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ScienceDirect
Renewable Energy 33 (2008) 293–298
RENEWABLE ENERGY
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Numerical simulation of the impurity photovoltaic effect in silicon solar cells

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Available online 3 July 2007

Abstract

Recently, the impurity photovoltaic effect (IPV) was proposed to improve the solar cell performance. Free electron–hole pairs can be generated in a two-step process involving an impurity level in the energy gap and two lower-energy photons: first electrons are optically excited from the valence band to the defect level and then from the defect level to the conduction band. The IPV effect will thus enhance the long-wavelength response of the cell.

A significant amount of theoretical work has been carried out on IPV effect in the literature, particularly on silicon solar cells with indium impurities as defect. However, the lack of an easily available solar cell simulator including the IPV effect is a handicap.

In this work, the numerical solar cell simulator SCAPS of the ELIS group was extended to include IPV in collaboration between the ELIS and the LPDS groups. Also, some special features are implemented, such as the calculation of electron and hole photoemission cross-sections of the impurity using the model of Lucovsky. The functionality of new SCAPS version was checked against existing results in the literature. Also, new results are presented such as the evolution of solar cell parameters with the indium density. We find that increasing indium concentration can improve silicon solar cell parameters, especially the short-circuit current and the efficiency, without drastically decreasing the open-circuit voltage. This is possible if a suitable structure for the cell is chosen. The optimum indium density should be equal around the base region density to obtain a positive benefit from the IPV effect.

Light trapping, which is related to the internal reflectance at the front and the back of the cell, is very important in the IPV study. Reflectivity at the front and the back should exceed 99.9% to obtain a real efficiency increase. We calculate an improvement of about $6\,mA/cm^2$ in the photocurrent, and about 2% for the efficiency, which is due to the enhancement of long-wavelength absorption by the IPV effect.

Keywords: Silicon solar cell; IPV effect; SCAPS-1D; Light trapping

1. Introduction

The impurity photovoltaic effect (IPV) has attracted much attention as an approach to improve solar cell performance by introducing sub-band gap absorption mechanisms [1–3]. It can be exploited by intentionally adding impurities, acting as defect levels lying deeply within the forbidden gap. Photons having energies below the band gap E_g of the host material can excite electrons and holes from the defect to the conduction and valence band, respectively, thereby increasing the short-circuit current J_{sc} of the solar cell: this is called IPV effect. It is however also recognized that the deep defect states also act as recombination centres and hence reduce the open-circuit voltage V_{oc} [1].

In 1994, Keevers and Green [2] presented a theoretical study of the IPV effect where one optical impurity process was combined with effective light trapping. They studied a silicon solar cell with a large density of indium impurities, which produce a relatively deep acceptor level at 157 meV above the valence-band edge. They showed that an efficiency increase of 1–2% absolute could be obtained. In a numerical

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0960-1481/$ - see front matter
doi:10.1016/j.renene.2007.05.027

study of the IPV effect, Schmeits and Mani [3] confirmed that an improvement of silicon solar cell performances is possible by choosing a p–n–n^+ structure solar cell.

In this work, we present a numerical study of the IPV effect in indium-doped crystalline silicon solar cells with SCAPS [4]. SCAPS is a one-dimensional solar cell device simulator, developed at ELIS, University of Gent, which is freely available to the PV research community. The user can define a solar cell as a series of layers with different properties, such as thickness, doping densities and defect distribution. It is then possible to simulate a number of common measurements: *I–V*, *QE*, *C–f*, and *C–V*. In this joint ELIS/LPDS study, a new version of SCAPS was developed which takes into account the IPV effect. To test the validity of the new SCAPS version, we first checked the results of Ref. [3], and found a good agreement. In the next step, we studied the influence of the indium defect concentration and light trapping on the photovoltaic parameters of the cell. For the calculation of the electron and hole optical cross-sections, the Lucovsky model [5] was introduced into the new version of SCAPS.

