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Research Paper

Light management in Perovskite thin-film Solar Cells using multiple Gratings

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Abstract:
In this study, we developed a new method based on uniform and graded gratings on the back surface of perovskite ultrathin film solar cells to enhance light absorption. The proposed gratings were designed in two configurations including penetrating the active layer and placing on it. These structures increase absorption by scattering and diffracting light and enlarging the optical path of photons. Simulations based on the finite element method showed that graded gratings can significantly enhance the absorption in the visible and infrared regions. The maximum current density and efficiency obtained from dense gratings placed on the back surface of the active layer were 27.59 and 25.52% mA/cm^2, conventional PSCs that suffer from reduced efficiency under angled light incidence, our cell with graded gratings maintains high light absorption even at angles up to 45 degrees.

Keywords:
Thin-Film Solar Cells Perovskite,Graded Gratings,Absorption, Plasmonic, Scattering

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1.INTRODUCTION

Thin film (SC) is of interest because of its capabilities for less money, flexibility, and easier manufacturing compared to conventional solar cells [1]. These advantages can be realized with various materials, including amorphous and crystalline silicon, GaAs, CIGS, CdTe, and perovskites [2-4]. Perovskites, a unique class of hybrid organic-inorganic materials, hold particular promise for SC applications. They offer ease of fabrication, impact resistance, and high flexibility – all highly desirable for thin-film technologies [5].Additionally, perovskites boast long exciton diffusion lengths, suitable bandgaps, and strong light absorption coefficients, making them prime candidates for high-performance thin-film (PSCs) [6,7].Recent research has yielded significant progress in PSC efficiency. Studies have demonstrated that incorporating randomly dispersed plasmonic nanoparticles within the active layer can achieve efficiencies exceeding 26% [8]. Similarly, other approaches, such as utilizing surface plasmons from silver nanoparticles, have shown promise in enhancing light absorption and current generation(reaching 21.25 mA/cm2)[8].Notably, perovskite/silicon tandem solar cells have even pushed the boundaries of efficiency, reaching a remarkable 32.5% [9]. However, one key area for improvement in PSCs remains their light absorption compared to other types of solar cells. One key strategy to overcome the light absorption limitation and achieve even higher efficiencies in solar cells (SCs) involves light trapping methods [10,11]. These methods leverage photonic and plasmonic structures to improve light absorption within the cell by exciting specific modes of light interaction. Since SC efficiency hinges on effective light trapping or enhancement, these methods offer a promising approach. Photonic structures, such as gratings and nanowires, manipulate light propagation to achieve this goal. Gratings, with their periodic variations in refractive index, cause light to scatter and diffract within the cell, increasing its path length [24]. Nanowires, on the other hand, effectively trap light through a phenomenon called total internal reflection (TIR) [12,13]. Plasmonic structures offer a complementary approach. These structures, including metallic nanostructures and nanoparticles, utilize their interaction with light to excite surface plasmon resonances (SPRs) at the interface with surrounding materials. This enhances light absorption within the cell [14-16]. It's important to note that advancements in SC efficiency extend beyond light trapping. Phenomena from quantum mechanics, such as the introduction of intermediate bands and hot carrier extraction, are also being explored as potential avenues for further improvementaBeyond light trapping methods, researchers are exploring additional avenues to boost solar cell (SC) efficiency. Two promising approaches include intermediate bands and hot carrier extraction [17-20].

