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Evidences of the defect pool model in the dark current-voltage characteristics of hydrogenated amorphous silicon based p-i-n devices

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Abstract

In the scientific literature the density of states of hydrogenated amorphous silicon has been assumed to be either uniform or spatially variable inside the intrinsic layer of p-i-n solar cells. The dependence of the dark current voltage characteristics of amorphous silicon based solar cells with respect to the intrinsic layer thickness and to the mobility gap of a thin interfacial layer grown at the p/i interface is explored with numerical techniques. Our results indicate that the reported experimental trends can be adequately explained with the defect pool model and not by assuming an uniform density of states in the intrinsic layer.
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1. Introduction

Computer modeling has become a helpful tool in seeking for more efficient devices and in achieving a deeper knowledge on the transport physics that controls the shape of the output characteristics. It is well known that the electrical transport and the performance of a-Si:H based solar cells is strongly influenced by the presence of gap states. Trapping of free carriers at tail and mid-gap states could deteriorate the electric field in regions where light is absorbed and recombination of electron-hole pairs could reduce the final number of collected carriers. Both effects might have a serious impact on the final solar cell efficiency. Hence the accurate knowledge of the density of gap states in the intrinsic layer of p-i-n structures becomes a key issue in modeling of a-Si:H based solar cells. There is clear consensus about the presence of two tails, one with acceptor-like states and the other with donor-like states. There is also agreement in describing dangling bonds (DB) with deep or mid-gap amphoteric-like states but remains some controversy in modeling the density of DB inside the intrinsic layer of a-Si:H cells as uniform [1–3] or as non-uniform [4,5] using the algorithms derived in the defect pool model [6–8]. These two different representations of the density of DB in a-Si:H will be recognized in our manuscript with the symbols UDM (Uniform Density Model) and DPM (defect pool model).

In previous publications we showed that although the characteristics curves of a-Si:H based p-i-n solar cells could be modeled and matched by using either the UDM or the DPM the improvement of the solar cell efficiency when the mobility gap is graded inside the intrinsic layer can be reproduced only with the DPM [9–10]. The difficulties found in matching the Fill Factor (FF) of solar cell light current-voltage (J–V) curves with the DPM, specially in thick samples, were discussed and overcome in preceding papers [10,11]. The adoption of Freezing Temperatures (T_{FR}) below the one proposed by Powell and Deane (T_{FR}=500 K) [7] was crucial to match FF [10,11]. Although in many contributions T_{FR} was assumed 500 K [6,7,12] some authors have adopted in their contributions lower values of T_{FR} like 490 K [13], 473 K [14] and 463 K [8]. Among the characteristic curves that we were able to match with either the UDM and the DPM was the dark J–V characteristic. The dark current at low forward voltages is

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controlled by recombination through mid-gap states [15,16]. Hence the final shape of the dark J–V curve at low forward voltages is dependent of the distribution of DB adopted in the intrinsic layer. The DPM predicts a highly non-uniform density of DB inside the intrinsic layer of p-i-n devices with more defects near the interfaces [6–8].

Using numerical techniques we discuss in this paper the experimental dark J–V characteristics of a-Si:H based p-i-n devices published by Deng at al [17]. Deng at al have compared the dark J–V curves of p-i-n structures with different intrinsic layer thicknesses grown under similar conditions. In their devices an extra 20 nm thick interfacial layer with a variable mobility gap was included between the p-doped and the intrinsic layer. This extra layer allows for some control on the relative contributions coming from bulk recombination and from interface recombination to the total dark current. We evaluate the dark J–V curves of the different structures studied by Deng et al. assuming that the DB density is either uniform or spatially varying accordingly with the DPM. We also briefly describe the transport mechanisms controlling the dark J–V curves of a-Si:H p-i-n heterostructures. We show that the DPM model is able to capture the trends experimentally observed by Deng et al. while the UDM gives rise to predictions that are in contradiction with the experimental findings.

