Calculation of the position-dependent inner collection efficiency in PIN solar cells using an electrical–optical model

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Abstract

The position-dependent inner collection efficiency (PDICE) is defined as the probability for an electron–hole pair generated at a certain depth inside a solar cell to be collected. The quantum efficiency (QE) of a PIN solar cell yields the I-layer carrier collection probability as a function of the wavelength, whence only a crude idea of its position dependence can be obtained. Hence for optimizing carrier collection within the intrinsic layer, knowledge of its PDICE is also important. So far PDICE has been calculated by matrix inversion from external QE measurements, a procedure that leads to non-physical oscillations. In this report we determine PDICE in thin film solar cells using our electrical–optical model, which solves the Poisson’s equation and the continuity equations. Our method requires the simulation of a large number of experimental results, from which the parameters reproducing the characteristics of a given device are extracted. These parameters are then used to calculate PDICE. To the best of our knowledge this is the first time that such a model has been used to calculate PDICE. We next apply the method to calculate PDICE in PIN solar cells prepared under various conditions.

1. Introduction

The position-dependent inner carrier collection efficiency (PDICE – also designated as the dynamic inner collection efficiency or DICE), under given bias voltage and illumination conditions, is an important quantity to calculate. This is because it indicates at which positions inside the device carrier collection is weak, so that the problem maybe rectified. PDICE cannot be obtained directly from experiments and has to be extracted from measurable quantities. Takahama et al. [1] and Fischer [2] have calculated PDICE for amorphous silicon (a-Si:H) PIN solar cells using QE experiments. Electron beam-induced current (EBIC) technique at variable electron beam energy has also been used to calculate PDICE [3]. In these methods PDICE at ‘m’ grid points in the device, must be calculated using the measured QE’s at ‘n’ photon wavelengths or electron beam energies, using matrix inversion. The problem is that generally $m \gg n$, since in typical solar cells, under operating illumination conditions, the electric field is strongly position dependent. On the other hand, appreciable response from a-Si:H cells is obtained only over a relatively small wavelength range. We are thus led to oscillatory solutions [2,4].

In the present formalism, we simulate a large number of experimental characteristics of a given device, e.g. the $J–V$ and QE data under various conditions of a solar cell, using our electrical–optical model (ASDMP) based on the solution of the Poisson’s and the continuity equations. The simulations are used to extract the parameters characterizing the cell (e.g. as given in Table 1), which are then used via the procedure described in Section 3, to calculate the PDICE profile under given bias illumination and voltage conditions.

2. Simulation model

The one-dimensional electrical–optical model ASDMP [5] (Amorphous Semiconductor Device Modeling...
Program) used in this study solves the Poisson’s equation and the two carrier continuity equations under steady state conditions for the given device structure and yields the $J-V$ and QE characteristics. The electrical part of the program [6] is similar to the AMPS computer program [7]. The gap state model used in these calculations consists of the tail states and two Gaussian distribution functions to simulate the dangling bond states. The TCO/P and the N/aluminum contact barrier heights have been taken respectively as 1.34 and 0.2 eV. The generation term in the continuity equations has been taken as $G_{\text{generation}} = 1.34$ and $G_{\text{generation}} = 0.2$ eV. The gap state model used in these calculations consists of the tail states and two Gaussian distribution functions to simulate the dangling bond states.

### 3. Calculation of PDICE of a solar cell using ASDMP

Table 1 shows the parameters extracted by modeling the experimental characteristics of the cells. PDICE($x_i$) can then be calculated as follows: The PIN cell is divided into a large number of segments (typically 600), so that the calculated PDICE may be sensitive to the internal electric field, under a given bias light (BL) and voltage $V$. BL is assumed to enter through the P-layer, and the start of this layer is designated as $x = 0$. For the purpose of calculating PDICE at $x_i$, we produce with the help of our model, generation of BL in all the 600 segments, and additional $G(x_i)$ generation in only the segment at $x_i$. Similarly for calculating PDICE($x_{i+1}$) we produce additional $G(x_{i+1})$ generation in segment $x_{i+1}$. $G(x_i)$ maybe produced by any light signal, but it must have a delta function position dependence, being non-zero only in the required segment $x_i$, where PDICE is being calculated. The normalized collection, $C_{p,0}(G(x_i), BL, V)$ of holes at $x = 0$, due to $G(x_i)$ at $x_0$ is defined as

$$C_{p,0}(G(x_i), BL, V) = \frac{\text{Abs}(J_{p,0}(BL + G(x_i)), V) - \text{Abs}(J_{p,0}(BL, V))}{q G(x_i)}$$