Intermediate bands introduce new energy levels within the forbidden bandgap of a solar cell.These additional levels allow for the absorption of lower-energy photons that wouldn't normally excite electrons across the full bandgap. This translates to increased overall light absorption within the cell [21, 22]. Hot carrier extraction tackles a different challenge. High-energy photons can lose their excess energy as heat before being converted into electricity. Hot carrier extraction focuses on capturing these energetic electrons before thermalization occurs, maximizing their potential for electrical generation [23,24]. Beyond the well-established benefits of gratings for light trapping, recent research explores their potential to enhance light absorption through localized surface plasmons (LSPs). This approach affects the interaction between light and metal nanostructures at the interface with surrounding materials [25]. Studies by Yue et al. exemplify this concept, where incorporating silver nanoparticles within the solar cell significantly boosted near-infrared absorption (by 58.2%) due to LSP excitation by the nanoparticles [26]. The use of gratings for combined light trapping and absorption enhancement is not a new avenue. Tooghi et al. employed gratings on both the front and back of the cell, achieving substantial improvements in current density and efficiency by exciting both photonic and plasmonic modes [27]. This approach highlights the LSPR and light scattering within active layer. Similarly, Abdelraouf et al. proposed using optimized nanostructures for light capture, combining photonic and plasmonic properties. They utilized finite-element method (FEM) simulations to identify ideal grating sizes for maximizing absorption [28]. Our own research aligns with these advancements, demonstrating a significant increase (nearly threefold) in near-infrared light absorption through the incorporation of multiple backside gratings. This ultimately translates to an impressive 8.44% improvement in overall cell efficiency [29]. This paper investigates the incorporation of graded gratings into a silver back reflector for perovskite solar cells (PSCs). The proposed cell structures with graded gratings are depicted in Figure 1. The cells are categorized into five cases: Case 1 (typical gratings), Case 2 (two different grating sizes), Case 3 (three different sizes), Case 4 (four different sizes), and Case 5 (five different sizes).The designed PSCs feature a multilayer structure consisting of a silver back reflector and back contact, (CuSCN) as HTL, methylammonium lead iodide ($CH_3NH_3PbI_3$) as the active layer, (TiO_2) as ETL, and (ITO) as the front contact. The thicknesses of these layeres are 400 nm, 20 nm, 500 nm, 50 nm, and 75 nm, respectiveley. ITO and silver are placed on the front and back surfaces, respectively, serving as an anti-reflective coating layer to reduce light reflectance and suppress light transmission from the cell. The silver layer is sufficiently thicker than its skin depth, and the ITO layer thickness is calculated based on [30]. In Case 1, the unit cell periodicity is assumed to be $P0 = 300$ nm. For the other cases, the periodicity is multiplied by the respective grating number (Pi = i×P0) where i = 1, 2, 3, 4, and 5.The grating width is denoted as wg, and the grating height is set to hg. In previous studies, the grating heights were varied in the z-direction (hg1, hg2, hg3, hg4, hg5), and the grating widths were varied in the x-direction (w1, w2, w3, w4, w5). For the current study, the grating width wg remains constant, while the heights vary as h1to h5. [31].

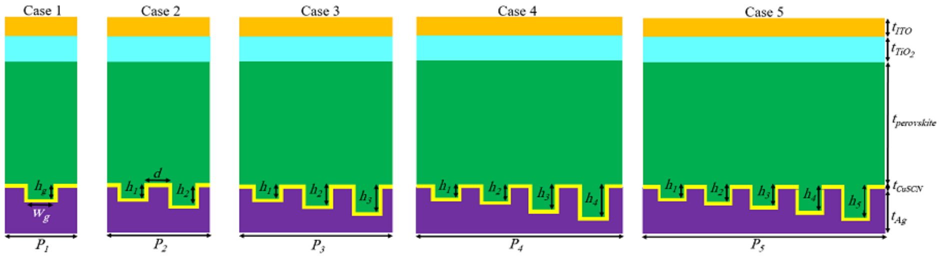


Fig. 1. Schematic of the proposed PSCs with d = 150 nm, t_{Ag} = 400 nm, t_{CuSCN} = 20 nm, $t_{perovskite}$ = 500 nm, t_{TiO2} = 100 nm, t_{ITO} = 75 nm, and $P_i = i \times P_0$, P_0 = 300 nm (i = 1, …, 5), for: a) Case 1, b) Case 2, c) Case 3, d) Case 4, and e) Case 5.

2.MATHEMATICAL FORMULATIONS

To assess the performance (PSCs), light absorption is a critical parameter. It quantifies the cell's capability to capture incident light and can be expressed as In this equation, λ0 represents the central wavelength, to set 550 nm. The refractive index of ITO at the central wavelength, n(λ0), is assumed to be 1.83. The refractive indices of other layers are obtained from references [32,33].

$$d = \frac{\lambda_0}{4n(\lambda_0)} \quad (1)$$

$$A(\lambda) = 1 - R(\lambda) - T(\lambda) \quad (2)$$

The presence of a highly reflective silver layer on the cell's backside effectively eliminates the transmission component, T(λ), in Equation 2. Therefore, the equation reduces to:

$$A(\lambda) = 1 - R(\lambda) \quad (3)$$

While Equation 3 calculates absorption of the Sc, to determine absorption individual layers, we employ the following equation, as described in [34]:

$$A(\lambda) = \frac{\omega\varepsilon''}{2P_{in}} \int_v |E(\lambda)|^2 \, dV \quad (4)$$

In the aforementioned equation, ω represents the angular frequncy, ε" denotes the imaginaray part permitivity, |E(λ)| signifies the electeric field intensity, and Pin represents the incedent solar power. Subsequently, Jsc and η are computed as follows:

$$J_{sc} = \frac{q}{hc} \int_{\lambda_{min}}^{\lambda_{max}} S(\lambda) A(\lambda) \lambda d\lambda \quad (5)$$

$$\eta = \frac{\int_{\lambda_{min}}^{\lambda_{max}} S(\lambda) A(\lambda) \frac{\lambda}{\lambda_g} d\lambda}{\int_{300\,nm}^{4000\,nm} S(\lambda) d\lambda} \quad (6)$$

In this equation, q, h, c, λg, and S(λ) represent the elementary charge, Planc constant, speed of light, perovskite bandgap wavelength, and solar radiation spectrum, respectively. Coupling is done in the wavelength domain λmin to λmax, as defined in reference [34].A diffraction grating, A periodic structure refracts the incident light acts differen angle and acts as a scattering elemen separates the constituent wavelength of a light spectrum. The diffraction angle are determined by the incident angle (θin), grating period (Λ), and wavelength landing light (λ), It is explained by the following equation [35]:

$$\theta_m = \sin^{-1}(\sin\theta_{in} + m\lambda/\Lambda); \quad |m| \leq \Lambda/\lambda, \quad m = 0, \pm 1, \pm 2, \ldots \quad (7)$$

By manipulating dimensions a diffuse grating, it thereby increases the absorption and absorption of light in the material.