2. Methodology

The p-i-n devices characterized by Deng. et al. contain a 25 nm thick front p-doped layer of a-SiC:H, a 35 nm thick back n-doped layer of n-μc-Si:H, an intrinsic a-Si:H layer of variable thickness, and a 20 nm thick a-Si:H interfacial layer (IL) between the p-layer and the i-layer of variable mobility gap. The devices resulting from varying the width of the intrinsic layer will be recognized with the letters VILTD (Variable Intrinsic Layer Thickness Devices) and the devices resulting from varying the mobility gap of the interfacial layer will be recognized with the letters VILMGD (Variable Interfacial Layer Mobility Gap Devices). The mobility gaps of the intrinsic and interfacial layers, grown with the Plasma Enhanced Chemical Vapor Deposition (PECVD) technique, were conveniently adjusted by using molecular hydrogen (H_2) dilution ratios $R=[H_2]/[SiH_4]$ of $R=0$, $R=10$, and $R=40$ that, according to their work, correspond to mobility gaps of 1.8 eV, 1.86 eV, and 1.95 eV respectively [17].

The dark J–V characteristics were evaluated with the computer code D-AMPS that was described elsewhere [18]. Our electrical and optical input parameters were calibrated by fitting dark and light J–V curves and the spectral response characteristics of a-Si:H based p-i-n solar cells prepared also with the PECVD technique but at the Debye Institute from Utrecht University, the Netherlands. The key electrical parameters describing the density of DB of our intrinsic a-Si:H are listed in Table 1 [10,11]. These parameters resulted from fitting characteristic curves of p-i-n devices in the initial state. We have to keep in mind that the electrical parameters that are common to both models (UDM and DPM) do not have to be identical [10,11].

The peaks of the three amphoteric-like Gaussians describing the DB in the UDM approach were assumed 0.3 eV spaced in energy. They were displaced by $\Delta E_G/2$ with respect to the valence band edge when the mobility gap was increased by ΔE_G. For the sake of simplicity the global density of DB was adopted independent of the dilution ratio R. This point will be discussed below. In the DPM the most likely energy formation of DB, i.e. the parameter E_P of Table 1 was also displaced by $\Delta E_G/2$ when the mobility gap was increased by ΔE_G. The density of DB was evaluated with the improved algorithm proposed by Powell and Deane adopting a Freezing Temperature of $T_{FR}\sim 460$ K [11] to

Table 1
Some of the key electrical parameters resulting from fitting J–V and QE curves of a-Si:H based p-i-n PECVD cells

	E_D (meV) E_A (meV)	t_N^+, t_P^- (cm^2) t_N^o, t_P^o (cm^2)	D^- (cm^{-3}) D^o (cm^{-3}) D^+ (cm^{-3})	E_D^- (eV) E_D^o (eV) E_D^+ (eV)	σ_N^+ (cm^2) σ_P^- (cm^2)	σ_N^0 (cm^2) σ_P^0 (cm^2)
UDM	50	9×10^{-15} both	2×10^{15}	0.55	4×10^{-15}	4×10^{-16}
	30	2×10^{-16} both	1×10^{15}	0.85	Both	Both
			2×10^{15}	1.15		
UDM*	49	9×10^{-15} both	2×10^{15}	0.55	3×10^{-15}	3×10^{-16}
	25	2×10^{-16} both	1×10^{15}	0.85	Both	Both
			2×10^{15}	1.15		

	E_D (meV) E_A (meV)	t_N^+, t_P^- (cm^2) t_N^o, t_P^o (cm2)	Δ (eV)	T_{FR} (K)	E_P (eV)	σ_N^+ (cm^2) σ_P^- (cm^2)	σ_N^0 (cm^2) σ_P^0 (cm^2)
DPM	45	9×10^{-15} both	0.35	460	1.26	4×10^{-15}	4×10^{-16}
	30	2×10^{-16} both					
DPM*	45	9×10^{-15} both	0.45	460	1.26	10^{-15}	10^{-16}
	30	2×10^{-16} both					

Parameters that are common to the UDM and to the DPM models: E_D and E_A, the valence and conduction tail slopes, t_N^+, t_P^- are the cross sections of electrons and holes for charged tail states; t_N^0 and t_P^0, the cross sections corresponding to neutral tail states; σ_N^+ and σ_P^-, the cross sections of electrons and holes corresponding to mid-gap states; σ_N^0 and σ_P^0, the cross sections corresponding to neutral mid-gap states. Parameters that are specific to the UDM model: D^-, D^o, and D^+, the density of DB enclosed by each of the Gaussian distribution of states; E_D^-, E_D^o, and E_D^+, the corresponding peak energies. Parameters that are specific to the DPM model: Δ, the energy separation between the doubly occupied D^- state and the empty state D^+; T_{FR}, the Freezing Temperature; E_P, the most likely energy formation energy for DB.

