Impact of defect-pool model parameters on the lifetime in c-Si/a-Si:H heterojunction solar cells

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Impact of defect-pool model parameters on the lifetime in c-Si/a-Si:H heterojunction solar cells

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Abstract

We present here a study of the recombination at the hetero-interface of solar cells based on amorphous silicon / crystalline silicon (a-Si:H/c-Si). The volume defects in the amorphous silicon are modeled with the defect-pool model and we study whether the surface defects in c-Si at the a-Si:H/c-Si interface can be considered as a projection of the defects in a-Si:H close to the surface. We study the impact of the defect-pool model parameters on the surface defect density and on the effective lifetime. We show that the calculation of interface defects from the defect-pool model is compatible with experimental results only if the width of the valence band tail is decreased when the thickness of the buffer layer is increased.

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Keywords: Amorphous silicon, Heterojunction, Defect Density, Recombination, Lifetime, Surface Passivation, Buffer Layer, Modelling, Solar cells

1. Introduction

Thin film heterojunction solar cells combining hydrogenated amorphous silicon (a-Si:H) and crystalline silicon (c-Si) have attracted broad research interest and market share due to their high stability, high efficiency and low temperature fabrication process which leads to a fabrication cost reduction in comparison with the high temperature

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diffused homojunction technology. The efficiency record of a-Si:H/c-Si heterojunction solar cells has been broken by Panasonic in April 2014 reaching 25.6% [1]. One of the key steps in this device optimization is the insertion of an intrinsic (i)a-Si:H buffer layer which results in a decrease of surface defects at the c-Si/a-Si:H interface. These surface defects attributed to silicon dangling bonds are still a limiting parameter to reach higher efficiency. The bulk defect distribution in a-Si:H is governed by the defect-pool model [2,3] which describes the density of dangling bonds (DB) in a-Si:H according to the position of the Fermi level, thus leading to a non uniform spatial DB distribution due to the band bending. The band bending in a-Si:H close to the a-Si:H/c-Si interface leads to modifications of the DB density according to the position in the a-Si:H layer.

We have developed a calculation program to self consistently solve Poisson's equation and determine the DB density profile in a-Si:H using the defect-pool model [4]. The surface defect density $D_{it}(E)$ is then inferred from the obtained DB density at the interface. This model allows us to study the impact of the parameters of the defect-pool model and the thickness of the (i)a-Si:H buffer layer on the $D_{it}(E)$, and consequently on the effective lifetime minority carriers.

2. Simulation method

In order to study whether the surface defects at the a-Si:H/c-Si interface that determine carrier recombination in c-Si can be considered as a projection of the defects in a-Si:H, we followed the following steps : (1) we used our calculation program to self consistently solve Poisson's equation and determine the DB density profile, (2) we modeled the DB density by monovalent state distributions, (3) we calculated the surface defect density at the a-Si:H/c-Si interface as a projection of the defects in a-Si:H close to the surface, (4) we studied the influence of the calculated a-Si:H/c-Si defect density and of the (i)a-Si:H buffer layer thickness on the effective carrier lifetime in symmetrical structures through a 1D numerical simulation (Silvaco Atlas).

2.1. Structure

We modeled a symmetrical (p)a-Si:H/(i)a-Si:H/(n)c-Si/(i)a-Si:H/(p)a-Si:H structure. The (n)c-Si absorber was standard 280 µm thick with a donor density of 1.7×10^{15} cm^{-3}. The (p)a-Si:H emitter thickness was set to 10 nm. The (i)a-Si:H thickness $d(i)$ was varied between 0 nm (no (i) a-Si:H) and 10 nm. The band gap was set to 1.7 eV in all the a-Si:H layers and to 1.12 eV in c-Si. The total density of states (DOS) in the a-Si:H was considered as the sum of the amphoteric DB states calculated using the defect-pool model, and the monovalent band tail distributions.

In the studied structure, the Fermi level in a-Si:H is always much closer to the valence band edge than to the conduction band edge, even close to the hetero-interface. The defect-pool provides, in this case, an important DB distribution in the upper part of the gap that can be reproduced by a Gaussian distribution $D(E)$. Moreover, this DB distribution can be approximated in terms of one-electron density of states by two monovalent states distributions, one being of acceptor type, $g_A(E)$, the other being of donor type, $g_D(E)$, so that the total monovalent DOS $g(E)$ can be represented by $g(E) \approx g_D(E) + g_A(E)$ with $g_D(E) \approx D(E) + kT\, ln(2)$ and $g_A(E) \approx D(E - U - kT \ln(2))$ where E is the energy, k is the Boltzmann constant, T the temperature and U the correlation energy.