3.RESULTS

3.1. OPTIMAL DIMENSION

For investigations of high input light absorption in (PSCs), we utilized the (FEM), a powerful wave-based simulation technique for optoelectronic devices. Figure 2.a presents the absorption spectera for reference cell Cases 1 to 5. Additive gratings significantley increase the absorption in (IR) region of solar spectrum, which is primarily attributed to the excitations localzed surface plasmon (LSPs) and light condensation. Excitaton of localzed surface plasmon (LSPs) increases the electric field around gratings, leading to a significant enhancement in absorption, as absorption is proportinal to square of the electrics field magnitude |E(λ)|. Additionally, the scattering of light within the active layer increases the optical path length photon, resulting in a higher generation rate and

Photo current. To quantitatively evaluate the impact of backside graded gratings on active layer absorption and gain insights into the underlying light absorption phenomena, the absorption enhancement can be calculated as ratio of the proposed PSCs' absorption to that of reference cell. As showen in Figur 2.b, an enhancement of nearly fourfold is achieved in certain near-IR wavelength.

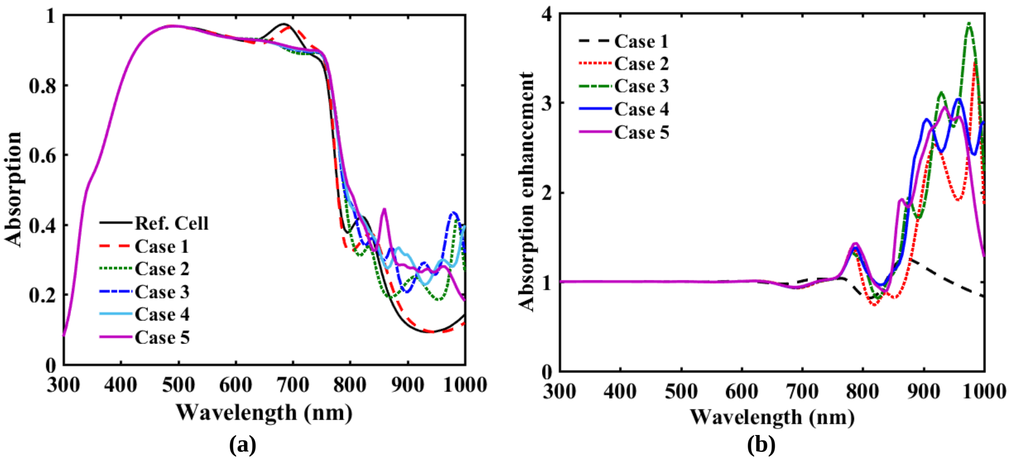


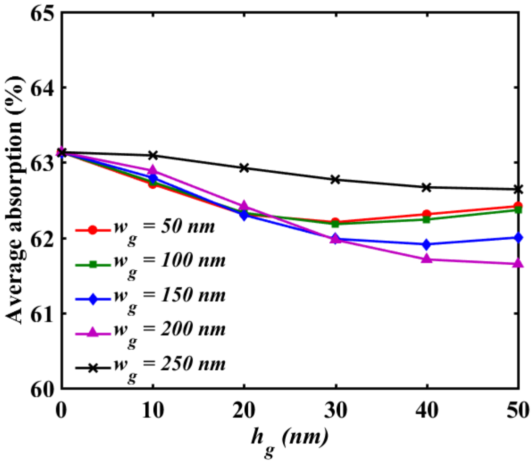
Fig. 2. a) Absorption spectra vs. wavelength for reference cell and proposed SCs, b) Absorption enhancement vs. wavelength for Case 1 to Case 5.

To quantitatively evaluate the impact of graded gratings, Table 1 presents the average absoroption, Short circuit current density, and power conversion Efficiency of reference cell and propse structure. As shown, the highest averag absorption 67.1%, current density 27.59 mA/cm², and power conversion efficiency of 25.52% are achieved in Case 4. For this case, an enhancment of 6.3%, 5.2%, and 4.3% is obtained compared to the reference cell, respectively. Notably, Case 1 exhibits a lower absorption than the reference cell, while graded gratings generally lead to higher absorption. These findings suggest that single gratings are not suitable for design high-absorption solar cell based on our simulation.