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properly match the FF of the light J–V curves. The correlation energy U was assumed 0.2 eV and the energy offsets at the p/i and i/n interfaces were divided in equal proportions between the conduction and the valence bands in both the UDM and the DPM approaches [11].

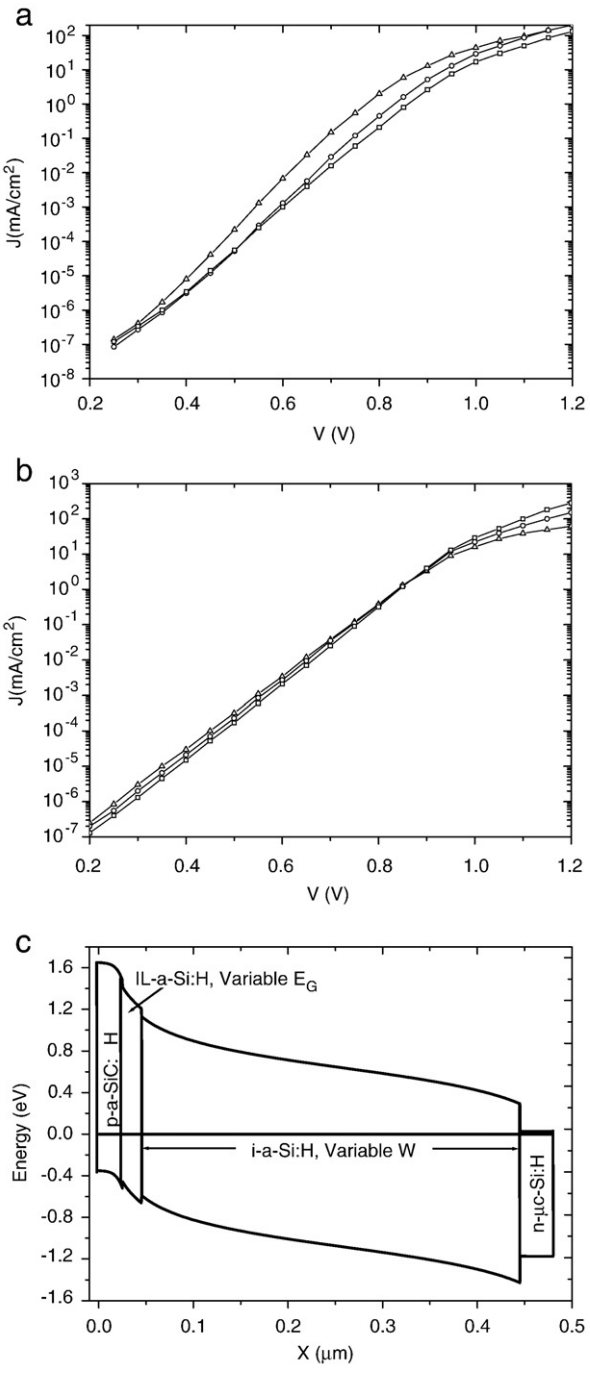

Fig. 1. The experimental dark J–V characteristics measured by Deng. et al. in a-Si:H based p-i-n devices: (a) for different mobility gaps in the 20 nm thick interfacial layer (IL) at the p/i interface: 1.72 eV (triangle), 1.77 eV (circle), and 1.87 eV (square) and (b) for different intrinsic layer thicknesses: 400 nm (triangle), 800 nm (circle), and 1500 nm (square); (c) Band diagram in equilibrium of the p-i-n devices under study. The doped layers are: a 25 nm thick p-a-SiC:H layer and a 35 nm thick n-μc-Si:H layer. Experimental data were digitized in voltage steps of 0.5 V.

As the computer code D-AMPS was calibrated fitting undiluted ($R=0$) samples that were prepared at Utrecht University some of our parameters resulted different from the ones found by the team conducted by Prof. Wronski from Penn State University, USA [17]. In particular the mobility gap that corresponds to $R=0$ was of 1.72 eV, instead of 1.8 eV. The use of mobility gaps higher than 1.72 eV resulted in a clear overestimation of the open circuit voltage of our a-Si:H p-i-n solar cells [11]. Hence in our simulations the mobility gaps reported by Deng et al. [17] for different dilutions ratios R; i.e. 1.8 eV, 1.86 eV, and 1.95 eV were proportionally scaled down to 1.72 eV, 1.77 eV and 1.87 eV respectively. Nevertheless we will show in this paper the dark J–V curves predicted for the mobility gaps reported by Deng et al. [17].

