

Characteristic curves of hydrogenated amorphous silicon based solar cells modeled with the defect pool model

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Abstract

Using the improved expression of the defect pool model proposed by Powell and Deane we match the experimental current–voltage and the spectral response characteristic curves of hydrogenated amorphous silicon solar cells. We compare the electrical parameters resulting from using the different defect pool models published in the literature and from assuming a uniform density of dangling bond in every device layer. We discuss the applicability of the algorithm derived by Schumm for the stabilized state exploring its sensitivity to the sample history. Finally we propose an expression for stabilized cells adapting Schumm's ideas to the expression derived by Powell and Deane.

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1. Introduction

Hydrogenated amorphous silicon (a-Si:H will be abbreviated as a-Si) thin films are currently used in solar cells and numerous electronic devices. The low processing temperatures and the large area manufacturability facilitate the cost-effective production of solar cells. Intrinsic plasma deposited a-Si prepared by Plasma Enhanced Chemical Vapor Deposition (PECVD) can be considered as device quality material when properties like the dark conductivity, the photoconductivity, the optical gap, the mid-gap electronic density of states (DB), the absorption coefficient, etc., meet pre-established criteria [1]. The a-Si density of states (DOS) consists of parabolic conduction (CB) and valence bands (VB) (extended states) that exponentially decay inside the gap into the conduction band tail (CBT) and valence band tail (VBT) respectively and of mid-gap states (DB) that are usually described by three Gaussian distributions containing

amphoteric states recognized as D^+ , D^0 and D^- . It was a common practice in the past two decades to assume the presence of a uniform density of DB (UDM) on the whole a-Si intrinsic layer of a-Si based solar cells [2–4] and to adopt a higher density of DB in the stabilized state than in the initial state [4,5]. The Gaussian distribution of DB does not contain information about the origin of these states. Nonuniform densities of DB in the intrinsic layer of a-Si solar cells were also proposed by few authors with some success [6,7]. The defect pool model (DPM), taking shape in the beginning of the nineties [8–11], suggested that DB result from the conversion of Si–Si weak-bonds (WB) ($WB \leftrightarrow DB$) through chemical-type reactions involving DB, Si–Si WB, and Si–H bonds. The equilibrium state distribution of DB resulting from minimizing the entropy of this system appropriately described the defect structure in doped and undoped a-Si in thermal equilibrium as well as the metastable defect formation under non-equilibrium [7,9]. The Si–Si WB distribution is associated with the VB tail [12]:

$$G_D(E) = G_{DO} \exp(-E/E_{DO}) \quad (1)$$

where E_{DO} is the VBT slope, E is the gap state energy referred to the valence band edge and G_{DO} is the density of states value at the valence band edge. The distribution of available defect

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sites $P(E)$ where DB are created, or defect pool, is described by the Gaussian distribution:

$$P(E) = \frac{1}{\sqrt{2\pi}\sigma_{DP}} \exp \left[-\frac{(E-E_{DP})^2}{2\sigma_{DP}^2} \right] \quad (2)$$

where σ_{DP} is the standard deviation of the pool and E_{DP} is the peak or pool center (or the most probable DB energy). Powell and Deane derived this expression for the DB density [9]:

$$N_{DB}(E) = \gamma \left[\frac{2}{F_{EQ}^0(E)} \right]^{\frac{\rho k T_{FR}}{E_{DO}}} P \left[E + \frac{\rho \sigma_{DP}^2}{E_{DO}} \right] \quad (3)$$

where F_{EQ}^0 is the equilibrium occupation of neutral DB states and E_{DO} is the VBT slope. The scaling factor γ is given by a complex expression and ρ can be expressed as [9]:

$$\rho = 2E_{DO}/(2E_{DO} + ikT_{FR}) \quad (4)$$

where i indicates the number of Si–H bonds mediating in the WB $\leftrightarrow$ DB reaction. This number could be 0, 1, or 2. The pool width σ_{DP} is not a free input parameter and it can be extracted from the following expression [9]:

$$\Delta = \frac{2 \cdot \rho \cdot \sigma_{DP}^2}{E_D(T_{FR})} - U = E_{D^+} - E_{D^*} \quad (5)$$

