Photoemission cross section: A critical parameter in the impurity photovoltaic effect*

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A numerical study has been conducted to explore the role of photoemission cross sections in the impurity photovoltaic (IPV) effect for silicon solar cells doped with indium. The photovoltaic parameters (short-circuit current density, open-circuit voltage, and conversion efficiency) of the IPV solar cell were calculated as functions of variable electron and hole photoemission cross sections. The presented results show that the electron and hole photoemission cross sections play critical roles in the IPV effect. When the electron photoemission cross section is $< 10^{-20}$ cm^2, the conversion efficiency η of the IPV cell always has a negative gain ($\Delta\eta < 0$) if the IPV impurity is introduced. A large hole photoemission cross section can adversely impact IPV solar cell performance. The combination of a small hole photoemission cross section and a large electron photoemission cross section can achieve higher conversion efficiency for the IPV solar cell since a large electron photoemission cross section can enhance the necessary electron transition from the impurity level to the conduction band and a small hole photoemission cross section can reduce the needless sub-bandgap absorption. It is concluded that those impurities with small (large) hole photoemission cross section and large (small) electron photoemission cross section, whose energy levels are near the valence (or conduction) band edge, may be suitable for use in IPV solar cells. These results may help in judging whether or not an impurity is appropriate for use in IPV solar cells according to its electron and hole photoemission cross sections.

Keywords: solar cell, impurity photovoltaic effect, photoemission cross section, conversion efficiency

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1. Introduction

The impurity photovoltaic (IPV) effect has attracted considerable attention since solar cells employing it can additionally absorb the sub-bandgap photons and thus enhance the photogenerated current.[1–8] The principle of the IPV effect is to introduce an energy level within the material bandgap by doping. The energy level acts as a stepping stone and causes photons with energies less than the bandgap energy to be collected via a two-step absorption mechanism, in which a sub-bandgap photon excites an electron from the valence band to the impurity level and then another sub-bandgap photon pumps it from there to the conduction band. However, the addition of impurities can increase the chance of recombination and thus decrease the open-circuit voltage V_{oc} of the solar cell because the introduced impurities can also work as recombination centres. For this reason, Güttler and Queisser[9] argued that the IPV effect cannot improve solar cell performance. Karazhanov[4] also held that the IPV effect has negligible influence on improving efficiency. However, Schmeits and Mani[3] illustrated that the open-circuit voltage of a solar cell has a slight degradation if a proper solar cell structure p–n–n$^+$ is implemented. Khelifi *et al.*[6] demonstrated that a silicon solar cell using the IPV effect will yield a positive benefit (~ 6 mA/cm^2 in the photocurrent and $\sim 2\%$ in the absolute efficiency) if the reflectivities at the front and the back of the cell both approach unity. In our previous work,[10] we showed that a positive gain of conversion efficiency for IPV silicon solar cells doped with indium would be achieved if the electron thermal capture cross section of the impurity is $< 10^{-20}$ cm^2. These results indicated that some factors can enlarge or weaken the potential of the IPV effect. To make better use of the IPV effect for improving solar cell performance, the relevant factors should be fully clarified. One of the important factors in raising solar cell efficiency by the IPV effect is the photoemission cross section of the impurity in the host semiconductor. We think that the role of photoemission cross sections in the IPV effect should be clearly revealed; however, to the best of our knowledge, published reports about the IPV effect do not focus on this issue.

In the present work, we evaluated the influence of the photoemission cross section of indium in silicon on IPV solar cell performance. The role of photoemission cross sections in

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the IPV effect was studied by using the SCAPS program.[11,12]

2. Theory

Figure 1 shows the operation principle of an IPV solar cell. Besides the conventional Shockley–Read–Hall (SRH) mechanism,[13,14] there are two impurity optical transitions in the model. These two transitions are made by two sub-bandgap photons with energies $h\nu_1$ and $h\nu_2$. An electron–hole pair can be generated via the two transitions. A modified SRH model is applied for the addition of the IPV effect. The net recombination rate U via the impurity is expressed as[6]

$$U = \frac{np - (n_1 + \tau_{n0} g_{nt})(p_1 + \tau_{p0} g_{pt})}{\tau_{n0}(p + p_1 + \tau_{p0} g_{pt}) + \tau_{p0}(n + n_1 + \tau_{n0} g_{nt})}, \quad (1)$$

with

$$\tau_{n0} = \frac{1}{\sigma_n^{th} \upsilon_T N_t}, \quad \tau_{p0} = \frac{1}{\sigma_p^{th} \upsilon_T N_t}, \quad (2)$$