The results obtained by Deng. et al are shown in Fig. 1a and b[1]. The band diagram of one of the devices under study (with our mobility gaps) is shown at equilibrium conditions in Fig. 1c. In VILTD samples Deng et al. studied the dependence of the dark J–V curves with the intrinsic layer thickness. The 20 nm thick interfacial layer has a dilution ratio of $R=40$ (our $E_G=1.87$ eV) and the intrinsic layer of undiluted a-Si:H has a variable thickness of 400 nm, 800 nm, and 1500 nm. The higher mobility gap of the IL prevents that the recombination taking place at the p/i interface and inside the interfacial layer could make a significant contribution to the dark current. Hence the inclusion of the high gap IL at the p/i interface guarantees that the dependence of the J–V characteristics with respect to the intrinsic layer thickness will not be masked by the contribution coming from interface states. In the VILTD samples. At low forward voltages the current J is controlled by recombination of electron-hole pairs through deep states In this regime quasi-Fermi levels, split by the applied voltage, do not considerably enter into tails.

In the VILMGD samples the intrinsic layer thickness is of 400 nm and the dilution ratio is fixed to $R=10$, i.e. E_G is set to $E_G=1.77$ eV (our value). The mobility gap of the IL is varied from 1.72 eV ($R=0$) up to 1.87 eV ($R=40$). By doing this the dark current is probed with respect to the contribution coming from the interfacial layer. In particular the combination E_G(IL)= 1.72 eV and E_G(i-layer)=1.77 eV maximizes the contribution coming from the interfacial layer.

3. Results

The dark J–V curves predicted by D-AMPS for the VILTD samples using the parameters of Table 1 are shown in Fig. 2 (solid lines and full symbols). The comparison of Fig. 2a and b indicates that when the density of DB in the intrinsic layer is assumed uniform (UDM) the dark J–V curve at low forward voltages results much more sensitive to the intrinsic layer thickness than when the DPM is adopted. However when the DPM is implemented there is still some dependence of the dark J–V curve with respect to the intrinsic layer thickness. The

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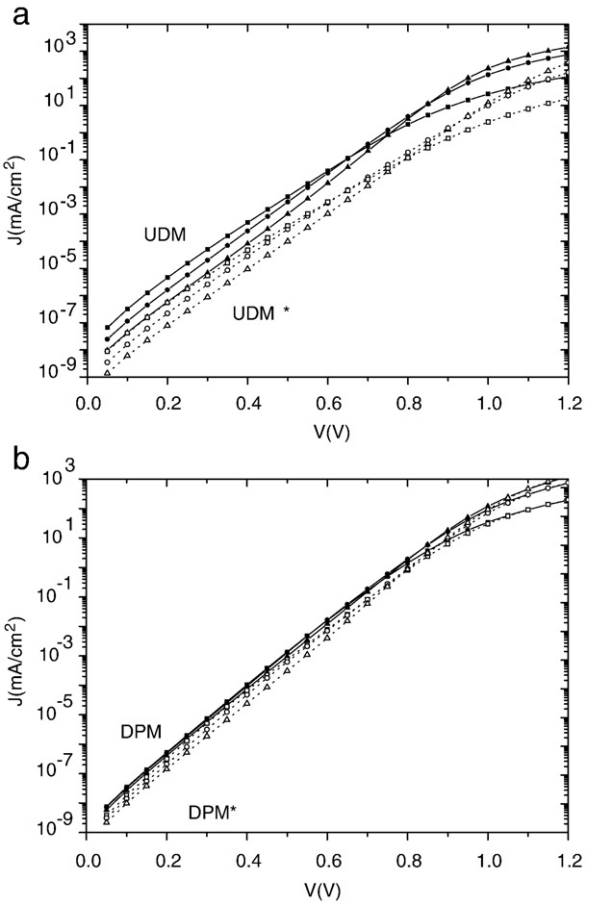

Fig. 2. Dark J–V curves predicted with (a) UDM and with (b) DPM for a-Si:H p-i-n devices with different intrinsic layer thicknesses: 400 nm (triangle), 800 nm (circle), and 1500 nm (square) (solid lines, full symbols). The gap of the 20 nm interfacial layer is of 1.87 eV and the gap of the intrinsic layer is of 1.72 eV. The dot lines with empty symbols correspond to the dark J–V curves predicted with (a) UDM when some of the electrical parameters proposed by the team of Wronski from PSU are used (UDM*) and with (b) DPM when slightly different electrical parameters that result in a closer resemblance to the experimental curves are used (DPM*).