2. Generation and recombination in IPV

In the IPV effect, the presence of a deep state within the energy gap adds two impurity optical transitions to the traditional Shockley–Read–Hall recombination model (SRH; e.g. [6]). As illustrated in Fig. 1, electron and hole transition through the impurity is governed by capture, thermal and optical emission of carriers. The net recombination rate U via the impurity is given by [2]

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

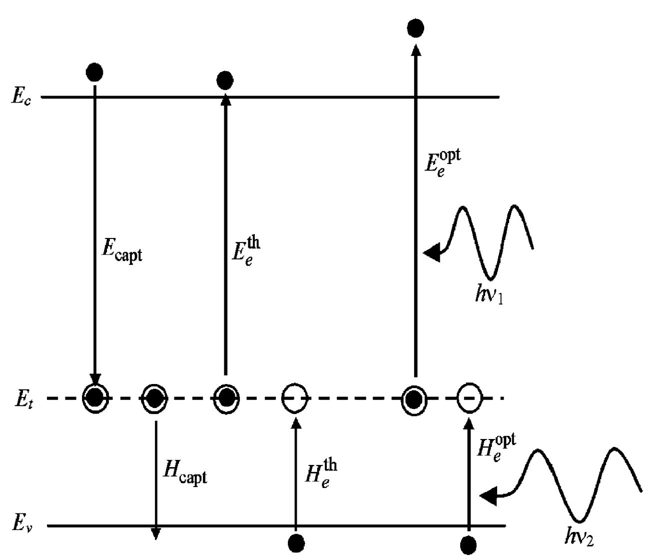

Fig. 1. The carrier transitions of the modified SRH recombination model. E_{cap} and H_{cap} are the electron and hole capture, E_e^{th} and H_e^{th} are the electron and hole thermal emission, respectively. The electron and hole photoemissions E_e^{opt} and H_e^{opt} constitute the IPV effect.

where n_1 and p_1 are the electron and hole concentrations when the Fermi level coincides with the impurity level, and

$$\tau_{n0} = \frac{1}{c_n N_t} \quad \text{and} \quad \tau_{p0} = \frac{1}{c_p N_t}, \tag{2}$$

$$g_{nt} = N_t \int_{\lambda_{n\ \min}}^{\lambda_{n\ \max}} 2\sigma_n^{\text{opt}}(x,\lambda)\phi_{\text{ph}}(x,\lambda)\,d\lambda,$$

$$g_{pt} = N_t \int_{\lambda_{p\ \min}}^{\lambda_{p\ \max}} 2\sigma_p^{\text{opt}}(x,\lambda)\phi_{\text{ph}}(x,\lambda)\,d\lambda, \tag{3}$$

where $\sigma_n^{\text{opt}}(\lambda)$ and $\sigma_p^{\text{opt}}(\lambda)$ are the electron and hole photoemission cross-sections of the impurity, and N_t is the defect density. The terms in g_{nt} and g_{pt} describe the IPV effect.

In a Lambertian cell, the photon flux $\phi_{\text{ph}}(x,\lambda)$ at a depth x for photon wavelength λ is given by the following expression [2]:

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

where R_f and R_b are the internal reflection coefficients at the front and back of the cell, L is the total length of solar cell and $\phi(\lambda)$ is the external incident photon flux. Eq. (4) and the parameters R_f and R_b describe the light trapping in the solar cell. Several optical mechanisms contribute to the total absorption coefficient α_{tot} in Eq. (4) [2]:

$$\alpha_{\text{tot}}(\lambda) = \alpha_{\text{e-h}}(\lambda) + \alpha_n(\lambda) + \alpha_p(\lambda) + \alpha_{\text{fc}}(\lambda). \tag{5}$$

Here $\alpha_{\text{e-h}}(\lambda)$ is the band-to-band absorption coefficient. The defect absorption coefficients α_n (λ) and α_p (λ) are given by

$$\alpha_n(\lambda) = f_t N_t \sigma_n^{\text{opt}}(\lambda) \quad \text{and} \quad \alpha_p(\lambda) = (1 - f_t) N_t \sigma_p^{\text{opt}}(\lambda), \tag{6}$$

where the occupancy f_t of the impurity level is given [2] by an equation similar to Eq. (1). The free carrier absorption α_{fc} (λ) in Eq. (5) is given by [7]

$$\alpha_{\text{fc}}(\lambda) = C_{\text{fc}}^n \lambda^2 n + C_{\text{fc}}^p \lambda^2 p, \tag{7}$$

where C_{fc}^n and C_{fc}^p are empirical parameters.