$$n_1 = N_C \exp\left(-\frac{E_C - E_t}{kT}\right), \quad p_1 = N_V \exp\left(-\frac{E_t - E_V}{kT}\right), \quad (3)$$

$$g_{nt} = N_t \int_{\lambda_g}^{\lambda_{n,max}} \sigma_n^{opt}(x,\lambda)\, \phi_{ph}(x,\lambda)\, d\lambda, \quad (4)$$

$$g_{pt} = N_t \int_{\lambda_g}^{\lambda_{p,max}} \sigma_p^{opt}(x,\lambda)\, \phi_{ph}(x,\lambda)\, d\lambda, \quad (5)$$

$$\phi_{ph}(x,\lambda) = \phi_{ext} \frac{1 + R_b e^{-4\alpha_{tot}(\lambda)(L-x)}}{1 - R_f R_b e^{-4\alpha_{tot}(\lambda)L}} e^{-2\alpha_{tot}(\lambda)x}, \quad (6)$$

$$\alpha_{tot} = \alpha_{e-h} + \alpha_n + \alpha_p + \alpha_{fc}, \quad (7)$$

$$\alpha_n(\lambda) = f_t N_t \sigma_n^{opt}(\lambda), \quad \alpha_p(\lambda) = (1 - f_t) N_t \sigma_p^{opt}(\lambda). \quad (8)$$

In these expressions, n and p are the electron and hole concentrations, τ_{n0} and τ_{p0} are the lifetimes for electrons and holes, n_1 and p_1 are the electron and hole concentrations when the Fermi level coincides with the impurity level, g_{nt} and g_{pt} are the photoemission rates from the impurity for electrons and holes, N_t is the impurity concentration, E_t is the impurity energy level, σ_n^{th} and σ_p^{th} are the thermal capture cross sections for electrons and holes, υ_T is the thermal velocity (10^7 cm/s), N_C and N_V are the effective densities of states in conduction and valence bands, E_C and E_V are the conduction and valence band edges, σ_n^{opt} and σ_p^{opt} are the photoemission cross sections of the impurity for electrons and holes (i.e., optical cross sections of electrons and holes from the impurities), ϕ_{ext} is the external incident photon flux, $\phi_{ph}(x,\lambda)$ is the photon flux at depth x from the incident surface for wavelength λ, R_f and R_b are the internal reflection coefficients at the front and back surface of the cell, L is the total thickness of the cell, α_{e-h} is the intrinsic absorption coefficient, α_n and α_p are the impurity absorption coefficients for electron and hole photoemission from the IPV impurity, α_{fc} is the absorption coefficient for free-carrier absorption, and f_t is the occupation probability of the impurity level, respectively.

In the SCAPS program, the Si solar cell considered in this study is a p–n–n^+ form as shown in Fig. 1. The thicknesses of p, n, and n^+ layers are set as 1, 100, and 5 μm, respectively. The carrier concentrations of p, n, and n^+ layers are set as $N_A = 10^{18}$ cm^{-3}, $N_D = 10^{17}$ cm^{-3}, and $N_D = 10^{18}$ cm^{-3}, respectively. The acceptor-type IPV impurity indium (8×10^{16} cm^{-3}) is introduced only into the n base layer. The main parameters for the indium impurity and Si solar cell at 300 K are listed in Table 1.[1,6,15] The absorption of free carriers is ignored. The illumination is AM 1.5 G, 100 mW/cm^2. R_f and R_b are both set to 0.999.

Table 1. Basic parameters for the indium impurity and Si solar cell used in this work (at 300 K).

Parameter and unit	Value
Band gap E_g/eV	1.12
Relative dielectric constant ε	11.9
Electron affinity χ/eV	4.05
Effective density of states in conduction band N_C/cm^{-3}	2.80×10^{19}
Effective density of states in valence band N_V/cm^{-3}	2.65×10^{19}
Electron mobility μ_e/cm^2·V^{-1}·s^{-1}	1350
Hole mobility μ_h/cm^2·V^{-1}·s^{-1}	450
Surface recombination velocity S/cm·s^{-1}	10^4
Electron thermal capture cross section σ_n^{th}/cm^2	1.0×10^{-22}
Hole thermal capture cross section σ_p^{th}/cm^2	5.07×10^{-15}
Indium energy level E_t–E_V/eV	0.157

