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Ideal Efficiency of Resonant Cavity-Enhanced Perovskite Solar Cells

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Abstract

Perovskite solar cells (PSCs) have attracted significant attention in recent years due to the rapid increase in device efficiency (reaching over 25% in 2019), ease of fabrication, and the potential to produce low-cost photovoltaic modules. In this paper we have determined the ideal power conversion efficiency and quantum efficiency of PSCs with the *p*-*i*-*n* device structure, where *p* is the hole transport layer, *i* is the perovskite absorber layer, and *n* is the electron transport layer. The absorption of incident light occurs in a thin perovskite layer, the thickness of which is comparable to the wavelength of absorbed light. We take into account interference effects when the PSC structure is represented by a Fabry-Perot resonator. The optical flux within the absorbing layer is calculated as a function of the spatial coordinate (in the direction of the layer thickness), for a certain wavelength, at the normal incident light. The power quantum efficiency is calculated assuming that the incident light source is a blackbody at the temperature of the Sun, as well as for the AM1.5g standard solar spectrum. The results obtained by using the derived expressions that take into account the interference effects are compared with those obtained by neglecting these effects.

Keywords Perovskite · Solar cell · Resonant cavity · Efficiency

1 Introduction

The global installed solar photovoltaic (PV) capacity exceeded 500 GW at the end of 2018, while the estimated additional 500 GW of PV capacity is projected to be installed in the next five years (Haegel 2019). In this way, humanity is entering the era of a terawatt installed PV capacity. Our current global power needs amount to about 15 TW annually, and it is expected that they will reach 30 TW in 2050 (Cherrette 2018). If sunlight is efficiently captured and converted to electrical energy, it potentially supplies 67 TW (Cherrette 2018). Hence, solar energy has the potential to satisfy our present and future

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energy needs. PV is already cost-competitive with conventional electricity generation in many parts of the world.

Perovskite solar cells (PSCs) (Kojima 2009) have attracted significant attention in recent years due to the rapid increase in device efficiency (reaching over 22% in 2016 (Sherkar 2017), and even 25.2% in 2019 (Zhang 2019)), the ease of fabrication (simple fabrication technology, active layer formation at temperatures not much higher than room temperature), and the potential to produce low-cost photovoltaic modules. The high power conversion efficiency (PCE) is enabled by the fact that perovskite is a direct semiconductor with a high light absorption coefficient (~ 10^5 cm^{-1}), and has favorable semiconductor parameters (mobility and carrier lifetime). The focus of the research is on ultrathin solar cells (active layer thickness ~ 100 nm) and further increase in solar cell efficiency (Chen 2019, Chen 2018, Steenhoff 2015). However, the high PCE, comparable to the best obtained in Si solar cells, has been achieved in organic-inorganic hybride halide lead perovskite solar cells. Due to the inherent instability associated with both organic constituents and the interlayer diffusion of dopants, as well as the environmental toxicity of lead (Benmessaoud 2016), extensive research efforts are being made to obtain stable organic-free, lead-free, and dopant-free PSCs (Miyasaka 2019), but there is a long way for them to achieve sufficiently high efficiency levels.

This paper presents investigation of the maximum efficiency of PSCs in resonant cavity structures. In addition to optical losses, the main factors limiting the efficiency of solar cells are known to be surface and volume recombination processes in the structure. One reason for using a resonant structure is the fact that multiple light absorption in the active layer allows for obtaining a sufficiently high efficiency at the absorption layer thickness of ~ 100 nm. Such a small thicknesses enables reduced material use, and decreases the impact of recombination processes that depend on the absorber volume, thereby approaching the ideal efficiency, assuming a low surface recombination effect (i.e. highly selective electron and hole transport layers and low density of surface defects (Sandberg 2019)). Such structures are suitable for all types of PSCs, including organic-free, lead-free, and dopant-free PCSs, where the recombination losses due to volume defects are more pronounced.

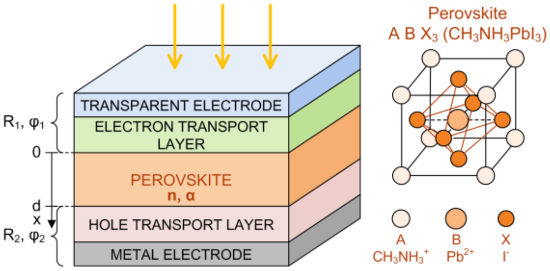

Fig. 1 Illustration of the structure of a resonant cavity perovskite solar cell (left) and perovskite crystal structure (right).

