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Modeling a-Si:H p–i–n solar cells with the defect pool model

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Abstract

Using self-consistent computer modeling we find that the experimental current–voltage (J–V) and the spectral response (SR) characteristic curves of a-Si:H p–i–n solar cells can be fitted by either assuming a uniform density of dangling bonds (DB) in each device layer (UDM) or by relying on the defect pool model (DPM). Fittings within the DPM were achieved using the algorithms proposed by Powell and Deane and Schumm. One Si–H bond mediating in the creation of dangling bonds in the first expressions proposed by Powell and Deane and Schumm are appropriate for modeling solar cells in the initial state. The applicability of the algorithm proposed by Schumm for a-Si:H in the stabilized state is also discussed in solar cells. Using DPM we have explored the optimum doping and band gap profile in the intrinsic layer leading us to the maximum efficiency of a-Si:H p–i–n cells.

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1. Introduction

Hydrogenated amorphous silicon (a-Si:H) has been widely investigated as a viable material for inexpensive and efficient solar cells. a-Si:H and its alloys contain a large number of localized states: tail states (TS) and dangling bonds (DB). In the defect pool model (DPM) DB result from the breaking of weak or strained bonds (WB) [1–3]. The equilibrium DB density predicted by DPM is strongly influenced by the energy of the Fermi level and results quite non-uniform within the intrinsic layer of a p–i–n structure. The detailed knowledge of the DB density and the understanding of defect formation mechanisms are of vital importance to appropriately model the defect structure and the density of metastable defects for devices applications. It was a common practice to assume an increasing uniform density of DB (UDM) in the intrinsic layer to simulate the degraded state of a-Si:H [4]. Nowadays we can rely on more advanced formalisms like the ones proposed by Powell–Deane (two algorithms) [1,2] and Schumm [3] (one algorithm). We will identify their models with the initials DPM1, DPM2, and DPM3 respectively.

In this paper we show that for a-Si:H p-i-n solar cells the current–voltage (J–V) can be fitted by using either the UDM or the DPM approaches and that any of the three different DPM proposed in the literature can be used in the initial state under certain restrictions. We also can fit light J–V of a-Si:H p–i–n cells in the stabilized state using either the UDM or the DPM3 representation. We explore as well the most appropriate band gap and doping profile in the intrinsic layer to maximize the solar cell performance. The design of the optimum profile in the intrinsic layer of a-Si:H p–i–n solar cells was shown to have an strong influence on the drift diffusion length [5].

2. Experiments

Single p–i–n a-Si:H solar cells were grown by plasma enhanced chemical vapour deposition (PECVD) in an ultra high vacuum multi-chamber system (PASTA). Cells were deposited on SnO_2 coated glass (Asahi U-type) in the super-strate configuration SnO_2/p-aSiC:H/i-a-Si:H/n-a-Si:H/Ag. Three thin layers (0.5 nm) with decreasing content of carbon were included between the p and the intrinsic layer. Cells were deposited with different i-layer thicknesses: 215, 500, and 1000 nm. Absorption coefficient and refractive indexes of each

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individual a-Si:H-layer were determined by $R@T$ measurements. The total density of DB (5×10^{15} cm^{-3}) and the Urbach tail (48 meV) were extracted with the CPM technique. The activation energies of doped layers were obtained from temperature dependence of the dark conductivity (0.47 and 0.24 eV in the p, and n-layer respectively). Single a-Si:H p–i–n solar cells were characterized by measuring AM1.5 light J–V, SR and low-forward dark J–V characteristics.

3. Modeling

Our simulations were performed with the computer code D-AMPS [6]. The density of states in the UDM is described by three Gaussian distributions recognized as D^-, D^0, and D^+. The ratio of charged to neutral defects is adopted 4:1 and the separation Δ between the non-occupied D^+ peak and the double occupied D^- peak is set to 0.4 eV for any band gap. The hydrogen concentration H is adopted 3.5×10^{21} cm^{-3}, and the freezing temperature 500 K in DPM. The correlation energy U is assumed 0.2 eV. The most probable energy E_p in the distribution of available states is used as fitting parameter but keeping its value close to the D^+ peak used in UDM. The Pool width is appropriately selected to reproduce the UDM value of Δ, or close, in each layer. Since there is not a clear picture available for the distribution of energy offsets we split them equally between the conduction and the valence band.