3. Numerical results and discussion

Our structure is a crystalline silicon p^+–n–n^+ solar cell, where the indium impurity concentration is zero in the n^+ layer. The corresponding thicknesses and shallow doping densities of the layers are respectively (2 μm, $N_A = 10^{18}\,\text{cm}^{-3}$), (100 μm, $N_D = 10^{17}\,\text{cm}^{-3}$) and (20 μm, $N_D = 10^{18}\,\text{cm}^{-3}$).

The parameters characterizing Si and the indium impurity at 300 K are summarized in Table 1. To calculate the electron and hole photoemission cross-sections of the impurity, we used both the models presented in [2] and the model of Lucovsky [5].

Note that all are assumed zero for photons of energy above the band gap. Free carrier absorption was not

Table 1
Silicon and indium impurity parameters used in this study (at 300 K) [2,3]

Property	Symbol	Value	Unit
Energy gap	E_g	1.12	eV
Electron mobility	μ_n	1350	$cm^2/V\,s$
Hole mobility	μ_p	480	$cm^2/V\,s$
Dielectric constant	ε_s	11.7	
Surface recombination velocity	$v_{sn} = v_{sp}$	$10–10^4$	cm/s
Indium energy level from the top of the valence band	$E_t–E_V$	0.157	eV
Defect type		Acceptor	
Electron thermal capture cross-section	σ_n^{th}	1.0×10^{-22}	cm^2
Hole thermal capture cross-section	σ_p^{th}	5.07×10^{-15}	cm^2

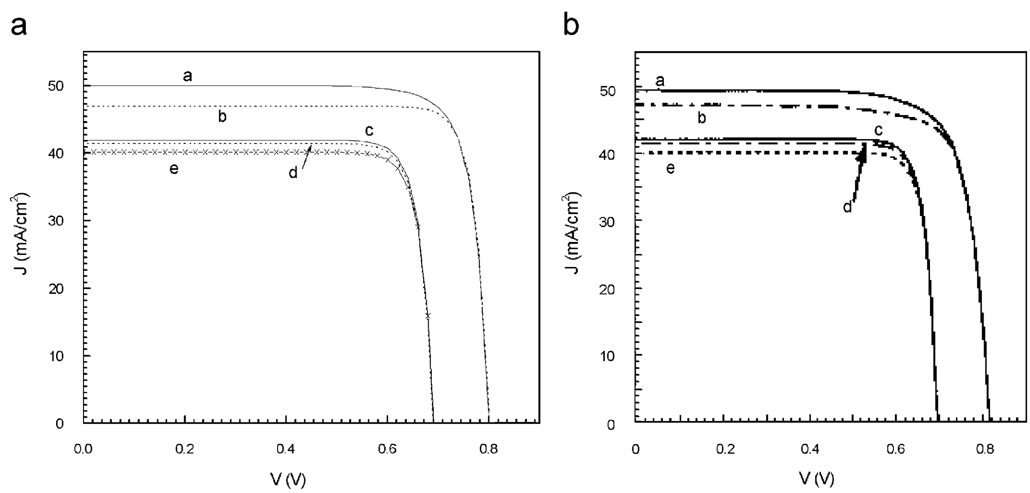

Fig. 2. Current–voltage characteristics for the p^+–n–n^+ silicon solar cell with In impurity concentration $N_t = 10^{17}\,cm^{-3}$. (a) Results calculated with SCAPS (this work); (b) results calculated in [3]. In both (a) and (b), curves a and b are for $R_b = R_f = 1$, curves c and d are for $R_b = 0.97$, $R_f = 0.93$. For b and d, the electron and hole optical generation rates are switched off. In curve e indium concentration is set to zero.

included into the model. In this numerical study, we varied indium concentration N_t, and the light trapping parameters R_f and R_b.