In this study we determine both the ideal quantum and power conversion efficiency of PSCs with the *p-i-n* device structure (Fig. 1), where *n* is the electron transport layer

(ETL), *i* is a thin perovskite absorber layer, and *p* is the hole transport layer (HTL). In the considered structure, the contact junctions are made of transparent indium-tin-oxide (ITO) on the front side, and silver on the back side. In the optical sense, we represent the contact and ETL and HTL layers (top and bottom mirrors) with the corresponding complex reflection coefficients, whose modules are r_1 and r_2, and phases φ_1 and φ_2, and $R_1=r_1^2$ and $R_2=r_2^2$, as shown in Fig. 1. In that way, the PSC structure is represented by a Fabry-Perot resonator.

The aim of the analysis is to investigate the influence of interference effects on the ideal efficiency. This is significant because in most investigated PSCs, the thickness of the absorber layer is comparable to the incident light wavelength. Power efficiency is calculated assuming that the incident light source is a blackbody at the temperature of the Sun, and also for the AM1.5g standard solar spectrum. The results obtained by using the derived expressions that take into account the interference effects are compared with those obtained by neglecting these effects.

2 Theory

Ideal efficiency assumes neglecting of the recombination effects and other losses due to the imperfect structure of solar cells. By using the method described in (Djurić 1997; Pettersson 1999; Djurić 2001), the optical flux $I(x,\lambda)$ within the absorbing perovskite layer when interference effects are taken into account is proportional to the square of the total electric field (which is the sum of the incident and reflected) in the spatial coordinate x, for a certain wavelength of the incident light λ (assuming normal incident light).

$$I_{\text{int}}(x,\lambda)=I_0(1-R_1)\frac{e^{-\alpha x}+R_2e^{-\alpha(2d-x)}+2\sqrt{R_2}e^{-\alpha d}\cos\left(\frac{4\pi n(x-d)}{\lambda}+\varphi_2\right)}{1+R_1R_2e^{-2\alpha d}-2\sqrt{R_1R_2}e^{-\alpha d}\cos\left(\frac{4\pi nd}{\lambda}+\varphi_1+\varphi_2\right)} \tag{1}$$

When interference effects are neglected the optical flux is obtained as the sum of incident and reflected light optical fluxes, including the effects of reflection on the back side (Djurić 1983)

$$I_i(x,\lambda)=I_0(1-R_1)\frac{e^{-\alpha x}+R_2e^{-\alpha(2d-x)}}{1-R_1R_2e^{-2\alpha d}} \tag{2}$$

Here, d is the active (absorber) layer thickness, and n and α are its refractive index and absorption coefficient, respectively.

The incident number of photons per unit area and unit time emmited by blackbody at the temperature of Sun T_s is (Shockley 1961)

$$I_0=\frac{2\pi}{c^2}\frac{\nu^2}{e^{h\nu/(k_BT_s)}-1} \tag{3}$$

where v is the frequency of the incident light, c is the speed of light, h is the Planck constant, and k_B is the Boltzmann constant.

Quantum efficiency is given by the expression (Djurić 2001)

$$QE(\lambda) = \int_0^d \alpha(\lambda) \frac{I(x,\lambda)}{I_0} dx \,, \tag{4}$$

where it is necessary to take $I=I_{int}$ (Eq. (1)) or $I=I_i$ (Eq. (2)) for cases with interference and no interference, respectively. After calculating the integrals, expressions for quantum efficiency are obtained for these two cases

$$QE_{\text{int}}(\lambda) = (1-R_1)\frac{(1-e^{-\alpha d})(1+R_2e^{-\alpha d}) + \dfrac{\alpha\lambda}{\pi n}\sqrt{R_2}e^{-\alpha d}\sin\left(\dfrac{2\pi nd}{\lambda}\right)\cos\left(\dfrac{2\pi nd}{\lambda}+\varphi_2\right)}{1+R_1R_2e^{-2\alpha d} - 2\sqrt{R_1R_2}e^{-\alpha d}\cos\left(\dfrac{4\pi nd}{\lambda}+\varphi_1+\varphi_2\right)} \tag{5}$$

$$QE_i(\lambda) = (1-R_1)\frac{(1-e^{-\alpha d})(1+R_2e^{-\alpha d})}{1-R_1R_2e^{-2\alpha d}} \tag{6}$$