4. Results

We found that the experimental J–V and SR characteristic curves of a-Si:H p-i-n solar cells can be fitted with D-AMPS using either the UDM or the DPM approach. Among the different microscopic chemical reactions proposed in DPM1 and DPM3 we selected the reaction where only one Si–H bond is involved in the reaction WB $\rightarrow$ DB. Reactions where zero or two Si–H bonds participate give rise to a quite low or to a quite high density of DB what results in too optimistic or too pessimistic efficiencies. However two Si–H bonds are involved in the WB $\rightarrow$ DB reactions of the DPM2 but the density of DB results lower than the density predicted by DPM1 with two Si–H bonds. We show in Fig. 1 our fittings of the light J–V curve corresponding to a p–i–n with a 500 nm thick i-layer. DPM predicts a highly non-uniform density of defects: more DB near the p/i and i/n interfaces than in the bulk (see Fig. 2). This DB profile reinforces the electric field at the edges of the intrinsic layer and weakens the electric field in the bulk making more difficult the task of reproducing experimental FF in thicker p–i–n solar cells. To minimize the bulk electric field deterioration we found convenient in DPM to increase the electron and hole mobilities to 30(20) and 3(2) cm^2/V/s respectively and to decrease the Urbach tail slope to 45(48) meV. We also introduced a background uniform density of around 2×10^{15} cm^{-3} fully ionized acceptor states in the intrinsic and band-gap graded layers to improve our FF. The i-layer mobility gap was adopted 1.72 eV to reproduce FF and V_{oc}. Scattering at rough surfaces was needed to match the short circuit current (J_{sc}) and SR at red and longer wavelengths [7]. Using identical inputs DPM3 gives rise to more DB than DPM1. This undesired effect was counter balanced by adopting slightly higher values of E_p in buffer and i-layers. Using similar input values light J–V and SR of a-Si:H solar cells with 215 and 1000 nm thick i-layers were also fitted. We show all our light J–V fittings in Table 1. SR characteristics are not included in this paper for lack of space. The dark J–V curve at low forward voltage was also satisfactorily reproduced (see Fig. 3).

The current at low forward biases and under dark conditions is controlled by i-layer bulk recombination in a-Si:H p–i–n cells [8]. In UDM recombination is dominated by deep states (DB) at lower biases and by tail states at higher voltages. Tail and deep states contribute mostly to recombination near the interfaces and in the bulk respectively. On the other hand in DPM

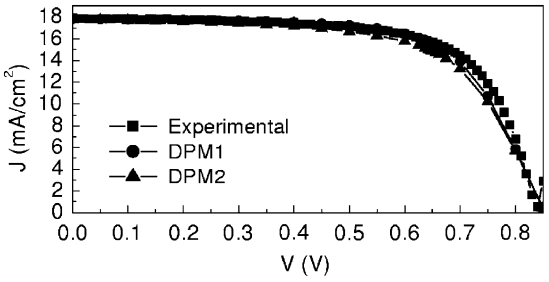

Fig. 1. Fittings of the light J–V curve achieved with D-AMPS using DPM1 and DPM2. The i-layer thickness is 500 nm. The cell is in the initial state.

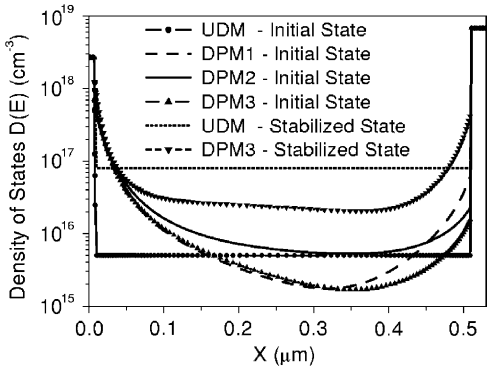

Fig. 2. Density of dangling bond profiles resulting from our fittings of p–i–n solar cell characteristic curves for the different models used in this paper. The i-layer thickness is 500 nm.