3.1. Validation of the numerical model

In Fig. 2 we show the current–voltage characteristics for the p^+–n–n^+ structure with $N_t = 10^{17}\,cm^{-3}$ in the p^+ and n region. Our SCAPS simulations (Fig. 2a) are compared with the result calculated in [3] (Fig. 2b). In both Fig. 2(a) and (b), ideal light trapping ($R_b = R_f = 1$) is assumed in curves a and b, while more realistic values $R_b = 0.97$ and $R_f = 0.93$ are assumed in curves c and d. In curves b and d the optical generation via In impurities is switched off, but they can still contribute to the net doping and to the recombination. The curve e corresponds to the case where there is no In at all in the cell. We noticed a good agreement between our results (Fig. 2a) and those of [3] (Fig. 2b). The IPV effect clearly increases J_{sc} (compare curves a with b, and c with d), but this advantage is appreciable only when ideal light trapping is assumed (compare curves a with c).

3.2. The effect of indium concentration

Fig. 3 shows the effect of indium impurity concentration N_t on the photovoltaic parameters: open-circuit voltage V_{oc}, photocurrent density J_{sc} and the efficiency η. Both J_{sc} and η increase with increasing N_t when $N_t \leqslant N_D$ and decrease above this concentration. An In concentration N_t lower than the base concentration N_D keeps the indium level fully occupied which allows sub-band gap photons to be absorbed by the electron photoemission process (from the In level to the conduction band). When indium concentration compensates the base doping ($N_t > N_D$), the hole photoemission process (from the In level to the valence band) is maximized. It competes with the first photoemission process and also with electron hole pair creation by intrinsic band-to-band absorption, which reduces the available photon flux and photocurrent of the cell. We observed a slight increase in the open-circuit voltage for concentrations lower than $10^{17}\,cm^{-3}$, after that it drops.

We notice that the studied structure is p^+–n–n^+, which has the advantage to keep a high value for the built-in voltage and thereafter keeps the indium level occupied. In addition, the n^+ layer introduces a back surface electric field that improves the cell electric characteristics, particularly the open-circuit voltage by reducing the recombination current. Note that it is difficult to shift the condition $N_t = N_D$ for maximal IPV effect to higher values: first, N_D should not exceed about $10^{18}\,cm^{-3}$ to prevent band gap narrowing and a shift of intrinsic band-to-band absorption to lower energies [8], second, N_t is limited because the maximum solid solubility of indium in silicon is about $10^{18}\,cm^{-3}$ [9].

