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Charge collection in amorphous silicon solar cells: Cell analysis and simulation of high-efficiency *pin* devices

Michael Stuckelberger *, Yannick Riesen, Brice Perruche, Matthieu Despeisse, Nicolas Wyrsch, Christophe Ballif

Ecole Polytechnique Fédérale de Lausanne (EPFL), Institute of Microengineering (IMT), Photovoltaics and Thin Film Electronics Laboratory, Rue Breguet 2, CH-2000 Neuchâtel, Switzerland

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ABSTRACT

The drift length $L_{drift}=\mu\tau E$ within the *i* layer of a-Si:H solar cells is a crucial parameter for charge collection and efficiency. It is strongly reduced not only by light-induced reduction of $\mu\tau$, but also by electric field deformation ΔE by charges near the *p*–*i* and *i*–*n* interfaces. Here, a simple model is presented to estimate contributions of free carriers, charges trapped in band tails and charged dangling bonds to ΔE. It is shown that the model reproduces correctly trends observed experimentally and by ASA simulations: charged dangling bonds contribute most to ΔE of meta-stable cells. Electrons trapped in the conduction band tail near the *i*–*n* interface lead to the strongest field deformation in the initial state, while positively charged dangling bonds near the *p*–*i* interface get more important with degradation under AM1.5g spectrum. The measurable parameter V_{coll} is proposed as an indirect parameter to estimate the electric field, and an experimental technique is presented that could enable the distinction of defects near the *p*–*i* and the *i*–*n* interfaces.

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1. Introduction

One of the main efficiency limitations in hydrogenated amorphous silicon (a-Si:H) based solar cells remains to be the electrical performance degradation arising from metastable defect creation in the form of dangling bonds under light exposure (Staebler–Wronski-Effect (SWE) [1]). These defects reduce the mobility lifetime product $\mu\tau$ and, with it, the drift length $L_{drift}=\mu\tau E$. As the cells are drift driven, this affects seriously the charge collection and efficiency of the cells.

With a degraded mobility-lifetime product, the strength of the electric field within the absorber layers gets crucial for the preservation of a sufficiently high charge extraction from the intrinsic (*i*) layer. In addition, charges trapped not only in the doped *p* and *n* layers, but also in *i* layers lead to a deformation of the electric field ΔE. Using for simulations and deposited cells in the following always the same doped layers, we concentrate on the *i* layer and discuss in this article the influence of (a) free carriers, (b) charges trapped in valence and conduction band tails, and (c) charged dangling bonds on the electric field and hence on the charge collection. As the electric field within solar cells is experimentally hardly accessible, results from a very simple instructive model are compared with simulations with the ASA program [2] and experiments, including the measurement of parameters that allow to deduce information about the electric field within the *i* layer.

One of these parameters is the measurable collection voltage V_{coll} as discussed in [3–5]. It obtains its physical meaning by the link to the collection function or -efficiency χ that is defined as:

$$\chi=\frac{Q_{coll}}{Q_{photo}}=\frac{J_{coll}}{J_{photo}}=1-\frac{\int R(x)dx}{\int G(x)dx}, \quad (1)$$

with $Q_{coll,photo}$, $J_{coll,photo}$ the collected and photogenerated charge and current densities; R and G are the e^-/h^+-pair recombination and generation rates. Different terms for χ have been derived in literature for various recombination models [3,6–9]. In all these cases, the fractional collection losses (in percent of the generated current) do not depend on G and are therefore proportional to J_{photo}. Describing the solar cell by the simple equivalent circuit [3], between high illumination regime with dominant series resistance losses and low illumination regime with dominant parallel resistance losses, there exists a medium illumination regime, where the recombination term is dominant. In this regime, one finds independently of the form of χ the collection voltage

$$J_{sc}\cdot R_{sc}\approx\chi|_{V=0}\cdot\left.\frac{\partial V}{\partial\chi}\right|_{V=0}\doteq V_{coll} \quad (2)$$

that does not depend on J_{photo}. Thanks to its independence from the collection model and other parameters such as parallel and series resistance, V_{coll} is a good parameter for intrinsic charge collection that can provide additional information to e.g. quantum efficiency or fill

* Corresponding author.
E-mail address: michael.stuckelberger@epfl.ch (M. Stuckelberger).
URL: http://pvlab.epfl.ch (M. Stuckelberger).