Table 1
Fittings of light J–V curves

IS	E-500	UDM	DPM1	DPM2	DPM3	E-215	DPM1	DPM3	E-1000	DPM1	DPM3
V_{oc}	0.836	0.858	0.852	0.854	0.85	0.815	0.824	0.817	0.818	0.845	0.839
FF	0.683	0.68	0.667	0.638	0.655	0.64	0.656	0.638	0.601	0.588	0.574
J_{sc}	17.95	17.85	17.83	17.76	17.67	14.77	14.89	14.92	19.08	19.17	19.17

SS	E-500	UDM	DPM3	E-215	DPM3	E-1000	DPM3
V_{oc} (V)	0.81	0.818	0.808	0.795	0.79	0.865	0.798
FF	0.522	0.553	0.538	0.533	0.549	0.427	0.468
J_{sc} (mA/cm^2)	16.22	16.03	16.24	13.74	13.58	15.98	15.93

E stands for experimental data and the number besides is the i-layer thickness in nm. IS refers to cells in the initial state and SS refers to cell in the stabilized state.

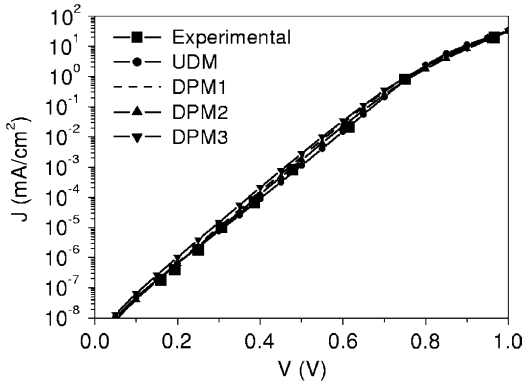

Fig. 3. Fittings of the dark J–V curve achieved with D-AMPS using UDM, DPM1, DPM2 and DPM3. The i-layer thickness is 500 nm. The cell is in the initial state.

recombination is controlled entirely by deep states. Adopting wider tails and higher cross sections in UDM helps us in compensating the higher recombination introduced by deep states near interfaces by DPM. The strategy followed in our fittings was to obtain a similar integrated recombination (cm^{-2} s^{-1}) on the whole i-layer in UDM and DPM. Under dark conditions this was achieved on the voltage range shown in Fig. 3 and under light conditions the i-layer integrated recombination rate has to be similar only for voltages approaching V_m (maximum power point) and V_{oc} where recombination losses shape the light J–V curves. For different DPM models our inputs were selected such as having similar trapping and recombination profiles mainly in the front region of device where DB concentrations are higher.

Table 1 includes fittings of light J–V in the stabilized state performed with DPM3. Schumm assumes that the chemical reactions controlling the defect structure are identical in equilibrium and out of equilibrium. He proposes an expression where the effect of light soaking is to change the steady occupancy of defects and to introduce the extra factor $(np/n_0p_0)^B$ where n (n_0) and $p(p_0)$ are the free carrier concentrations out of (in) equilibrium. B is a function of the freezing temperature [3]. Interestingly this theory allowed us to match the light J–V and to reproduce the increase (decrease) of the low (high)-forward dark J–V_s experimentally observed under light soaking. Manipulating our input data we are able to match J–V curves using the n and p profiles predicted by D-AMPS at either short circuit or at open circuit voltage conditions. However, the experimental light J–V were obtained illuminating with AM1.5 light during 3000 h in a-Si:H p–i–n cells operating at V_{oc}. Fittings were achieved with the UDM increasing DB densities 16 times in the i-layer and 10 times in buffers (we have problems near V_{oc} in the 1000 nm thick solar cell). Similar fittings can also be obtained combining increases of cross sections and DB densities.