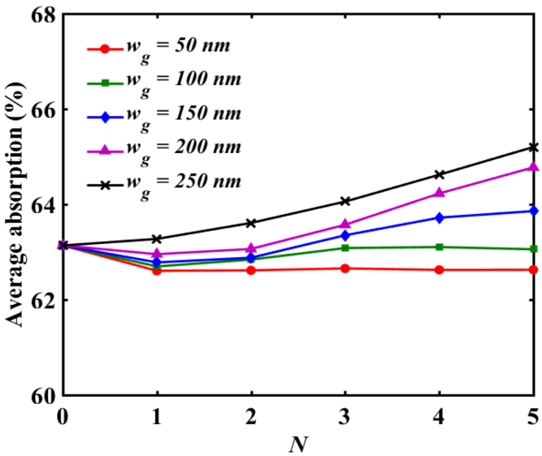
Table 1
The average absorption, short circuit current density, and efficiency of the reference cell, and Case 1 to Case 5

Type of SCs	Ref.Cell	Case 1	Case 2	Case 3	Case 4	Case 5
Averege absorption (%)	63.1	62.7	65.2	67	67.1	66.9
Short circuit current density (mA/cm^2)	26.22	26.20	26.86	27.53	27.59	27.51
Efficiency (%)	24.26	24.23	24.84	25.51	25.52	25.50

To optimize the dimension of the graded grating for high absorption, various grating widths were considered. The results indicate that increasing the grating size generally leads to a decrease in average absorption. This is *attributed* to the reduced efficiency of typical gratings in scattering light into the cell, coupled with increased parasitic losses in the silver-graded gratings, which ultimately diminish the net absorption. To enhance light scattering and absorption, graded gratings with varying depths were introduced, as described in [29].Figure 3.b illustrates the average absorption of Case 2 as a function of the N coefficient. The highest achieved value of 65.2% coresponds to graded grating a width of 250 nm and hights of 50 nm and 100 nm (N = 2). This suggests that Case 2 effectively scatters more light into the cell compared to Case 1.Figure 3.c presents the average absorption of Case 3 versus N for various grating widths [29]. The highst average absorption of 67% is achievd with a grating width of 250 nm and hights of 50 nm, 100 nm, and 150 nm (N = 5).Figure 3-d depicts the average absorption of Case 4 versus N. An average absorption of 67.1% is obtained with a grating width of 250 nm and height of 50 nm, 100 nm, 150 nm, and 200 nm (N = 4). this case, graded gratings effectively scatter more light withines the actives layer, resultings in enhanc absorptions.Figure 3-e shows the height achieved average absorption of Case 5, which is 66.9% and corresponds to a grating width of 250 nm and hights of 30 nm, 60 nm, 90 nm, 120 nm, and 150 nm (N = 3). In this structure, the average absorption is lower than in Case 4, indicating that Case 4 is a more efficient configuration.



(a)



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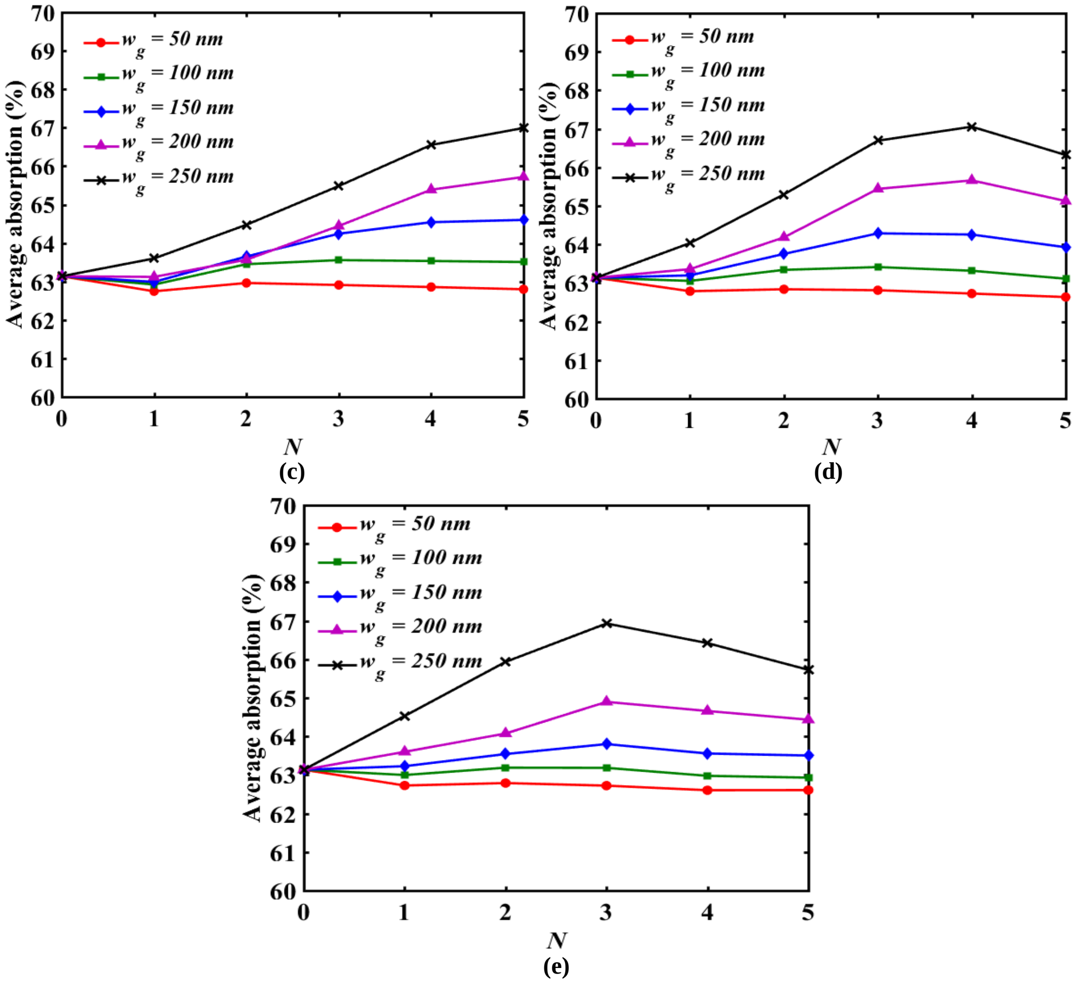