DPM does not predict that the dark J–V characteristic is insensitive to the intrinsic layer thickness as suggested by Deng et al. [17]. Both models predict a consistent and systematic increase of the dark J–V curve for thicker p-i-n samples as it is experimentally observed. This result can be attributed to the weaker field and to the higher number of DB present in thicker intrinsic layers.

The spread of the dark J–V curves with respect to the intrinsic layer thickness reported by Deng et al. (see Fig. 1b) is higher than the one predicted by our code when the DPM is implemented but lower than the one obtained with the UDM. In the last case the global DB density in the intrinsic layer was assumed of 5×10^{15} cm^3. In order to obtain a lower spread of the J–V curves with the UDM a lower global DB density should be invoked. We run few simulations with the electrical parameters that we could found in some of the previous papers published by the team conducted by Prof. Wronski from Penn State University. They have characterized the density of states of undiluted a-Si:H with Photoconductivity and with the Dual Beam Photoconductivity technique. They have reported density of DB around 4×10^{15} cm^{-3} – 6×10^{15} cm^{-3}, charged and neutral mid-gap cross sections in the range of 1×10^{-15} – 3×10^{-15} and 1×10^{-16} – 3×10^{-16}cm^2 respectively and an Urbach Tail of 49 meV [19,20]. Their values are not too dissimilar to ours except for their mobility gaps [17]. The dark J–V characteristics resulting from using their parameters are shown in Fig. 2a (dot lines and open symbols). The parameters corresponding to these simulations are also listed in Table 1 and they are identified with the symbol UDM*. A similar spread in the J–V curves with respect to the intrinsic layer thickness is obtained. Further simulations, that were not included in this paper, excluded the possible uncertainties present in the activation energies of the doped layers and in the energy offset alignments at the p/i and i/n interfaces as possible causes for the overestimated spread. The use of different number of Gaussians and peak positions and the donor-like and acceptor-like characters of their mid-gap states instead of the amphoteric-like character of ours mid-gap states could not either account for this wide spread.

The recombination rate profiles obtained, when the parameters of Table 1 are adopted, are shown for a forward voltage of 0.2 V in Fig. 3a. For low forward voltages the dark current is given by the integral of the recombination rate along the device that obviously must a function of the intrinsic layer thickness when the UDM is adopted. The same integral shows a weaker dependence with respect to the intrinsic layer thickness when the DPM is adopted. The DPM predicts that the peak of the recombination is located near the p/i interface, where the DB density results maximum, instead of at the intrinsic layer bulk as expected with the UDM. In the DPM the contribution coming from the recombination rate near the p/i interface is similar for different intrinsic layer thicknesses but the contribution coming from the bulk of the intrinsic layer is still dependent of the intrinsic layer thickness. The small spread observed in the J–V curves of Fig. 2b predicted by D-AMPS with the parameters found in our previous papers can be slightly magnified by adopting: (a) a higher energy separation Δ between the doubly occupied D^- state and the empty state D^+ ($\Delta=0.45$ eV instead of $\Delta=0.35$ eV) and (b) by assuming that the offsets at the front p/IL and IL/i interfaces are entirely located at the conduction band. By doing this the Fermi level results displaced farther from the valence band edge and the DPM generates a lower density of DB near the IL/i interface. Finally by decreasing the mid-gap state cross sections the dark current levels and the cross over of the J–V curves of different intrinsic layer thicknesses become more similar to the ones published by Deng et al. [17]. A lower freezing temperature would also be helpful but lower values were not reported yet ($T_{FR}=460$ K). The electrical parameters needed to achieve a better agreement with the experimental trends are also listed in Table 1 with the symbol DPM*. The resulting dark J–V curves are included in Fig. 2b (dot lines and open symbols). Interestingly when the input parameters are modified the separation between the dark J–V curves obtained for a 800 nm thick intrinsic layer and for a 1500 nm thick intrinsic layer become more noticeable. The general idea behind these changes is that lowering the density of