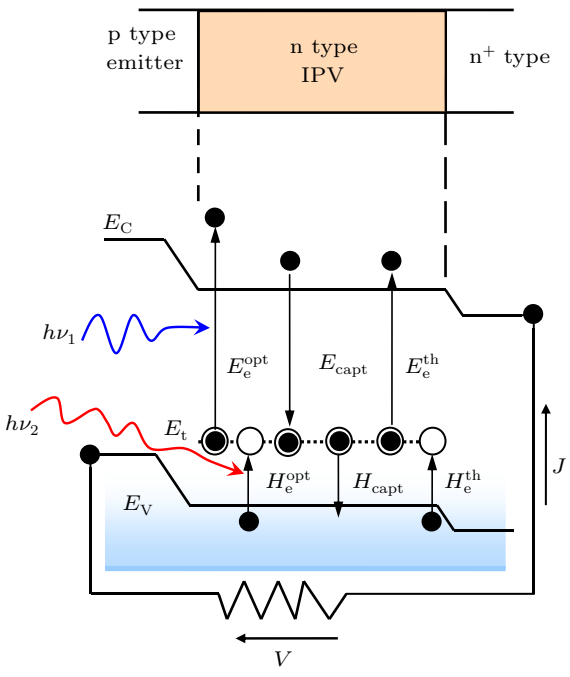


Fig. 1. (color online) Schematic structure and operation principle of the IPV solar cell.

The values of the electron and hole photoemission cross sections of indium in Si are related to the incident wavelengths. However, we found that these values in the wavelength range of interest nearly have the same order of magnitudes.[1] The photoemission cross sections of electrons and holes considered in this study are set to 10^{-21}–10^{-12} and

10^{-21}–10^{-10} cm^2, respectively. Therefore, for convenience, it is assumed that the photoemission cross sections have the same values for different incident wavelengths. In addition, the photoemission cross sections are assumed to be zero for photons with energy above the bandgap. The short-circuit current density J_{sc}, the open-circuit voltage V_{oc}, and the conversion efficiency η are calculated as functions of variable hole and electron photoemission cross sections.

3. Results and discussion

Figure 2 shows the short-circuit current density as a function of the hole photoemission cross section with different electron photoemission cross sections. It is found that the short-circuit current densities with different electron photoemission cross sections always have positive benefits when the hole photoemission cross sections are $< 10^{-16}$ cm^2. More benefits are obtained when increasing the electron photoemission cross sections. J_{sc} increases from 42.87 to 47.45 mA/cm^2 as σ_n^{opt} increases from 10^{-21} to 10^{-12} cm^2 if $\sigma_p^{opt} = 10^{-21}$ cm^2. J_{sc} is 42.57 mA/cm^2 in the case with no indium impurity (without IPV). Moreover, it is also observed from Fig. 2 that, when $\sigma_p^{opt} = 10^{-10}$ cm^2, J_{sc} always gains a negative benefit with different electron photoemission cross sections. These results indicate that larger electron photoemission cross section and smaller hole photoemission cross section can realize more benefits to J_{sc} for the IPV solar cell. The reasons are as follows.

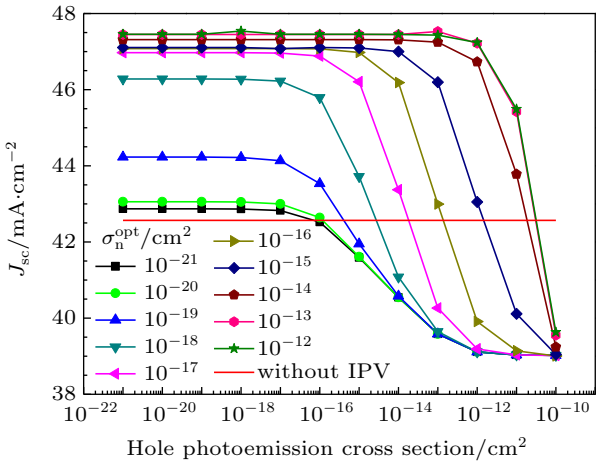


Fig. 2. (color online) Short-circuit current density J_{sc} as a function of the hole photoemission cross section with different electron photoemission cross sections.