Fig. 3. a) The average absorption in terms of h_g with various w_g for Case 1, the average absorption vs. N for various w_g for: b) Case 2, c) Case 3, d) Case 4, and e) Case 5.

3.2. CURRENT ABSORPTION

Figure 4-a illustrates the current and voltage (J-V) charcteristics of the proposed (SCs). The maximum Short circuit current of 27.59 mA/cm² is achievd in Case 4, representing a 5.2% increase compared to the reference cell. The proposed SCs exhibit an Voc of 1.1 volts, which is higher than the Voc voltage of

the SC-based SCs. Figure 4-b presents the Short circuit current and efficiency of all proposed SCs. The maximum efficiency of 25.52% is obtained in Case 4, showing a 5.2% increase compared to the reference cell.

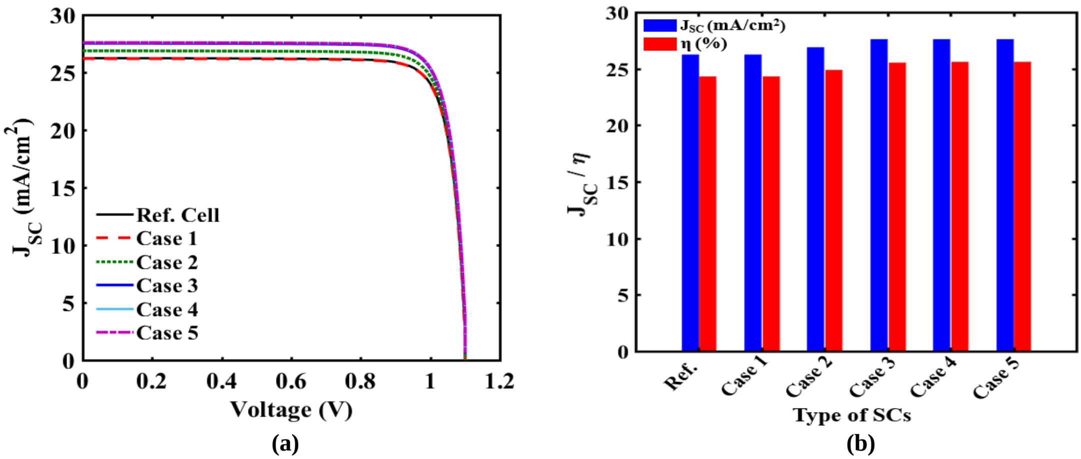


Fig. 4. a) The current-voltage characteristics, and b) The current density and efficiency for proposed SCs.

This section compares the findings of this research with similar studies, as presented in Table 2. Due to potential underestimation of losses in previous work, the comparison focuses on photocurrent derived the total absorption of perovskites layer. The results demonstrate that the proposd structure achieves the highst photocurent among compared devices.In [36,37], a study incorporated Al/SiO2 core-shell cluster nanoparticles within the perovskite layer. Their optimal configuration involved a 3 nm thick SiO2 shell, a central cluster NP with a 55 nm radius, and surrounding NPs with a 15 nm radius. In [38], another study used NPs with a 10 nm radius surrounded by 2 nm radius NPs. Compared to these approaches, the proposd structur offers a simpeler design while maintaining high performnces.Beyond Short circuit current, Efficiency, and Open circuit Voltage, additional crucial paramters for photovoltaic cells are photon absorption and carier transport. In thin absorber, photon absorption is the dominant factor governing solar cell performance, whereas charge carrier transfer becomes more critical in thicker absorbers. In this research, the thin perovskite layer facilitates efficient charge carrier transport to the electrodes, minimizing the potential for carrier recombination within the layer. The enhanced photon absorption achieved through plasmonic effects is expected to translate into increased solar cell efficiency for the proposed structure, as supported by prior research [39,40].