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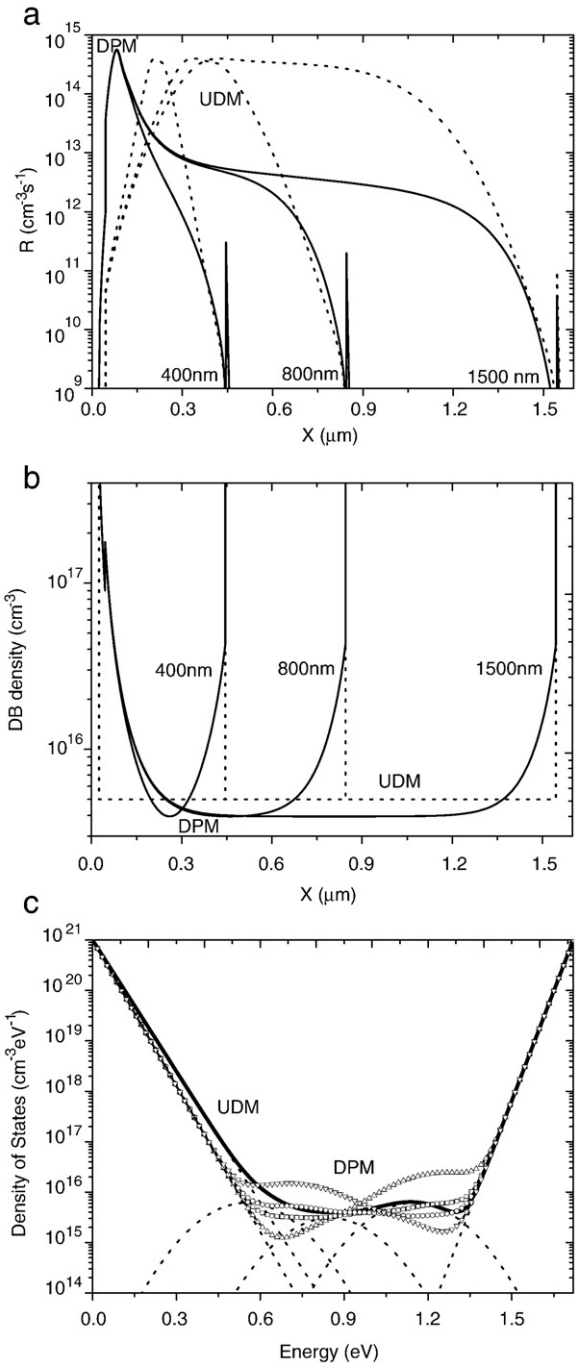

Fig. 3. (a) Recombination rate profiles obtained at V=0.2 V and (b) density of dangling bonds present in a-Si:H based p-i-n devices for different intrinsic layer thicknesses (400 nm, 800 nm, and 1500 nm) when the UDM (dot) and the DPM (solid) are adopted. The gap of the 20 nm interfacial layer is of 1.87 eV and the gap of the intrinsic layer is of 1.72 eV. In (c) the density of states obtained with DPM is plotted with respect to the gap state energy for a 800 nm thick intrinsic layer sample at: 100 nm (up triangle), 300 nm (square), 500 nm (circle), and 700 nm (down triangle) from the p/i interface. The solid line corresponds to the density of DB obtained with UDM. Tails and Gaussians (in UDM) are added as guide for the eye (dot lines).

DB near the p/i interface the dark J–V curves becomes more sensitive to the defects located in the bulk of the intrinsic layer. It is important to mention that other research groups have published experimental dark J–V curves of a-Si:H based p-i-n devices where a lower dependence with respect to the intrinsic layer thickness than the one reported by Deng et are observed [21,22]. These experimental results could only be explained with the DPM by appropriately tailoring the number of DB near the p/i interface.

The dependence of the dark J–V curve with respect to the intrinsic layer thickness predicted with the DPM becomes less and less important for thicker intrinsic layers (see Fig. 3a). Hence a more conclusive test to decide the validity of the DPM vs. the UDM would be the measurement of dark J–V curves of p-i-n devices with quite thick intrinsic layers where the current J might finally lose its dependence with respect to the intrinsic layer thickness in the DPM.