(1)

where the subscript ‘0’ of the hole current $J_{p}$ represents its value at $x = 0$ and $q$ is the electronic charge. This collection depends on the applied BL and $V$. We can similarly define the normalized collection $C_{n,0}(G(x_i), BL, V)$ of electrons at $x = 0$, due to $G(x_i)$ at $x_0$. Then

$$PDICE(x_i, BL, V) = C_{p,0}(G(x_i), BL, V) - C_{n,0}(G(x_i), BL, V).$$

(2)

The difference in the numerator of Eq. (1), $\Delta J_{p,0}$, is in general the sum of

$$\Delta J_{p,0} = J_{p,0}(G(x_i)) + \sum_k \frac{\partial J_{p,0}(BL, V)}{\partial x_k} \Delta x_k(G(x_i)).$$

(3)

The first term of Eq. (3) is the hole current at $x = 0$ due to the generation, $G(x_i)$, at $x_0$. The second term is the extra BL hole current at $x = 0$ (if any) due to the now well-known 'photogating effect' [9–11], where $\Delta x_k$ represents different parameters, a change of which may give rise to this effect, such as the electric field, $n/i$ potential barrier, etc. But for PDICE($x_i$) to be calculated from Eq. (2), the numerator of $C_{p,0}(G(x_i), BL, V)$ should be the first term of Eq. (3) alone. To minimize the effect of the second term of Eq. (3), $G(x_i)$ is chosen to be two orders of magnitude lower than the intensity of BL at $x_i$. Under these conditions, the second term in Eq. (3) is negligible.

### Table 1

Parameters extracted using model ASDMP to simulate the solar cell characteristics of different types of solar cells discussed in the text

<table>
<thead>
<tr>
<th>Parameter</th>
<th>P a-Si:H</th>
<th>I a-Si:H</th>
<th>I pm-Si:H</th>
<th>I Ar-dil a-Si:H</th>
<th>N a-Si:H</th>
</tr>
</thead>
<tbody>
<tr>
<td>Layer thickness (nm)</td>
<td>8</td>
<td>450–1000</td>
<td>530</td>
<td>450</td>
<td>25</td>
</tr>
<tr>
<td>Mobility gap (eV)</td>
<td>2.00</td>
<td>1.86</td>
<td>1.96</td>
<td>1.86</td>
<td>1.80</td>
</tr>
<tr>
<td>Activation energy (eV)</td>
<td>0.46</td>
<td>0.87</td>
<td>0.92</td>
<td>0.87</td>
<td>0.2</td>
</tr>
<tr>
<td>Characteristic energy (VB tail) (eV)</td>
<td>0.120</td>
<td>0.050</td>
<td>0.050</td>
<td>0.043</td>
<td>0.050</td>
</tr>
<tr>
<td>Characteristic energy (CB tail) (eV)</td>
<td>0.070</td>
<td>0.030</td>
<td>0.030</td>
<td>0.030</td>
<td>0.030</td>
</tr>
<tr>
<td>Tail prefactors $G_{\text{tail}}$, $G_{\text{mid}}$ (cm$^{-3}$ eV$^{-1}$)</td>
<td>$4 \times 10^{11}$</td>
<td>$4 \times 10^{11}$</td>
<td>$4 \times 10^{11}$</td>
<td>$4 \times 10^{11}$</td>
<td>$4 \times 10^{11}$</td>
</tr>
<tr>
<td>Electron mobility (cm$^2$/V s)</td>
<td>20</td>
<td>20</td>
<td>20</td>
<td>20</td>
<td>20</td>
</tr>
<tr>
<td>Hole mobility (cm$^2$/V s)</td>
<td>4</td>
<td>4</td>
<td>12</td>
<td>3</td>
<td>4</td>
</tr>
<tr>
<td>DOS (cm$^{-3}$) (initial)</td>
<td>$5 \times 10^{18}$</td>
<td>$5 \times 10^{15}$</td>
<td>$7 \times 10^{14}$</td>
<td>$2 \times 10^{15}$</td>
<td>$9 \times 10^{14}$</td>
</tr>
<tr>
<td>DOS (cm$^{-3}$) (stabilized)</td>
<td>$5 \times 10^{18}$</td>
<td>$1 \times 10^{17}$</td>
<td>$2 \times 10^{16}$</td>
<td>$4 \times 10^{16}$</td>
<td>$9 \times 10^{14}$</td>
</tr>
<tr>
<td>Neutral $\sigma$ (tails) (cm$^3$)</td>
<td>$10^{-17}$</td>
<td>$10^{-17}$</td>
<td>$10^{-17}$</td>
<td>$5 \times 10^{-17}$</td>
<td>$10^{-17}$</td>
</tr>
<tr>
<td>Charged $\sigma$ (tails) (cm$^3$)</td>
<td>$10^{-16}$</td>
<td>$10^{-16}$</td>
<td>$10^{-15}$</td>
<td>$5 \times 10^{-15}$</td>
<td>$10^{-15}$</td>
</tr>
<tr>
<td>Neutral $\sigma$ (midgap) (cm$^3$) (initial)</td>
<td>$10^{-17}$</td>
<td>$10^{-17}$</td>
<td>$10^{-15}$</td>
<td>$10^{-17}$</td>
<td>$10^{-17}$</td>
</tr>
<tr>
<td>Charged $\sigma$ (midgap) (cm$^3$) (initial)</td>
<td>$10^{-16}$</td>
<td>$10^{-16}$</td>
<td>$5 \times 10^{-15}$</td>
<td>$5 \times 10^{-16}$</td>
<td>$10^{-15}$</td>
</tr>
<tr>
<td>Neutral $\sigma$ (midgap) (cm$^3$) (stabilized)</td>
<td>$10^{-17}$</td>
<td>$2 \times 10^{-16}$</td>
<td>$10^{-15}$</td>
<td>$10^{-16}$</td>
<td>$10^{-17}$</td>
</tr>
<tr>
<td>Charged $\sigma$ (midgap) (cm$^3$) (stabilized)</td>
<td>$10^{-16}$</td>
<td>$2 \times 10^{-14}$</td>
<td>$2 \times 10^{-14}$</td>
<td>$5 \times 10^{-15}$</td>
<td>$10^{-15}$</td>
</tr>
</tbody>
</table>