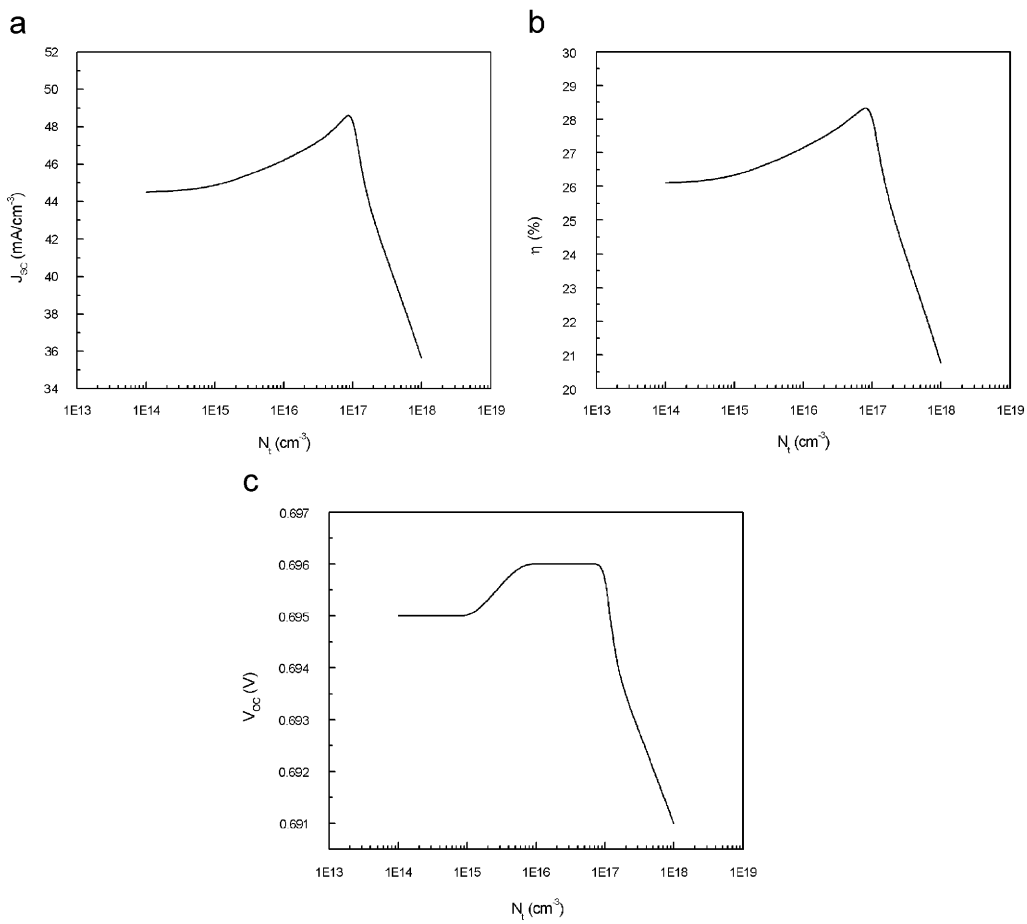

Fig. 3. Photovoltaic parameters of a silicon solar cell as a function of indium concentration: (a) short-circuit current density, (b) efficiency and (c) open-circuit voltage.

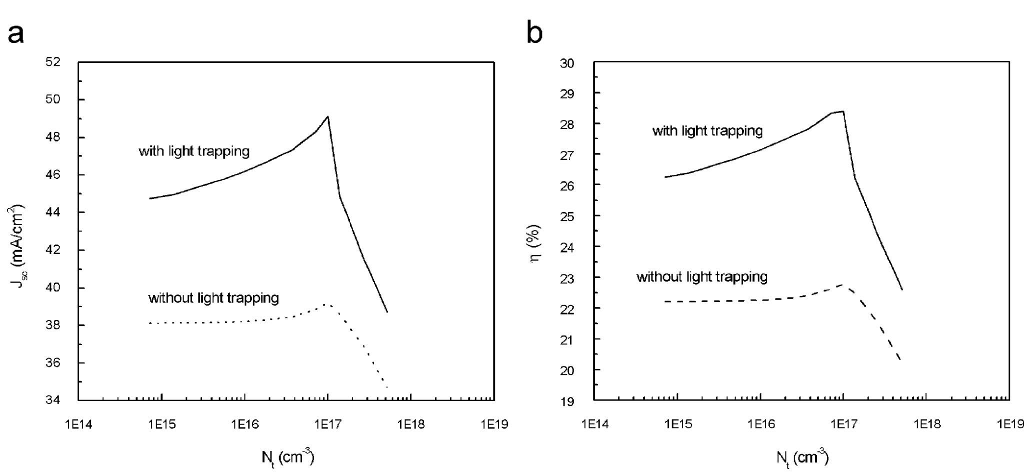

Fig. 4. Effect of light trapping on the IPV effect: (a) short-circuit current improvement and (b) efficiency improvement, with $N_t = 10^{17}\,cm^{-3}$.