where Δ is the separation between the non-occupied D^+ peak (E_{D^+}) and the double occupied D^* peak (E_{D^*} , where $E_{D^*} = E_{D^-} - U$). The neutrality condition in (i)-a-Si leads us to the relationship $E_{DP} = E_F + \Delta / 2$, where E_F is the Fermi level. Hence we have that $E_{DP} \sim E_{D^+}$. The factor γ and the expressions (3)–(5) are not identical in the other versions of the defect pool model published in the literature [9–11]. The dependence of F_{EQ}^0 with respect to the Fermi level in Eq. (3) gives rise to highly non-uniform density of DB along the intrinsic layer of a $p-i-n$ a-Si structure with a higher DB density near the interfaces than in the bulk. The DB distribution profile is evaluated in the solar cell at the freeze-in temperature T_{FR} (which is higher than the device operational temperature T). The temperature dependence of the VBT slope is accounted by [13]:

$$E_{VO}^2(T) = E_{VO}^2(T=0) + kT^2. \quad (6)$$

Powell–Deane published two different algorithms of the DPM [9,10] that we will recognize as DPM1 (Eqs. (1)–(5)) and DPM2 and Schumm proposed one expression for the initial state and other for the stabilized state that we will recognize as DPM3 and DPM4 respectively [11].

In previous publications we showed that although the experimental current–voltage ($J-V$) and spectral response (SR) characteristic curves of a-Si and a-SiGe $p-i-n$ based solar cells could be matched by adopting either the UDM or the DPM approach only the implementation of the DPM allowed us to achieve higher efficiencies in a-Si and a-SiGe $p-i-n$ solar cells when gap grading in the intrinsic layer was performed [14,15]. Particularly in a-SiGe $p-i-n$ cells the use of the UDM did not allow us to justify the gap grading regularly performed in the

intrinsic layer [16]. Using the DPM we found that the optimum band gap profile should have an exponential shape decreasing from the interfaces towards the intrinsic layer bulk [17]. A careful experimental analysis provided by the Rutherford Backscattering Technique confirmed our predictions [18]. In a-Si $p-i-n$ solar cells we could fit the dark $J-V$ curve in a $p-i-n$ cell with a 500 nm thick i -layer and the light $J-V$ in cells with 215, 500, and 1000 nm thick i -layers [15] using the UDM and different versions of the DPM. However we could not fit the same characteristic curves when two Si–H were participating in the WB $\leftrightarrow$ DB reaction ($i=2$), the option most widely accepted by the scientific community because this reaction has the highest probability and the uppermost entropy [9–11,19–21]. We predicted that the efficiency of the a-Si $p-i-n$ solar cell could also be improved by grading the gap and the boron concentration in the intrinsic layer following a similar approach as the described in a-SiGe solar cells [15].

In this paper we describe in detail the procedure followed to match the experimental a-Si solar cell characteristic curves and we compare the resulting electrical parameter values obtained with the UDM and with the different versions of the DPM. We discuss the difficulties associated to the use of the defect pool model in a-Si solar cell modeling. Finally we propose the improved algorithm of Powell and Deane (DPM2) as the best choice to model a-Si solar cells and we discuss how to overcome the bottle-necks that appear in the initial state and in the stabilized state.

2. Experimental details

Samples were grown by PECVD and characterized at Utrecht University, the Netherlands. The solar cells were deposited in the super-strate configuration: $\text{SnO}_2/p\text{-a-SiC:H}/i\text{-a-Si:H}/n\text{-a-Si:H}/\text{Ag}$. The intrinsic layer thickness was 215, 500, or 1000 nm thick. Three thin layers (0.5 nm) with decreasing content of carbon were included between the p - and the intrinsic layer. The total density of DB ($5 \times 10^{15} \text{ cm}^{-3}$) and the Urbach tail (48 meV) were extracted with the Constant Photocurrent Measurement technique. The activation energies of doped layers were obtained from temperature dependence of the dark conductivity as 0.47 eV and 0.24 eV in the p -, and n -layer respectively. To reach the stabilized state samples were light-soaked with a white light of 100 mW cm^{-2} intensity at controlled temperature ($T \sim 45^\circ \text{C}$) during 3000 h and under open circuit conditions.

3. Modeling

Our simulations were performed with the computer code D-AMPS [22] where trapping and recombination terms were conveniently modified to include the DPM. The hydrogen concentration $[H]$ was fixed to $3.5 \times 10^{21} \text{ cm}^{-3}$. The freezing temperature was initially set to 500 K following the work published by Powell and Deane [9,11]. The correlation energy U was assumed equal to 0.2 eV [9–11]. The most probable energy E_{DP} was adopted equal to the peak of the D^+ Gaussian resulting from fitting solar cell characteristics with the UDM and subsequently changed but keeping the activation energy

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