in Table 2. The maximum photogenerated current density of the silicon sub-cell is a function of ARC layer thickness and refractive index. The variation in the refractive index of ARC tends to change the current density and open-circuit voltage. The enhancement in open-circuit voltage $V_{oc}$ and short-circuit current $J_{sc}$ by introducing an intermediate anti-reflective layer is shown in Figs. 13 and 14.

In Table 2, ‘T’ and ‘E’ represent theoretical and experimental data of the different tandem solar cells.
| Computational model adopted | Device architecture                     | Antireflective coating (ARC) | Charge transporting layers | Efficiency (%) | References          |
|-----------------------------|----------------------------------------|------------------------------|-----------------------------|----------------|---------------------|
| Single-diode modeling       | Perovskite/Si Tandem Cell              | Present                      | TiO$_2$, Spiro-OMeTAD       | 31.78          | Davidson (2017)     |
| Single-diode modeling       | Cu$_2$O/Silicon Tandem Cell            | Not Present                  | ZnO, Cu$_2$O                | 31.23          | Mitroi et al. (2017) |
| One-diode model             | Perovskite/Si tandem solar cell        | Present                      | TiO$_2$, Spiro-OMeTAD       | 31.00          | Lehr et al. (2018)  |
| Transfer matrix modeling    | Perovskite/Si tandem solar cell        | Present                      | PCBM, Spiro-OMeTAD          | 31.00          | Altazin et al. (2018) |
| Single-diode modeling       | Perovskite/Si Tandem Cell              | Present                      |                             | 33.00          | This work           |
7 Quantum efficiency of the tandem solar cell

The External Quantum Efficiency (EQE) is calculated for the top and bottom cells. The optimized EQE spectra of the sub-cells reveal that complementary absorptions occur for the wavelength ranging from 300 to 1100 nm. The top cell is absorbing almost every wavelength. The limit between the two materials is very well defined due to the strong
absorption of the perovskite material. The increase in absorption in the overlying layers is the main reason for the increase in EQE over a wide range of the wavelength for an AR-coated device as compared to the device without an intermediate ARC layer as shown in Figs. 15 and 16, and 17.

8 Conclusion

The light trapping in the solar cell can enhance the light incoupling and minimize optical losses for developing highly efficient tandem solar cells. An increased light incoupling and a decrease in optical losses within the device can significantly improve the photon management of a perovskite/silicon tandem solar cell. The numerical simulation using a single-diode model is performed to investigate the optical and electrical properties of the perovskite/silicon tandem solar cell. In this article, ZnO and Si$_3$N$_4$ are used as anti-reflection coating layers for photon management in the perovskite/silicon tandem cell. At the optimal thickness of the ZnO anti-reflection coating layer, the near-infrared reflectance loss by the perovskite layer in the device structure is minimized and the transmittance of near-infrared energy to the silicon sub-cell is maximized. The innovative idea of using electron transport material ZnO as an anti-reflection coating layer in the perovskite-based top cell has minimized the reflection loss by nearly 20%. Si$_3$N$_4$ layer assisted the localization of transmitted near-infrared photon energy in the silicon sub-cell. The optimization of the refractive index and thickness of the intermediate Si$_3$N$_4$ anti-reflection coating layer is done to minimize the reflectivity in the bottom cell. The intermediate double anti-reflection Si$_3$N$_4$ layer is effective over the whole visible spectrum, whereas an intermediate single ARC layer can be non-reflective only at a specific range of wavelength, generally at the middle of the visible spectrum. The combination of top and bottom anti-reflection layers has improved the conversion efficiency of the tandem cell by 1% because the optical properties of the tandem cell are enhanced. The optimization of band gap energy and thickness of the perovskite top cell ensures the efficiency of the tandem solar cell reaches over 32%. The simulation results based on the single diode model are consistent with theoretical or experimental values for other types of tandem cells described in the literature with a 1–8% deviation. The deviations are caused because of the different device architectures and computational models. Therefore, the findings pave the path for the design and development of photon-managed tandem solar cells with high efficiency.

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Declarations

Conflict of Interest The authors declare that they have no conflict of interest.

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