3.3. Effect of light trapping

The importance of light trapping in IPV cells was suggested for the first time by Keevers and Green [2]. Light trapping increases the opportunity for photons to be absorbed by weak optical processes in a cell, such as the rate limiting electron photoemission process from the indium level.

In a silicon solar cell with a randoming top surface, a perfect antireflection coating and a planar back surface of reflectivity R_b, the degree of light trapping is adjusted by the value of R_b. Setting $R_b = 0$ corresponds to no light

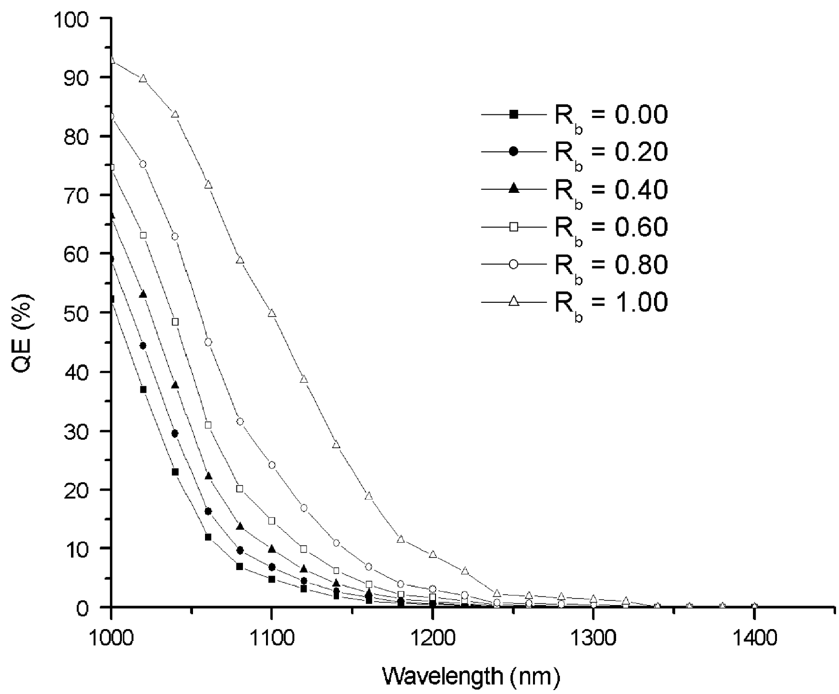

Fig. 5. Effect of light trapping on sub-band gap spectral response with $N_t = 10^{17}\,\mathrm{cm}^{-3}$.