After calibrating our code by matching experiments we used D-AMPS to explore the dependence of the a-Si:H solar cell efficiency with respect to doping and band gap profiling inside the intrinsic layer. Grading near the i/n interface introduce minor improvements in solar cell performance while grading near the p/i interface can significantly enhance the cell efficiency. Grading was performed accordingly to the exponential distribution (resembling experimental boron profiles) $\exp[-x/(CW)]$ where x is the distance from the p/i interface towards the bulk, W (nm) is the region thickness where band gap, boron doping or both are graded and C defines how steep is the exponential. These parameters can be adjusted to find the optimum distribution. Fig. 4 shows that once C has been optimized there is an optimum value of W that we will recognize as W^*. In our simulations we assume that the energy E_p, the pool width, mobilities, and tail slopes vary also accordingly within the region of thickness W. When the i-layer band gap is profiled we observe that for lower values of W such us $W < W^*$ ($W^* = 50$ nm), V_{oc} tends to decrease while for higher values of W such as $W > W^*$ FF and in less extend Jsc tend to decrease. Band gap grading reduces recombination and the electric field near the p/i interface while enhances the electric field in the bulk. Boron contamination weakens (strengths) the electric field near the p/i interface (in the bulk) what increases (decreases)

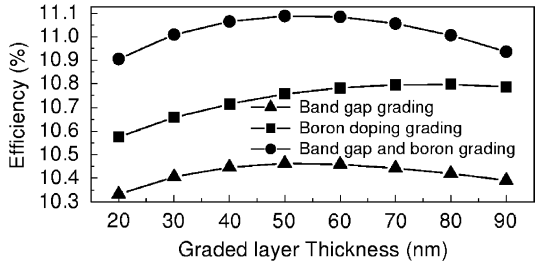

Fig. 4. Efficiency versus profiled region thickness W. Boron doping ($C = 0.1$), band gap ($C = 0.3$), and both ($C = 0.3$) are graded in the intrinsic layer (500 nm thick) near the p/i interface. Simulations performed with DPM1.

recombination near the p/i (in the i-layer bulk). We also obtain an optimum value W^* ($W^* = 80$ nm). In this case we observe a decrease in FF when we have $W < W^*$ and we observe a decrease of V_{oc} and J_{sc} when we have $W > W^*$. Exponential grading of both the band gap and the boron doping gives rise to the most significant enhancement (10% relative) of the solar cell efficiency. There is a reduction in the recombination losses over the whole i-layer because band gap is higher near the p/i interface and the electric field becomes stronger in the bulk. Our results are shown for DPM1 but similar trends were obtained for DPM2 and DPM3.

When the density of DB is modeled with UDM D-AMPS advice us the entire removal of buffer layers at the p/i interface. On the other hand, when the DPM is implemented our predictions are more in agreement with experimental evidence; i.e. we can justify the presence of buffer layers at the p/i interface and of band gap profiles in the intrinsic layer [9].

5. Conclusions

We were able to fit with D-AMPS the experimental J–V and SR characteristic curves of a-Si:H p–i–n solar cells having three different intrinsic layer thicknesses by either using uniform density of dangling bonds (UDM) in each device layer or with the defect pool model (DPM). Fittings were achieved in the initial and in the stabilized state of these solar cells. However in order to find the highest solar cell efficiency our predictions indicate that only the DPM is able to reproduce experimental trends. The three algorithms published in the literature for DPM can be used for this purpose but only the second version published by Powell and Deane allows us to assume that two Si–H bonds are involved in the DB creation. The theory proposed by Schumm for degraded a-Si:H can be used in solar cell modeling with caution. The a-Si:H cell efficiency can be significantly improved by profiling the band gap and introducing boron contamination in the intrinsic layer near the p/i interface.

Acknowledgements

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