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factor [10]. In a more intuitive approach, V_{coll} is the voltage that must be applied to the equivalent ohmic resistance R_{sc} for a current J_{sc} to flow.

2. Simple model to estimate $\Delta E(x)$

The main assumptions for this model are: (1) No recombination of holes and electrons in the *i* layer and (2) diffusion is negligible as charge transport mechanism compared to drift. Starting from a constant nominal electric field $E_{nom} = \frac{V_{bi}}{d_i}$ with the built-in voltage V_{bi} and the *i* layer thickness d_i, charge profiles and the electric field deformation $\Delta E = E - E_{nom}$ caused by such charges are calculated without iteration of the transport equations (limiting this model to cases, in which $\Delta E \ll E$). The aim of such crude simplifications is to provide intuitive insights in the physical processes of charge collection and explain measured trends.

The model is based on the intuitively plausible model of amphoteric defect states that can be charged positively (D^+), negatively (D^-) or remain neutral (D^0). As derived in [11], these states are occupied with the probabilities f^+, f^-, and f^0 which depend on the capture cross sections $\sigma_{p,n}^{+,0,-}$ of D^+, D^- and D^0 for holes and electrons and on the free carrier concentrations p_f and n_f. With assumption (1), we get the particle fluxes $\Phi_{p,n}(x)$ at position x in an *i* layer between $x=0$ (*p–i* interface) and $x=d_i$:

$$\Phi_p(x) = \int_x^{d_i} G(\xi)d\xi \quad \text{and} \quad \Phi_n(x) = \int_0^x G(\xi)d\xi. \tag{3}$$

With assumption (2), it is:

$$p_f, n_f(x) = \frac{\Phi_{p,n}(x)}{v_{p,n}^{th}} = \frac{\Phi_{p,n}(x)}{\mu_{p,n} \cdot E_{nom}} \tag{4}$$

with the thermal velocities v^{th}. Based on [12,13], we assume further $\sigma^{\pm} \equiv \sigma_p^- = \sigma_n^+$ and $\sigma^0 \equiv \sigma_p^0 = \sigma_n^0$ and write $\zeta \doteq \frac{\sigma^{\pm}}{\sigma^0}$, $\gamma \doteq \frac{\mu_n}{\mu_p} = \frac{v_n^{th}}{v_p^{th}}$, and $\eta(x) \doteq \frac{\Phi_n(x)}{\Phi_p(x)}$. For numerical calculations, we took $\zeta = 50$ and $\gamma = 3$ [13,14]. The occupation functions reduce then to:

$$f^+(x) = \frac{1}{1+\zeta\eta(x)+\eta^2(x)}, \quad f^-(x) = \frac{\eta^2}{1+\zeta\eta(x)+\eta^2(x)}. \tag{5}$$

Considering always only one type of charge carriers, the field deformation relative to the *p–i* (index *p*, considering holes) or to the *i–n* interface (index *n*, considering electrons), is calculated as:

$$\Delta E_{p,n}(x) = \frac{q}{\epsilon_0 \epsilon_r \int_{0,x}^{x,d_i} N_{p,n}(x')dx'}. \tag{6}$$

Depending on the charge type, $N_{p,n}(x')$ is either the free charge carrier concentration p_f, n_f calculated with Eq. (4), or the concentration of charge carriers trapped in band tails $p_{bt}, n_{bt} = \frac{p_f}{\Theta_p}, \frac{n_f}{\Theta_n}$ (with the Rose trapping factors $\Theta_p \approx 0.005$ and $\Theta_n \approx 0.1$), or the concentration of charged dangling bonds $p_{db}, n_{db} = f^{+,-} \cdot N_{db}$ with the dangling bond concentration N_{db}. The choice of the remaining parameters $G(x)$ and $N_{db}(x)$ is principally the same as in the ASA simulations (see Section 3) and will be discussed in Sections 4 and 5.

From $\Theta_{p,n} \ll 1$ follows directly that $\Delta E_{p,n}$ caused by free carriers can be neglected with respect to $\Delta E_{p,n}^{bt}$.

3. Experimental

An *i* layer thickness series (100–1000 nm) of ~0.25 cm^2 a-Si:H cells was deposited by PECVD in superstrate configuration on glass with 2 μm thick boron-doped zinc oxide (LPCVD) TCO layers on both sides (a second series deposited in another system lead to very similar results). Typical cell efficiencies are above 10% in initial state and above 8% stable.