The series A a-Si:H and pm-Si:H cells, have a 3 nm a-Si:C:H buffer layer. The DOS here is $5 \times 10^{17}$ cm$^{-3}$ (a-Si:H cell) and $10^{19}$ cm$^{-3}$ (pm-Si:H cell) as evaluated by simulation. Also an intermediate layer with DOS between that in the buffer and main I-layers had to be assumed. The series B cells have no buffers but a P/I IL with DOS $\sim 10^{17}$ cm$^{-3}$ is assumed.
often negligible, but when it is not, PDICE has to be renamed a ‘position dependent carrier collection response’ instead of ‘efficiency’. Also then, PDICE\(_i\) becomes a function of the intensity of \(G(x_i)\). We would like to emphasize however, that in all experiments on QE and calculations of PDICE ([1,2] present method) the modifications described by the second term of Eq. (3) actually exist, and when non-negligible, can even give rise to QE or PDICE higher than unity. The value of PDICE\(_i\) calculated by Eq. (2) is identical to its value from

\[
\text{PDICE}(x_i, BL, V) = C_{n,L}(G(x_i), BL, V) - C_{p,L}(G(x_i), BL, V),
\]

where \(C_{n,L}(G(x_i), BL, V)\) and \(C_{p,L}(G(x_i), BL, V)\) are the normalized collection of electrons and holes respectively, at \(x = L\) (the \(N\)-layer/metal back contact junction), due to the generation \(G(x)\) at \(x_i\).

4. Experiments

One set of PIN diodes having either standard amorphous silicon or polymorphous silicon intrinsic layers, were deposited by the standard plasma enhanced chemical vapor deposition (PECVD) process in a multi-plasma monochamber reactor [12] at LPICM, Ecole Polytechnique, France. We will refer to these as series A cells. The standard a-Si:H films were produced by the dissociation of pure silane at 40 mTorr under an RF power of 10 mW cm\(^{-2}\). Polymorphous silicon (pm-Si:H) films on the other hand, were prepared by the dissociation of a 3% silane in hydrogen mixture at 1800 mTorr under an RF power of 90 mW cm\(^{-2}\). pm-Si:H is a nanostructured silicon thin film produced by PECVD, under conditions close to powder formation. It has a lower initial and stabilized density of states (DOS) and a considerably higher hole mobility (\(\mu_p\)) than a-Si:H; but lower light absorption coefficients [13]. Another set of a-Si:H PIN cells (to be referred to as series B) was fabricated at IACS, Kolkata, India, also by the PECVD technique, with the intrinsic layer deposited under two conditions: using (a) undiluted silane and (b) 90% argon (Ar) diluted silane. The depositions were carried out in an interconnected four-chamber ultra-high vacuum deposition system. Ar-diluted a-Si:H also has a lower DOS than standard a-Si:H, and a lower valence band tail characteristic energy \(E_D\) [14]. In all solar cells the TCO, SnO\(_2\), has a textured surface. Series A cells have an intrinsic a-Si:C:H buffer layer at the P/I interface. \(J-V\) characteristics have been measured for all cells. For the series A samples QE was measured under AM 1.5 bias light; while for series B, QE was measured without bias light. Light-soaking was done under 100 mW cm\(^{-2}\) light.