Fig 1 shows the calculated DOS in a-Si:H at the a-Si:H/c-Si interface with the standard defect-pool parameters given in Table 1. In order to represent the surface defect density as described in the third step above, we have introduced a very thin defective (n)c-Si layer (<0.5nm). The DOS in this defective layer has been evaluated as the volume DOS calculated at the second step restricted to the bandgap of c-Si with a band offset $\Delta E_v = 0.4\ eV$ [5].

The effective lifetime was calculated from the ratio $\Delta p_{av}/U_{tot,}$ where U_{tot} is the total recombination rate and Δp_{av} is the difference between the average concentration of minority carriers in c-Si under illumination and the average concentration in the dark. The total recombination is given by $U_{tot} = U_{Auger} + U_{rad} + U_{SRH}$ where U_{Auger} is the Auger recombination, U_{rad} is the radiative recombination and U_{SRH} is the Shockley-Read-Hall recombination [6,7] with a volumic lifetime $\tau_{SRH} = 10\ ms$. Band-to-band and Auger recombinations are taken into account according to the parameterization of Kerr and Cuevas [8].

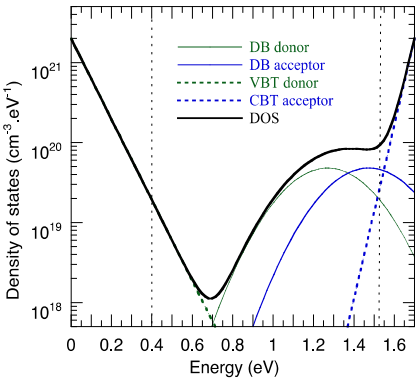

Fig. 1. One-electron density of states in a-Si:H at the hetero-interface. Two Gaussian distributions (DB donor and DB acceptor) represent the monovalent states transcription of the amphoteric dangling bonds calculated here with standard defect-pool parameters, VBT (CBT) is the valence (conduction) band tail distribution. The vertical dotted lines indicate the valence and conduction band edge for the c-Si defective layer.

2.2. Set of standard parameters

In order to study the impact of the defect-pool parameters on the DOS at the hetero-interface and then on the effective lifetime we have used the set of standard parameters [9] summarized in Table 1. We have varied independently the standard deviation of the Gaussian pool distribution σ_{DB}, the energy correlation U, the energy separation Δ and the capture cross-section of the carriers.

Table 1. Parameters of the a-Si:H layers.

	Emitter (p)a-Si:H	Buffer layer (i)a-Si:H
Equilibration temperature T^*	480 K	
Hydrogen concentration H	5.10^{21} cm^{-3}	
Concentration of electrons concentration in the silicon bonding states N_{SiSi}	2.10^{23} cm^{-3}	
Energy separation Δ	0.44 eV	
Energy correlation U	0.2 eV	
Standard deviation of the Gaussian pool distribution σ_{DB}	0.19 eV	
Effective DOS in the cond./val. band	5.0×10^{19} cm^{-3}	
Pre-exponential factors of the cond./val. band	2.0×10^{21} cm^{-3}.eV^{-1}	
Urbach energy of conduction band tail E_{U-cond}	0.040 eV	0.040 eV
Urbach energy of valence band tail E_{U-val}	0.086 eV	0.045 eV
Capture cross-sections		
Donor Gaussian distribution	$\sigma_n^+ = 1.3 \times 10^{-14}$cm^2	$\sigma_p^0 = 8.0 \times 10^{-15}$cm^2
Acceptor Gaussian distribution	$\sigma_n^0 = 2.7 \times 10^{-15}$cm^2	$\sigma_p^- = 2.0 \times 10^{-14}$cm^2
Valence band tail (donor)	$\sigma_n^+ = 1.0 \times 10^{-16}$cm^2	$\sigma_p^0 = 1.0 \times 10^{-18}$cm^2
Conduction band tail (acceptor)	$\sigma_n^0 = 1.0 \times 10^{-18}$cm^2	$\sigma_p^- = 1.0 \times 10^{-16}$cm^2