The dark J–V curves at high forward voltages are controlled by the electron space charge limited current [23] regime (partly shown in Figs. 1 and 2). The current in this regime results thickness dependent not only when the UDM is adopted but also when the DB density is evaluated with the DPM. Fig. 3b shows that the DB density predicted by the DPM is higher near the p/i interface than near the i/n interface (except when the offset at the conduction band of the i/n interface is assumed very low). This asymmetry in the DB density at both interfaces is caused by the parameter E_P (see Table 1) that must be adopted above mid-gap [11]. The barrier height and shape of the virtual cathode is controlled by electron trapping and in less extend by hole trapping. The physics behind the formation of the virtual cathode is similar in both the UDM and the DPM. The profiles of free carrier concentration, trap carrier concentration, recombination rate and electron and hole currents show similar shapes in both models. Interestingly the current level predicted by the DPM in thicker samples results slightly higher because the height of the virtual cathode barrier and of the virtual anode barrier result a bit lower. The field redistribution introduced by the DPM at high forward voltages gives rise to an stronger field in the intrinsic layer bulk (the DB density in the bulk results lower in the DPM than in the UDM) that might push more efficiently the free carriers towards the virtual cathode and the virtual anode lowering their barrier heights.

For illustration purposes the dependence of the density of states with respect to the gap energy is shown in Fig. 3c for a 800 nm thick sample at distances of 100 nm and 300 nm from the p/i and from the i/n interface respectively. The dependence of the density of DB predicted in the literature for p-type and n-type samples by the DPM can be observed in this figure near the p/i interface and near the i/n interface respectively [6].

The results obtained with the UDM and with the DPM for the VILMG devices are shown in Fig. 4. Our simulations for the alternative parameters listed in Table 1 (UDM* and DPM*) are also included. The dark J–V characteristics predicted by D-AMPS with the UDM for structures with interfacial layers of different dilution ratios resulted practically on the top of each other while visible departures can be observed when the DPM is invoked. The trends predicted for the dark J–V curves result quite similar to the trends measured by Deng et al. when the DPM is adopted (compare Figs. 1a and 4b). The results showed in Fig. 4 can be easily explained by inspecting the recombination rate profiles obtained at low forward voltages (see Fig. 5).

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The variable mobility gap of the interfacial layer give rise to quite different recombination rates specially inside of this region. In the UDM the recombination rate is dominated by the contribution coming from bulk states and in the DPM model the recombination is dominated by the contribution coming from states located near the p/i interface. In the UDM model the differences present in the recombination rates inside the interfacial layer can be clearly noticed in Fig. 5 but, due to their low values compared with the higher rates present in the bulk, they practically do not contribute to total current J given by the integral of the recombination rate on the total device length. The density of states enclosed by the Gaussians of diluted a-Si:H layers are similar or lower than the density of states corresponding to the Gaussians of non diluted a-Si:H layers [24]. The assumption of a lower density of DB in the diluted IL layer would make the contribution of the IL layers even lower. The scenario changes significantly with the DPM where the recombination rates inside the interfacial layer are much higher than with the UDM due to the presence of more