![Fig. 1](https://example.com/fig1.png)

**Fig. 1.** The experimentally measured and modeled QE characteristics of series A a-Si:H solar cells of different thickness, under AM 1.5 BL and short-circuit conditions: (a) in the initial state and (b) after LID. Lines for QE are experimental data and symbols represent the results of the model. The PDICE calculated using ASDMP for each case under AM 1.5 BL and 0 V are shown in (c) in the initial state and in (d) after LID.
from a 1 kW Xe-arc lamp in the open-circuit configuration at 50 °C for 1000 h.

5. Calculation of PDICE in solar cells

In this section we describe the procedure for calculating PDICE in the initial and light-stabilized states of the solar cells described above. The QE of series A a-Si:H cells of different thickness are compared to modeling results in Fig. 1(a) and (b), respectively in the initial state and after light-induced degradation (LID). Fig. 2 compares the QE’s of the other cells described in the experimental section to the results obtained by ASDMP. In Figs 1 and 2 the experimental QE curves are represented by lines, while symbols represent simulated data. We have also simulated the illuminated \( J-V \) characteristics of these cells. This range of simulations has enabled us to extract the parameters characterizing each device in the initial state and after LID (Table 1). The choice of several parameters have been dictated by the measured values of these quantities, e.g. low initial and stabilized DOS in pm-Si:H and Ar-diluted a-Si:H, higher \( \mu_p \) in the former and lower \( E_D \) in the latter [13,14]. The parameters chiefly determined by modeling are the properties of the P/I interface region and the capture cross-sections (\( \sigma \)'s) of all defect states in the device. Modeling indicates an extremely high density of states (DOS) in the P/I buffer region for pm-Si:H cells. In all cases an intermediate layer (IL), with DOS intermediate between the buffer and the main I-layer has been assumed. To match experimental results after LID, some capture cross-sections (\( \sigma \)'s) of the dangling bond (DB) states in the IL’s and main intrinsic layers had to be increased.

The parameters in Table 1 were then used by ASDMP, in conjunction with the procedure described in

![Fig. 2. A comparison of the experimentally measured and simulated QE characteristics at 0 V for the different types of solar cells studied (a) series A pm-Si:H cells under AM 1.5 BL, (b) series B a-Si:H cells without BL and (c) series B Ar-diluted a-Si:H cells without BL. Lines are experimental data and symbols represent the results of the model.](image1)

![Fig. 3. PDICE calculated using ASDMP and the parameters of Table 1, for series A a-Si:H and pm-Si:H cells, and series B a-Si:H and Ar-diluted a-Si:H cells; in the initial (a) and light-stabilized (b) states.](image2)
section 3 to calculate PDICE. The results are given in Fig. 1(c) and (d) for the series A a-Si:H cells in the initial and LID states. For all the cells a comparison of PDICE is given in Fig. 3(a) in the initial and in Fig. 3(b) in the stabilized state. As these devices are relatively thin (around 0.5 μm), the PDICE is high for all in the initial state. However large differences are seen in the stabilized state (Fig. 3b). For the series B cells, the Ar-diluted a-Si:H cell indicates better carrier collection than the a-Si:H cell after LID. This is due to the inherent lower stabilized DOS and lower ED for the former case. For the series A pm-Si:H cell, the trapped hole population and the electric field in front of the device fall due to an increase of the charged σ’s upon LID, specially over the defective intermediate layers near the P/I interface. This results in a fall in both the short-wavelength QE (Fig. 2(a)), and PDICE over the front of the device (Fig. 3b). The fall of the electric field in the front, results in field-redistribution and an increase of field towards the back of the cell, which, together with the lower stabilized DOS and higher μp of this material, ensures excellent collection from the back. In fact the improved back region field, generates some photogating effect here (Fig. 3b).

6. Conclusions

We have reported on how to calculate the depth profile of the inner carrier collection efficiency (PDICE) in PIN solar cells, using a model based on the solution of the Poisson’s equation and the continuity equations. In contrast to existing methods of PDICE calculation, which require matrix inversion and result in unphysical oscillations in the calculated values of PDICE, this method is based on the simulation of a large number of experimentally measured characteristics of the given device, from which the parameters characterizing the device are extracted. Such a calculation of PDICE is free from oscillations, so that fine structure in PDICE can be studied. It can also be easily extended to other device structures. The popularly used QE characteristic of a solar cell gives the collection efficiency as a function of the wavelength, from which only an approximate idea of the spatial dependence of carrier collection, can be deduced. Thus both PDICE and the QE characteristics are to be taken together, in order to visualize carrier collection within a device.

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