Total power generated in solar cell per unit area is

$$Q = h v_g \int_{v_g}^{\infty}\int_0^d \alpha I(x,v)\,dx\,dv \tag{7}$$

In the previous expression, I is I_{int} or I_i, as given by Eqs. (1) and (2), depending on whether or not interference is taken into account, and $v_g=E_g/h$, E_g is the energy bandgap of the perovskite active layer. The total incident power on unit area for blackbody radiation at temperature T_s is given by the Stefan-Boltzmann law (σ is the Stefan-Boltzmann constant)

$$P_s = \sigma T_s^4 \tag{8}$$

Power conversion efficiency can now be determined, as defined in (Shockley 1961)

$$\eta = Q / P_s \tag{9}$$

For the AM1.5g standard spectrum η is obtained using the previous expression, where Q is calculated based on data for spectral irradiance from (NREL 2011), and P_s=1000 W/m^2.

3. Results and discussion

We analyze the performance of resonant cavity-enhanced solar cells with a thin perovskite ($CH_3NH_3PbI_3$) absorber layer by using the theory presented in Section 2. Our goal is to investigate the PSC ideal efficiency in resonant cavity structures. The energy bandgap of $CH_3NH_3PbI_3$ is 1.55 eV (yielding $\nu_g=E_g/h\approx3.75\cdot10^{14}$ Hz and $\lambda_g=c/\nu_g\approx800$ nm), and data for the values of α and n for different λ are taken from (Manzoor 2018). The parameters R_1, R_2, φ_1 and φ_2 are obtained based on the expressions given in (Űnlű 1995). In the calculations we take T_s=5760 K (Kalogirou 2014).

Fig. 2 shows the dependence of the normalized optical flux I/I_0 on the spatial coordinate x, for three different values of λ (500 nm, 600 nm, 750 nm) and absorber thickness d=95 nm. The curves for the case when interference is taken into account (I_{int}/I_0) are shown by solid lines, and by dashed lines when they are neglected (I_i/I_0). The thickness of the resonant cavity corresponds to the first maximum of the power conversion efficiency curve calculated taking into account the interference effects (as shown in Fig. 4). As it can be seen in the diagram in Fig. 2, for a certain wavelength range the maximum of normalized optical flux and the area below the I/I_0 curve are enhanced when the interference effects exist, which is consistent with the results reported in (Chen 2018).

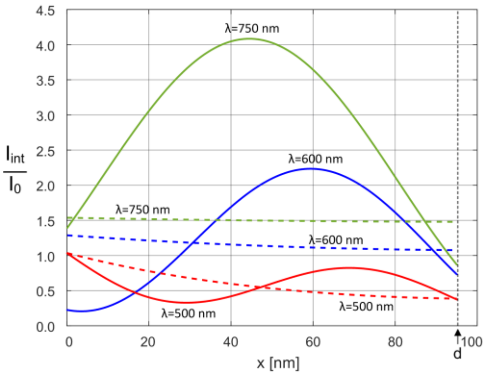

Fig. 2 Dependence of both I_{int}/I_0 (solid lines) and I_i/I_0 (dashed lines) on the spatial coordinate x for three different values of λ and perovskite (absorber) layer thickness d=95 nm.

The ideal quantum efficiency (calculated by using Eqs. (5) and (6)) of the analyzed PSC as a function of the wavelength of incident light is presented in Fig. 3 (for the perovskite layer thikness d=95 nm). It is given for the case when the interference is taken into account (solid line) and when it is neglected (dashed line). The diagram shows that, in the analyzed case, the interference effects increase the quantum efficiency for the wavelengths greater than about 550 nm.