Beside standard $J(V)$-curve measurements for the fill factor (*FF*), external quantum efficiency (EQE) measurements were used to determine V_{coll}: Varying the bias voltage V, V_{coll} can be determined as $V_{coll} = EQE(0V) \cdot \frac{\partial V}{\partial EQE}|_{0V}$ (details can be found in [4]). For the present study, $EQE(V)$ was determined with a probe beam at 420 nm and blue bias light that entered with the probe beam either from *p* or *n* side into the cell. This measurement is therefore sensitive mainly to charge collection near the *p–i* and *i–n* interface. [The absorption lengths of the probe beam at 420 nm and of the blue bias light are in the order of 25 and 65 nm, respectively.]

The ASA package (version 5 [2]) with the optical model GenPro3 was used for simulations. For the simulation parameters we took values obtained from layer measurements, where available, and reasonably chosen values otherwise.

4. Results

The correlation between V_{coll} and *FF* is discussed in [10,12]. Here, V_{coll} determined from EQE measurements is compared to the electric field deformation resulting from the simple model, and to a more precise simulation of the deposited cells (see Section 3) by the ASA package.

With the creation of dangling bonds by SWE during light soaking, field deformation by charges within the *i* layer reduces the charge collection additionally to the effect of new recombination centers: In ASA simulation, the dangling bond concentration in the *i* layer in initial state was set constant to $N_{db}^{ini}(x) = 3 \cdot 10^{15} \text{cm}^{-3}$. We simulate the degradation by a linear increase of N_{db} with $G(x)$ to $N_{db}^{deg}(x) = N_{db}^{ini} + c \cdot G(x)$ in the degraded state (we assumed $c = 2.5 \cdot 10^{-5}$s). [In the simple model, N_{db} is chosen 10 times smaller to reproduce qualitatively trends observed, without getting unphysically high ΔE that would no more justify the assumption $\Delta E \ll E$.] The ASA simulation of charge densities before and after light soaking is shown in Fig. 1. Fig. 2 shows the effect of these charges (ASA simulation and simple model calculations) on the electric field deformation.

The increased ΔE in the degraded state is confirmed by a decrease of V_{coll} after light soaking that can be seen in experiment (Fig. 3a) and ASA simulation (Fig. 3c). Not surprisingly, V_{coll} is smaller for *n* side illumination, as the slow holes have to cross the whole *i* layer and recombine more often than the electrons in the opposite case. To get a feeling for the voltage dependence of the charge collection, the parameter $V'_{coll} \doteq \frac{\partial V}{\partial \chi}\Big|_{V=0} = \frac{\partial V}{\partial EQE}\Big|_{V=0}$ (i.e. V_{coll} without normalization), has been investigated (see Fig. 3b). Interestingly, it shows a different behavior than V_{coll}. Namely, it increases strongly for thick cells, when illuminated from *n* side. The ASA simulation in Fig. 3d proves that this is not just a measurement artifact.

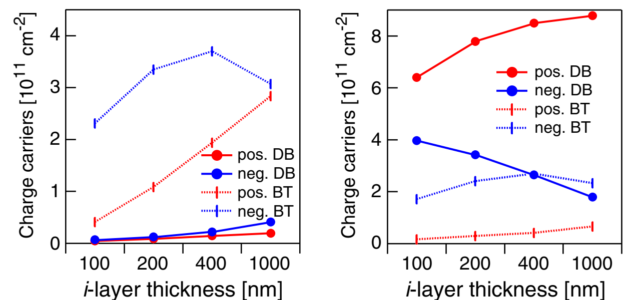

Fig. 1. ASA simulation of charge densities (integrated over whole *i*-layer thickness) in form of trapped charges in band tails (neg. BT for conduction band, pos. BT for valence band) and charged dangling bonds (DB) in initial (left) and degraded state (right) for cells with 100 to 1000 nm thick *i*-layers.

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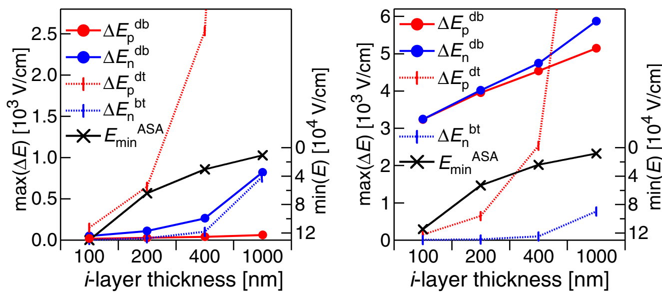

Fig. 2. Estimation of the field deformation ΔE due to positive (p) and negative (n) charges in band tails (bt) and dangling bonds (db) with the simple model in initial (left) and degraded state (right). E_{min} is the minimum electric field within the i layer from the corresponding ASA simulations.