The indium level is located 0.157 eV above E_V, so the values for n_1 and p_1 are 1.7×10^3 and 2.4×10^{16} cm^{-3} according to Eq. (3). The smallness of n_1 reveals that the electron photoemission is crucial for the IPV effect. The larger electron photoemission cross section can result in more transitions from the indium level to the conduction band. This action should yield more gains in J_{sc}. The magnitude of p_1 indicates that the transition from the valence band to the indium level is mainly contributed by thermal excitation. The thermal excitation transition ensures that the impurity level is mostly occupied and can provide adequate electrons for transiting from the impurity level to the conduction band. In this process, it does not need the contribution by optical excitation. The large hole photoemission cross sections will facilitate the absorption of the sub-bandgap photons and thus reduce the photon flux available for the electron photoemission process. So, a small σ_p^{opt} and a large σ_n^{opt} will result in greater short-circuit current densities.

Figure 3 illustrates the open-circuit voltage versus the hole photoemission cross section with different electron photoemission cross sections. It is clear that these open-circuit voltages with IPV have nearly the same values, ranging from 0.722 to 0.727 V. Moreover, the open-circuit voltages with IPV are always less than that without IPV (0.733 V). However, although the indium impurities are introduced into the solar cells, their open-circuit voltages have just a slight decrease. This advantage comes from the special solar cell structure p–n–n$^+$, which can maintain a high built-in voltage for the IPV solar cell, safeguarding the open-circuit voltage.[3]

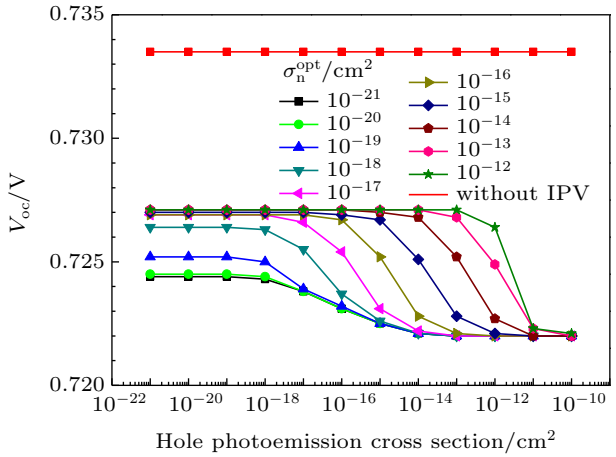


Fig. 3. (color online) Variations of open-circuit voltage V_{oc} with hole photoemission cross section for different electron photoemission cross sections.

Figure 4 depicts the variations of cell efficiency with hole photoemission cross section for different electron photoemission cross sections. It is observed that, when $\sigma_n^{opt} < 10^{-20}$ cm^2, regardless of the change of σ_p^{opt}, the IPV cell always has a negative gain ($\Delta\eta < 0$). When $\sigma_n^{opt} > 10^{-19}$ cm^2, for each σ_n^{opt} value, the conversion efficiency of the solar cell with IPV first achieves a positive benefit ($\Delta\eta > 0$) and then a negative benefit with increasing σ_p^{opt}. If σ_p^{opt} has the same size, first $\Delta\eta < 0$, and then $\Delta\eta > 0$ with increasing σ_n^{opt}. These results indicate that the photoemission cross section is crucial

to the performance of the IPV solar cell. To better understand the role of the photoemission cross sections in the IPV effect, current density–voltage (J–V) curves are plotted with different photoemission cross sections, as shown in Fig. 5. It can be seen that the combination of a small $\sigma_{\rm p}^{\rm opt}$ and a large $\sigma_{\rm n}^{\rm opt}$ will be helpful to obtain better device performance for the IPV solar cell. A very large electron photoemission cross section will enhance the absorption of sub-bandgap photons and strengthen the electron transition from the impurity level to the conduction band, and a very small hole photoemission cross section will reduce the sub-bandgap absorption and thus allow those sub-bandgap photons to be used for the transition from the impurity level to the conduction band since the transition from the valence band to the impurity level can be made by thermal excitation. As a result, more photocarriers will be created. The corresponding solar cell with the IPV effect would have a higher conversion efficiency.

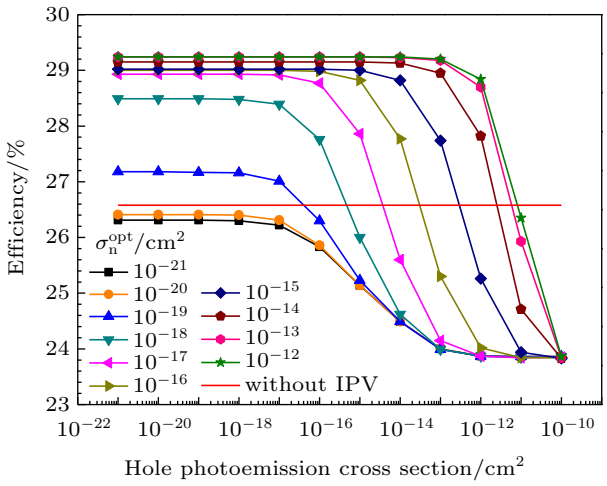


Fig. 4. (color online) Cell efficiency as a function of the hole photoemission cross section with different electron photoemission cross sections.