Table 2
Short-circuit current density in this research and other similar researches

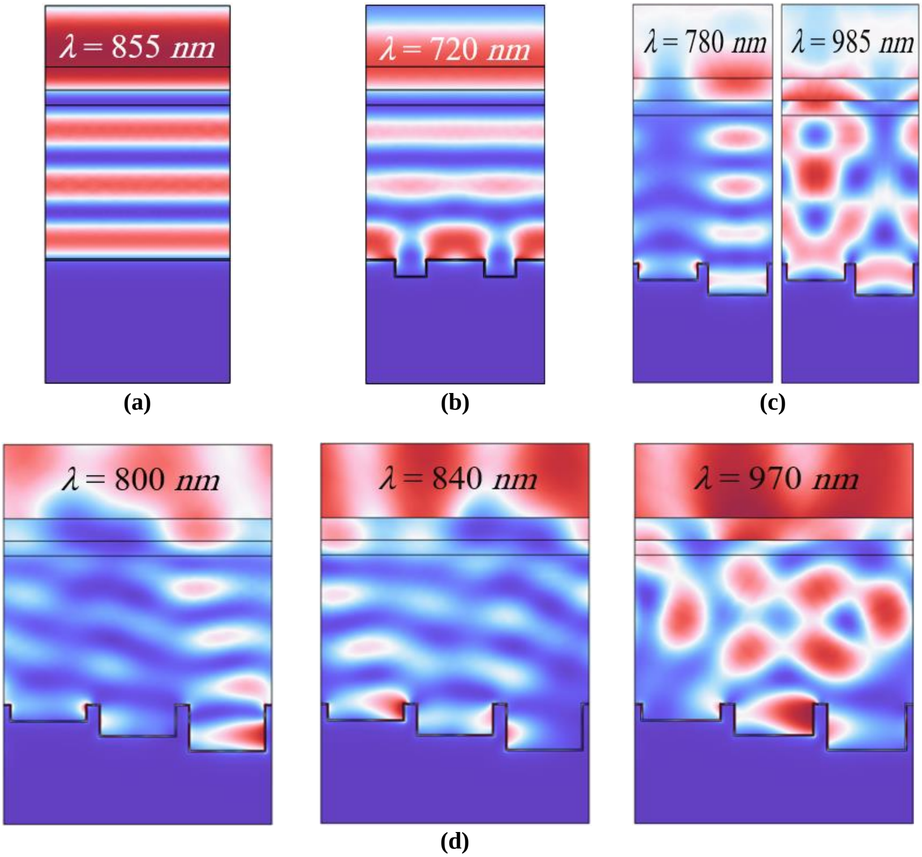
structure	Absorber thickness (nm)	Jsc (mA/cm^2)
This study	500	27.59
Al/SiO2 core-shell NPs [42]	250	22.28
lumpy Ag NPs[41]	50	22.05

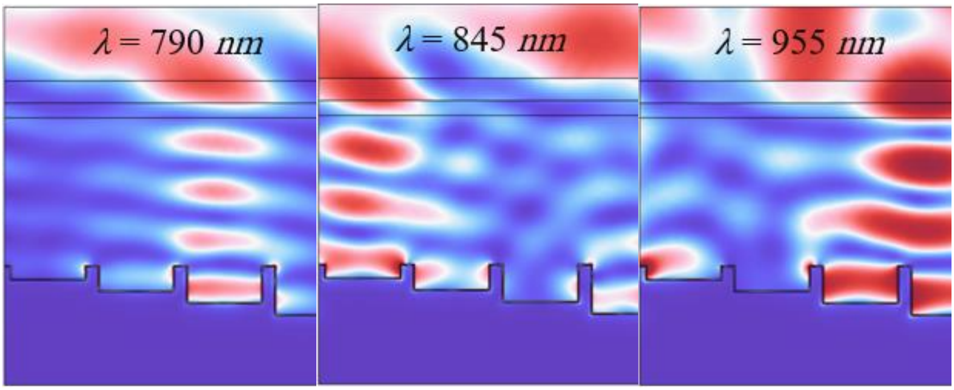
Additionally, a comparison between the obtained results and those from experimental studies is presented in Table 3. Experimental data were obtained for a perovskite active layer thickness of 680 nm, a silver layer thickness of 250 nm, grating width of 214 nm.