2.3. Impact of the defect-pool parameters

In Fig.2, we present the effective lifetime as a function of the excess minority carrier concentration calculated varying several parameters, namely the correlation energy U (energy difference between acceptor and donor states),

the standard deviation of the Gaussian pool σ_{DB} and the energy separation Δ (difference between negatively charged defects in n-type a-Si:H and positively charged defects in p-type a-Si:H). Fig 2a shows the effective lifetime curves calculated for five values of U in the range 0.15 eV to 0.35 eV. Fig 2b presents the impact of the modification of the standard deviation of the Gaussian pool σ_{DB} from 0.17 eV to 0.21 eV without changing the total DOS. Fig 2c shows effective lifetime curves calculated for three values of Δ in the range 0.35 eV to 0.50 eV. The simulated curves clearly show that these defect-pool parameters have a very small impact on the recombination and thus on the effective lifetime.

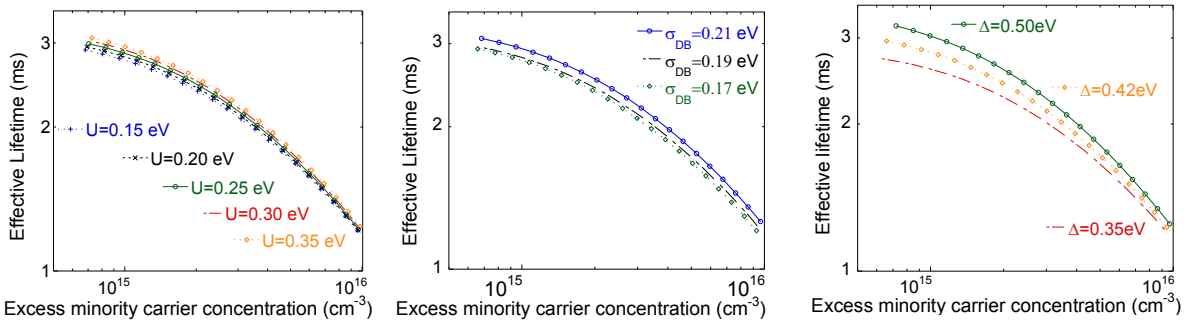

Fig. 2. Effective lifetime versus excess minority carrier concentration for several values of (a) the correlation energy U, (b) the standard deviation of the Gaussian pool σ_{DB}, and (c) the energy separation Δ.

Fig 3 shows the impact of the capture cross section on the effective lifetime. Each capture cross section of the Gaussian distributions has been increased by a factor of ten, keeping the others constant. We observe almost no effect of the capture cross section in the particular case of holes σ_p^0 and σ_p^-, a weaker impact is observed for the capture cross section of electrons of the acceptor Gaussian distribution σ_n^0 and a significant impact is pointed out for the capture cross section of electrons of the donor Gaussian distribution σ_n^+. This demonstrates that the capture of electrons by the donor Gaussian distribution ($D^+ + e^- \rightarrow D^0$) is the process that mainly determines the recombination properties. The reasons are that (i) electrons are the minority carriers at the heterointerface due to the strong band bending, (ii) the D^+/D^0 transition is deeper than the D^0/D^- one, and (iii) the D^+ states have larger capture cross sections for the electrons than the D^0 states.

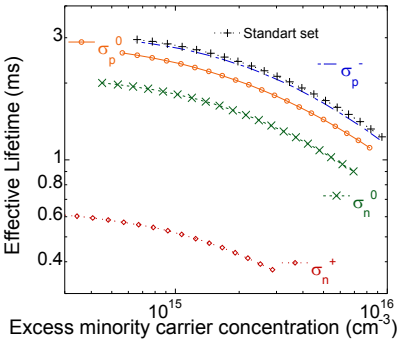

Fig. 3. Effective lifetime versus excess minority carrier concentration for several sets of capture cross section of deep defects.