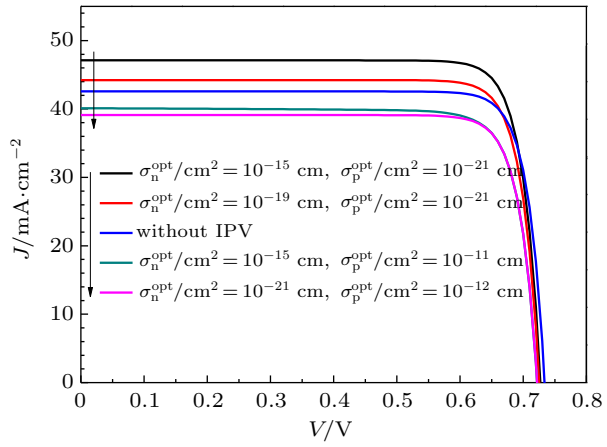


Fig. 5. (color online) Current density–voltage (J–V) curves with different hole and electron photoemission cross sections.

If the energy level formed by a donor-type impurity is close to the conduction band edge, a similar analysis of the IPV effect can be performed. It is concluded that a large $\sigma_{\rm p}^{\rm opt}$ and a small $\sigma_{\rm n}^{\rm opt}$ will be required for realising better device performance.

It is worth noting that the photoemission cross section has different values for the same impurity in different semiconductors. This is because the value of the photoemission cross section depends on the effective mass of the electron and hole, impurity energy level, dielectric constant, refractive index of the host semiconductor, and effective field ratio.[16–18] If an impurity is placed in different semiconductors, it would have different values for the effective mass of the electron and hole, impurity energy level, and effective field ratio. Moreover, different semiconductors have different dielectric constants and refractive indexes. All these can influence the value of the photoemission cross section. We can obtain the electron and hole photoemission cross sections through theoretical calculation[16–18] or experimental measurement.[19,20]

The above results indicate that the photoemission cross section plays a critical role in the IPV effect. We can assess the potential of an impurity used for the IPV effect to improve solar cell performance according to its electron and hole photoemission cross sections. Acceptor-type (or donor-type) impurities with large (small) $\sigma_{\rm p}^{\rm opt}$ and small (large) $\sigma_{\rm n}^{\rm opt}$, whose energy level is near the valence (or conduction) band edge, are not suitable for use in IPV cells.

4. Conclusions

We conducted a numerical study to explore the role of photoemission cross sections in the IPV effect for indium-doped silicon solar cells. It is found that $J_{\rm sc}$ has a positive benefit for different electron photoemission cross sections when $\sigma_{\rm p}^{\rm opt} < 10^{-16}$ cm^2 and more benefits can be obtained by increasing the value of $\sigma_{\rm n}^{\rm opt}$. If $\sigma_{\rm p}^{\rm opt} = 10^{-10}$ cm^2, $J_{\rm sc}$ always deteriorates for different electron photoemission cross sections. The value of $V_{\rm oc}$ with the IPV is always less than that without IPV; however, the decrease is slight. When $\sigma_{\rm n}^{\rm opt} < 10^{-20}$ cm^2, regardless of the change of $\sigma_{\rm p}^{\rm opt}$, the conversion efficiency of the IPV cell always has a negative gain ($\Delta\eta < 0$) when adding the IPV impurity. A large $\sigma_{\rm p}^{\rm opt}$ can adversely impact IPV solar cell efficiency. The photoemission cross section plays a critical role in the IPV effect. Furthermore, we can evaluate the potential of impurities used for the IPV effect to improve solar cell performance according to their electron and hole photoemission cross sections. Those impurities with small (large) $\sigma_{\rm p}^{\rm opt}$ and large (small) $\sigma_{\rm n}^{\rm opt}$, whose energy levels are near the valence (or conduction) band edge, may be suitable for use in IPV solar cells. These results are attractive for selecting a proper impurity in practical work with IPV solar cells.

Acknowledgments

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