Table 3
Short-circuit current density in this research and other similar researches

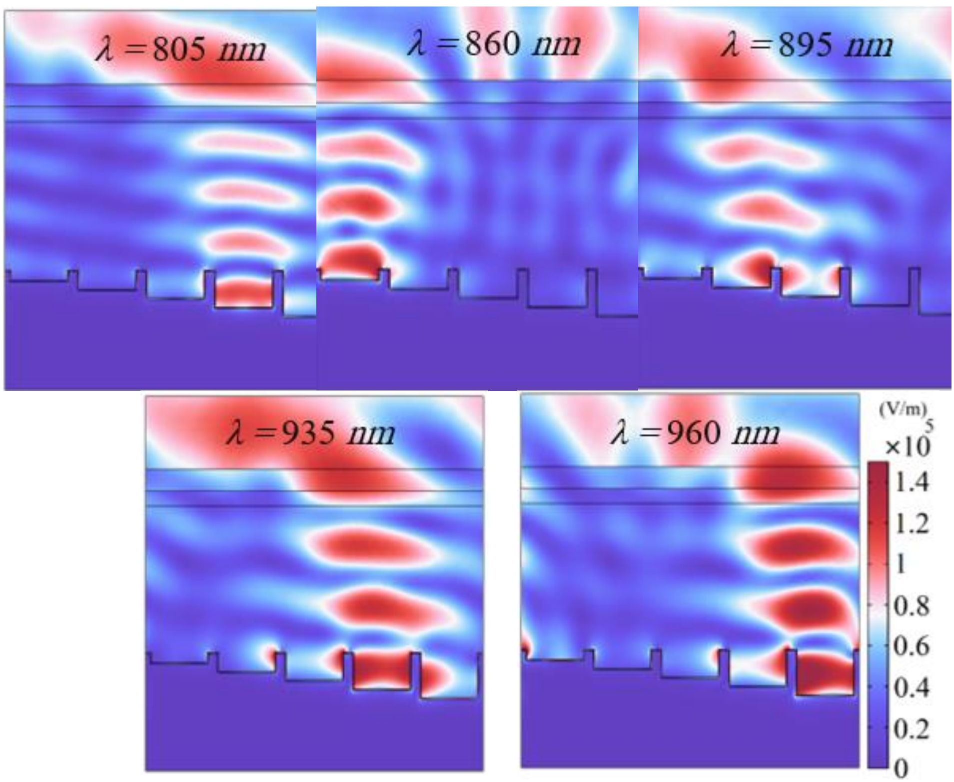
structure	Absorber thickness (nm)	Voc(mv)	Jsc (mA/cm^2)
This study	500	1100	27.59
Ag/ITO Thin Film Perovskite [43]	680	1160	23
Ag/ITO Thik Film Perovskite [43]	680	1106	20.08

To gain a deeper understanding of light absorption enhancement phenomena, we conducted a physical analysis [44,45]. As shown in Eqution 3, absroption directly proportional to squre the electric field intensity $|E(\lambda)|$. Figure 5 illustrates the electrc field intensities within the wavelength corresponding to the highest absorption.Figure 5-a depicts the relatively uniform electric field intensityes distribution within the referene cell its absorption peak of 855 nm. In contrast, Figure 5-b shows the excitaton of localizd surface plasmon (LSPs) at a wavelength of 720 nm above the gratings in Case 1, leading to enhanced electric field and increased absorption. However, the parasitic absorption of the silver back reflector in this case is relatively high, which can offset some actives layers absorption enhancment.Figure 5-c illustrtes the electric field intensities at wavelength of 780 nm and 985 nm for Case 2.The graded gratings effectively scatter light withen the actives layers, leading to enhnced absorption. For Case 3, the electrics field distributions wavelength of 800 nm, 840 nm, and 970 nm are shown in Figure 5-d. this cases, the scatterings of light withins the actives layers contributes to increased light trappings. Figure 5-e presents the electric field distribution in Case 4 wavelength of 790 nm, 845 nm, and 955 nm.The resonance wavelength strongly influenced by the dimensions of the gratings [29,46]. Graded gratings create"hot spots"characterized by high electric field concentrationes,which facilitate the generation of electron-hole paires. Finally, Figure 5-f shows the electrics field at wavelengths of 805 nm, 860 nm, 895 nm, 935 nm, and 960 nm for Case 5. In these cases, increased light scattering enhances absorption within the active layer, leading to a longer optical pathway for photons. This extended optical path increases the probability of absorption, resulting in a high generation rate of carriers and ultimately a high photocurrent.





(e)



(f)

Fig. 5. The electric field intensity for: a) reference cell at the λ = 855 nm, b) Case 1 at the λ = 720 nm, c) Case 2 at λ = 780 nm and 985 nm, d) Case 3 at λ = 800 nm, λ = 840 nm, and λ = 970 nm, e) Case 4 at λ = 790 nm, λ = 845 nm, and λ = 955 nm, f) Case 5 at λ = 805 nm, λ = 860 nm, λ = 895 nm, λ = 935 nm, and λ = 960 nm.