2.4. Thickness of the buffer layer

In order to study the impact of the interface, we chose an important value of the volumic lifetime $\tau_{SRH} = 100\ ms$ in this part. We have first studied the effect of the (i)a-Si:H layer thickness $d(i)$ without changing the other layer properties. To that purpose, we computed and illustrated the effective lifetime as a function of the excess carrier

distributions for a variation of $d(i)$ from 0 to 8 nm as presented in Fig. 4(a). We have observed that the lifetime first slightly increases and then decreases when the thickness of the buffer layer increases. These simulation results can be explained by the fact that the decrease of defects calculated from the defect-pool model is not sufficient to counterbalance the decrease of the field effect passivation. However, this is in contradiction with the experimentally observed behavior where the effective lifetime increases with the (i) layer thickness [10]. This discrepancy can be linked to the electronic properties of ultra-thin (i)a-Si:H layers (< 10 nm) which are reasonable poor compared to thicker layers. In order to take into account this fact we proposed to parameterize the valence band tail Urbach energy, E_U, versus $d(i)$:

$$E_U = \begin{matrix} E_{U,0} - a * d(i)^2 & d(i) < d_{lim} \\ E_{U,lim} & d(i) \geq d_{lim} \end{matrix}$$

where d_{lim} represents the thickness limit beyond which E_U is considered unvarying (=$E_{U,lim}$), $E_{U,0}$ is the Urbach energy for $d(i)$=0 and a is a parameterized factor used to describe the parabolic decrease of E_U. For the simulations we have used $E_{U,0} = 0.085$ eV, $E_{U,lim} = 0.045$ eV , $d_{lim} = 10$ nm and $a = 4.10^{-4}\text{eV.nm}^{-2}$.

With this new parameterization, it can be seen on Fig. 4(b) that the lifetime increases with *d(i),* which is now in agreement with experimental trends.

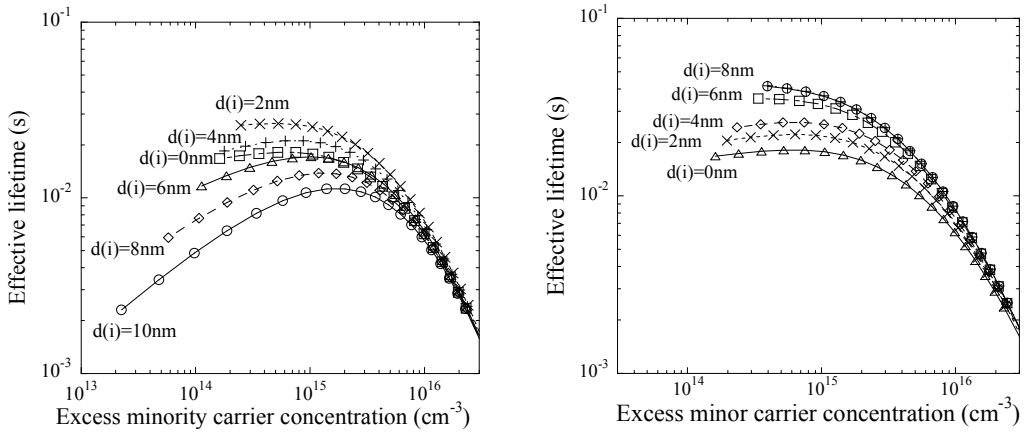

Fig. 4. Effective lifetime versus excess minority carrier concentration for several values of the (i)a-Si:H buffer layer thickness, $d(i)$, with a constant value of the valence band tail Urbach parameter, E_u, (Fig. 4a) and with a parabolic parameterization of E_u (Fig. 4b)

3. Conclusion

We have modeled surface defects at the a-Si:H/c-Si front emitter of heterojunction solar cells using the defect-pool model. The volume defects were self-consistently calculated according to this model in both the (i)a-Si:H buffer layer and (p) a-Si:H emitter layer. Surface defects were then introduced as a thin defective c-Si interface layer where the density of states was projected from the volume defects in a-Si:H close to the surface. Our simulations show that the defect-pool parameters values have no strong impact on the calculation of the surface DOS and on its dependence with the thickness of the (i)a-Si:H buffer layer. In order to reproduce the experimentally observed trend, namely that the effective lifetime increases with the (i) layer thickness, it is necessary to assume that the valence band tail Urbach energy decreases when this thickness increases. This is mandatory to have a sufficient increase of chemical passivation that can compensate the loss of field-effect passivation.

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