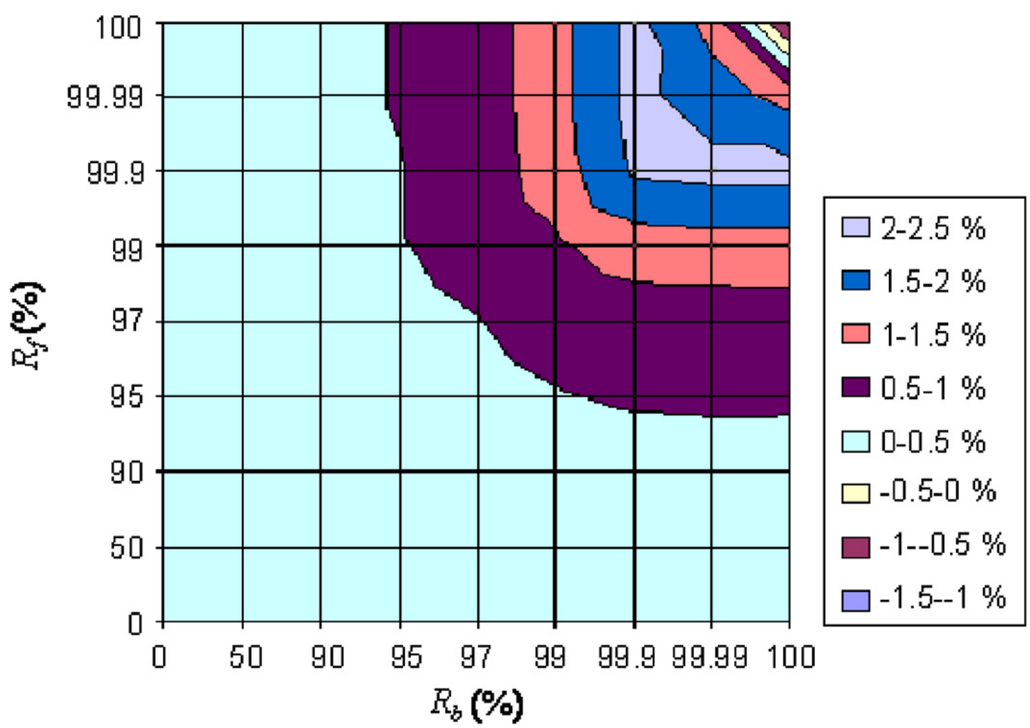

Fig. 6. Absolute efficiency as a function of front and back surface reflectivity, R_f and R_b, respectively.

trapping, however a perfectly back surface reflectivity is obtained by setting $R_b = 1$. Note that a reflectivity close to unity in the back surface of a silicon solar cell has been measured experimentally [8].

To examine how much light trapping affects the IPV effect and improves sub-band gap absorption in the solar cell, we show in Fig. 4 the $J_{sc}(N_t)$ and $\eta(N_t)$ curves with ($R_b = 1$) and without ($R_b = 0$) light trapping.

We see that light trapping increases the photocurrent by about 6 mA/cm^2, and the efficiency by about 2% (absolute) at the optimum indium concentration $N_t = 10^{17}\,\mathrm{cm}^{-3}$. This improvement is due to the enhancement of the IPV effect by improving long-wavelength absorption, as can be seen in Fig. 5 in which we observed an extension of the infrared response into the sub-band gap wavelength region, especially between $\lambda = 1100$ and 1350 nm.

A good internal reflection R_f at the front of the cell is also necessary to obtain a significant IPV effect. In Fig. 6 we show the absolute increase which could be obtained for the solar cell efficiency as a function of the reflection coefficients at the front and the back of the cell, R_f and R_b, respectively. Values approaching the unity are necessary for R_f and R_b otherwise no significant efficiency increase is obtained.

4. Conclusion

We have presented a numerical study of the IPV effect in silicon solar cell doped with indium as impurity, using a new version of the numerical solar cell simulator SCAPS, in which the electron and hole photoemission cross-sections of the impurity are calculated with the model of Lucovsky.

Checking existing results with the new version has shown a good agreement between our results and those of [3].

Our studies show that a significant improvement can be obtained in the short-circuit current and efficiency without sacrificing too much in open-circuit voltage. The benefits of IPV increase with increasing the defect concentration, until an optimum indium concentration, which equals around the base doping density.

This is due to the choice of the p^+–n–n^+ structure, which has the advantage to save the value of built-in voltage at the junction and by consequence that of V_{oc} and however reducing recombination process.

Light trapping is very important to give a positive benefit to the IPV effect by increasing the opportunity for photons to be absorbed by weak optical process in a cell, such as the electron photoemission process from the indium level. Both reflectivity at the front and the back of the cell should approach unity, and exceed 99.9%, to obtain a real efficiency increase.

It is still an open question whether the predicted advantages of the IPV effect can be realized experimentally. Possibly other host semiconductors and other impurities are better suited than the Si/In combination. The SCAPS simulation programme now can be used to explore the IPV effect in other materials such as wide-band gap semiconductors, e.g. GaAs and other III–V compounds.

Acknowledgments

This work is partly supported by Algerian ministry of higher education and research (CNEPRU Project No. D0801/01/05) (S.K., A.B.), and by the Research Fund of the University of Gent (BOF-GOA) (J.V., M.B.).

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