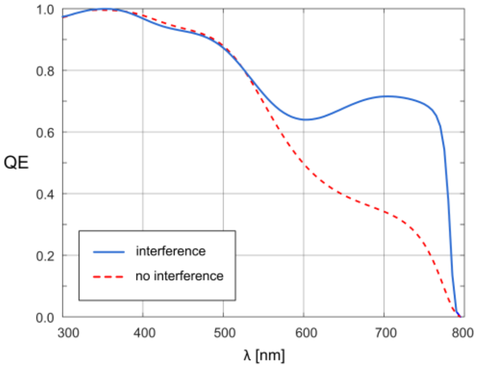

Fig. 3 Ideal quantum efficiency as a function of the wavelength of incident light when interference is taken into account and when it is neglected (*d*=95 nm).

Fig. 4 shows a solar cell ideal power conversion efficiency as a function of perovskite layer thickness when interference is taken into account (solid line) and when it is neglected (dashed line), obtained according to Eq. (9). It is calculated assuming that the incident light source is a blackbody at the temperature of the Sun, and also for the AM1.5g standard solar spectrum, which are typically used when considering the performance of flat solar panels (NREL 2011). For AM1.5g standard spectrum, η is calculated based on data for spectral irradiance from (NREL 2011).

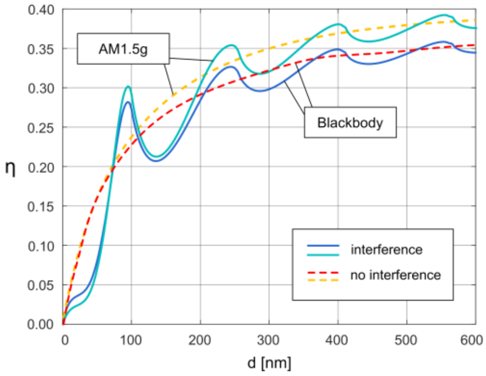

Fig. 4 Ideal power conversion efficiency as a function of perovskite layer thickness when interference is taken into account (solid lines), and when it is neglected (dashed lines), by using the spectrum of blackbody at the temperature of the Sun (T_s=5760 K) and AM1.5g spectrum.

It can be observed that the PCE obtained for the AM1.5g spectrum is greater than that for the black body radiation spectrum, which is in agreement with the results reported in (Belghachi 2015), given that the bandgap of the analyzed perovskite E_g=1.55 eV. PCE for cases where there are interference effects has pronounced maxima for certain thicknesses of the perovskite layer. The greatest difference between efficiencies when interference effects are taken into account and when they are neglected, corresponds to the first maximum, i.e. to the thickness of about 95 nm in the present case. As the thickness increases, the differences between the efficiencies calculated for the two cases decrease and they tend to have the same value. According to Fig. 3, the absorption is broadband for d=95 nm, which is the thickness corresponding to the first peak of the curves obtained taking into account the interference (Fig. 4). For that thickness the efficiency is not the greatest, but the interference exhibits the highest improvement: η reaches 30% (an increase of about 30% compared to the PCE without interference).

This analysis has shown that in the analyzed type of PSCs it is necessary to take into account interference effects when determining their parameters.

4. Conclusion

We have analyzed the ideal power conversion efficiency and quantum efficiency of perovskite solar cells (PSCs) with an active (absorption) layer placed in a Fabri-Perot cavity. The derived expressions used for the analysis refer to two cases. In the first case, which is generally valid, interference effects were taken into account, while in the second case, the interference effects were neglected, but the effects of reflection at the backside were taken into account. Since the thickness of perovskite layer is usually comparable to the wavelength of light, the model that takes into account the interference effects is suitable for general use.

The results of the analysis show that the ideal power conversion efficiency due to interference effects has pronounced maxima at certain thicknesses of the absorbing layer. The largest efficiency increase in the analyzed case (perovskite $CH_3NH_3PbI_3$) corresponds to the first maximum (95 nm thickness) and it is by about 30% higher than the corresponding value when interference is neglected. Quantum efficiency increases in the part of the spectrum relative to the case without interference.

The application of the presented theory is expected in the future stable, organic-free, lead-free, and dopant-free PSCs, in which the necessary increase in efficiency could be achieved by using a resonant cavity structure, since it allows for high efficiencies with a reduced thickness of the absorption layer, through the reduction of recombination losses in the volume of the active layer.

In our further work, the losses (both recombination and optical) that occur in the solar cell structure will be considered. This will allow us to identify and investigate the conditions under which resonant cavity thin perovskite solar cells have a higher actual power efficiency than the common ones (with a thicker absorbing layer).

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