To investigate influence of angle of incidence on the solar cells (SCs), we analyzed their performance under various angle [29,47-50]. Figures 6-a to 6-c present the averags absorptions, Short circuit current density, and Efficiency as a function of angle of incidence, respectively. Case 5 exhibits an average absorption exceeding 67% up to an angle of 30 degrees. The average absorption reaches a maximum of 68% at an angle of 15 degrees, primarily due to increased light scattering and trapping within the cell. The absorption remains relatively constant at around 65% up to an angle of 45 degrees, indicating that the proposed SCs are insensitive to illumination angle within ±45 degrees. Moreover, the current densities and efficiencies remain unchanged under oblique incidence lower than 45 degrees.

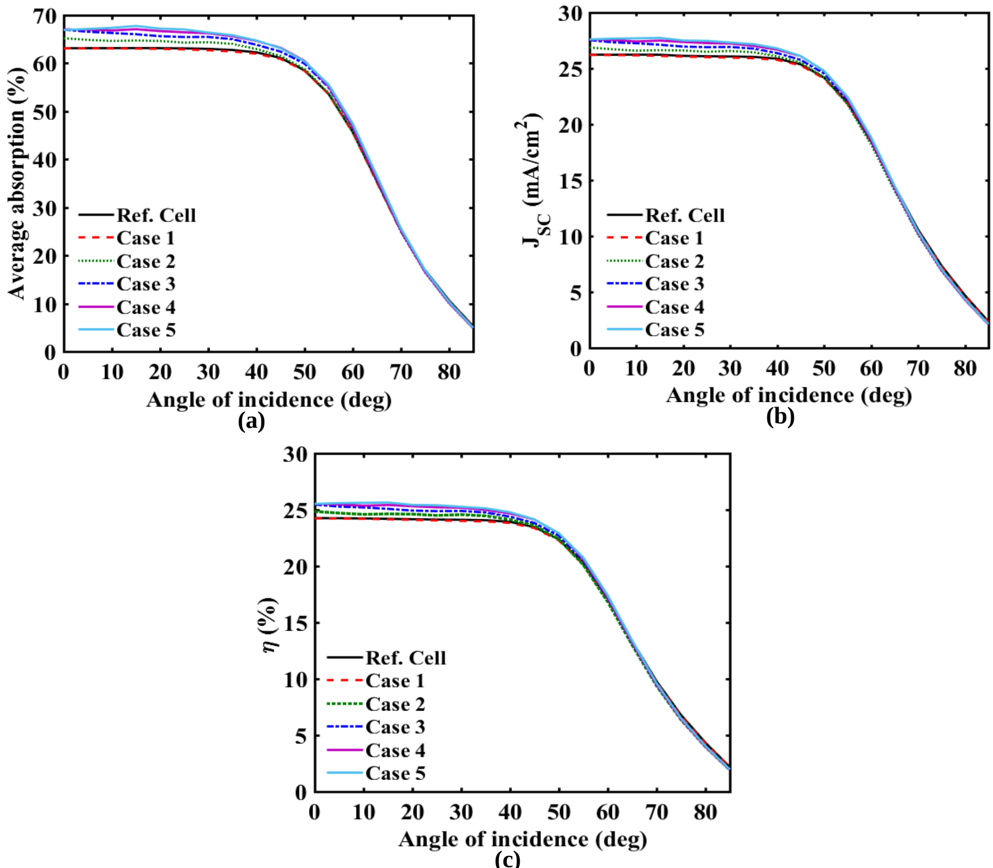


Fig. 6. a) Averags absorptions, b) short circuit currents density, and c) efficiency angle of incidence proposed SCs.

4.CONCLUSION

In this paper, for having absorption enhancement in the near-IR region of the Sun spectrum the graded gratings are proposed and extensively investigated for PSCs. For this purpose, firstly typical gratings are applied on the backside of the cell. It is revealed that this grating cannot dramatically enhance the absorption due to the parasitic loss of the sliver gratings on the backside of the cell. In order to overcome this issue, we applied graded gratings on the backside of the cell. Graded gratings enhance the absorption through the field enhancement caused by LSPs and the scattering of light inside the cell. It is depicted that by selecting the optimal size of the gratings, absorption in the near-IR is increased dramatically. The highest average absorption of 67.1%, the current density of 27.59 (mA/cm^2), and efficiency of 25.52% is obtained using four graded gratings which show an increase of 6.3%, 5.2%, and 4.3% compared to the reference cell, respectively. The simulation results under the illumination angles from 0 to 85 degrees show that graded gratings enhance the average absorption up to an angle of 45 degrees. For proposed PSCs, the light absorption up to an angle of 45 degrees is constant and near 65%, and thus, the proposed PSCs is not sensitive to the illumination angle up to ±45 degrees. Thus, a new type of grating is introduced to trap more light inside the cell and as a result, promises high-efficiency PSCs.

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