5. Discussion

While ΔE is dominated by the i–n interface in initial state (for constant N_{db}), the light induced increase of defect states mainly near the p–i interface strongly increases the contribution of the p–i interface to ΔE, as could be seen in Fig. 1: Most e^-/h^+-pairs are created near the p–i interface and the electrons need to travel much further, thus the mean electron flux $\overline{\Phi_n}(x)$ is much higher than the mean hole flux $\overline{\Phi_p}(x)$, over compensating the lower mobility of holes and leading to a higher electron concentration and dominating therefore ΔE following Eq. (6).

After light soaking, most defect states near the p–i (i–n) interfaces are, like before, in D^+ (D^-) state and deform the field. There are now more defects to be positively charged near the p–i interface. These lead to a larger electric field deformation than negatively charged dangling bonds near the i–n interface. [In actual solar cells, this effect is even more pronounced, as the p–i interface is already in initial state more defective than the i–n interface.]

Comparing the simple model (Fig. 2) with ASA simulation (Fig. 1), the effect of holes trapped in valence band tail seems to be strongly overestimated as compared to the electrons trapped in conduction band tail; this suggests that the ratio $\frac{\Theta_p}{\Theta_n}$ as given in [13] and used for the simple model calculations might be underestimated. The very strong maximum field deformation for cells with thick absorber layers shows the limitation of non-iteration in the simple model, where the error gets larger, the more ΔE is approaching the electric field.

A comparison of electric field and charge distributions from ASA simulations (not shown here) shows that the different behavior under p and n side illumination is a field deformation effect that is directly caused by the spatial separation of defects and e^-/h^+-pair generation in case of n side illumination (coincidence for p side illumination). Therefore, V'_{coll} could be a parameter that allows getting insight into the distribution of defects in the i layer of working solar cells — this will have to be studied further in detail.

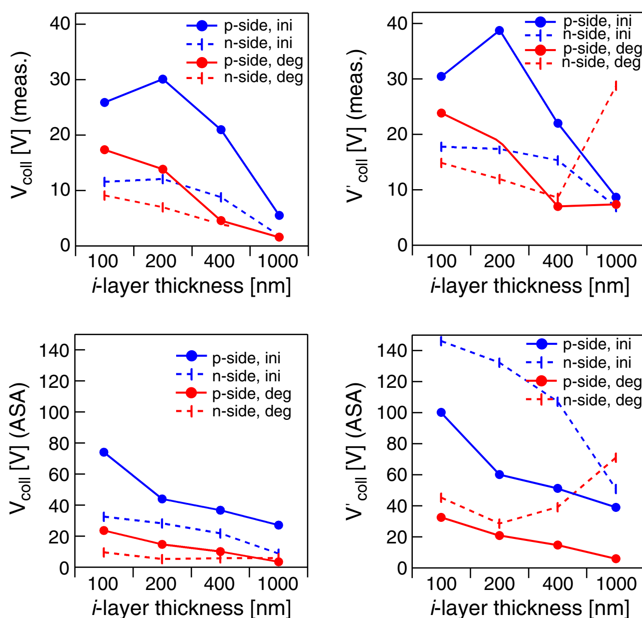

Fig. 3. V_{coll} and $V'_{coll} = V_{coll} \cdot EQE^{-1}(0V)$ determined from EQE measurements (top) and ASA simulation (bottom) with probe beam at 420 nm incident with blue bias light from p and n side for cells in initial state and after light soaking.

6. Conclusion

A simple model has been presented to estimate the electric field deformation in i layers of a-Si:H solar cells, caused by charges trapped in valence and conduction band tails as well as by charged dangling bonds. It has been compared to ASA simulations and measurements on an i layer series of deposited solar cells, where its good ability to describe observed trends, but also its limitations could be seen. It has been shown that field deformation is mainly governed by the i–n interface in the initial state, but that the p–i interface gets more important with light soaking from p side. Further, the use of the collection voltage V_{coll} and of the derived parameter V'_{coll} has been studied for an evaluation of the charge collection and internal electric field in the i layer.

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