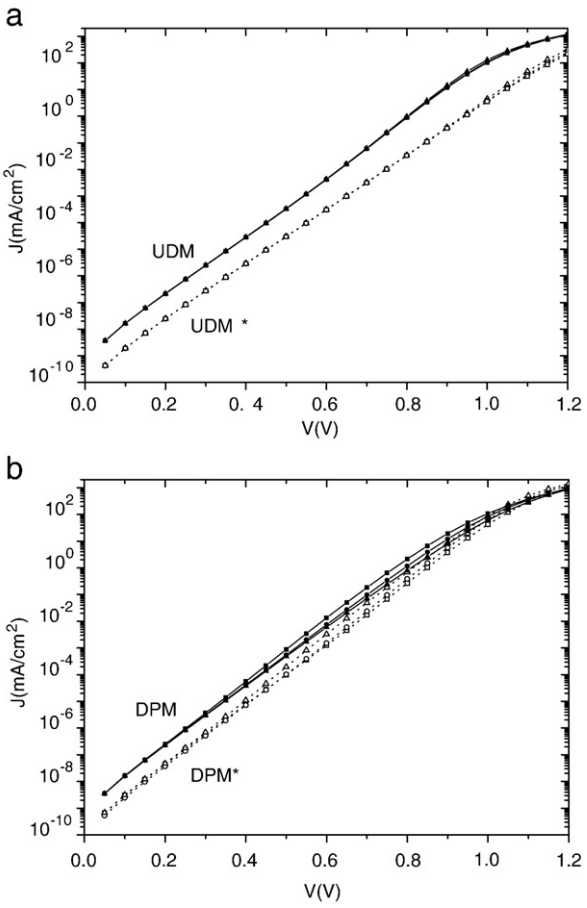

Fig. 4. (a) Dark J–V curves predicted with (a) UDM and with (b) DPM for a-Si:H based p-i-n devices when different mobility gaps are used in the 20 nm thick interfacial layer: 1.72 eV (triangle), 1.77 eV (circle), and 1.87 eV (square) (solid lines, full symbols). The intrinsic layer is 400 nm thick. The dot lines with empty symbols correspond to dark J–V curves predicted with (a) UDM when some of the electrical parameters proposed by the team of Wronski from PSU are used (UDM*) and with (b) DPM when slightly different electrical parameters that result in a closer resemblance to the experimental curves are used (DPM*).

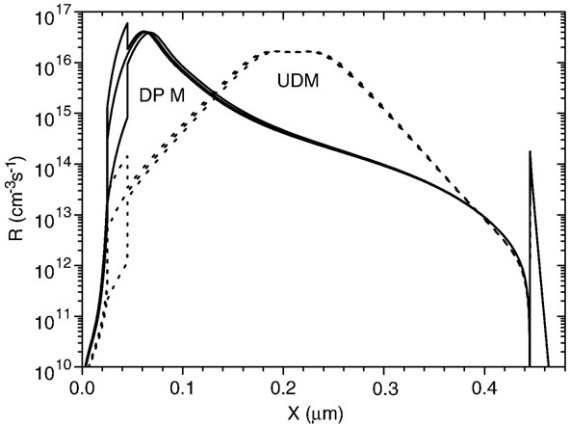

Fig. 5. Recombination rate profiles obtained with UDM (dot) and with DPM (solid) at a forward voltage of V=0.4 V in a-Si:H based p-i-n devices when different mobility gaps are used in the 20 nm thick interfacial layer (1.72 eV, 1.77 eV, and 1.87 eV). The intrinsic layer is 400 nm thick.

DB near the interfaces. In few words the dark J–V curves predicted with the UDM are practically insensitive to changes of the mobility gap of the interfacial layer in contradiction with the experimental findings of Deng et al. On the other hand the predictions coming from the DPM can reproduce the measured trends. In other words their experimental results are not in conflict with the predictions of our computer simulations performed with the DPM. These results are an example of how computer modeling could grab the experimental trends when the electrical properties are described with the appropriate physics.

Finally, different dark J–V curves could be obtained in p-i-n and in n-i-p devices with the DPM by assuming a non-uniform freezing temperature T_{FR} during the deposition of the intrinsic layer. This hypothesis, in our opinion, would unnecessarily complicate the computer of modeling of a-Si:H based solar cells. Of course our simulations predict identical dark J–V curves in p-i-n and in n-i-p when T_{FR} is adopted uniform on the whole device.

4. Conclusions

The experimental evidences presented by Deng et al. to prove the absence of non uniform distributions of defects inside the intrinsic layer of a-Si:H based p-i-n devices are actually evidences favoring the validity of the defect pool model. The most conclusive argument is the lack of sensitivity of the dark current voltage characteristics with respect to the mobility gap of an interfacial layer placed at the p/i interface that is predicted by our computer simulations when the density of deep defects is assumed to be uniform inside the intrinsic layer. On the contrary the defect pool model is able to predict the trends experimentally observed in the dark current voltage curves. The dependence with respect to the intrinsic layer thickness obtained in these curves when the density of mid-gap states is assumed constant results stronger than the one measured. The electrical parameters needed to reproduce the measured spread of the dark current curves for different intrinsic layer thicknesses must be

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appropriately selected when the defect pool model is used. A more conclusive experimental test for the defect pool model would be the measurement of the dependence of the dark current voltage characteristic of p-i-n a-Si:H devices with respect to very thick intrinsic layers.

Acknowledgments

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