AMPS-1D investigations of interface properties on heterojunction silicon solar cells

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Amorphous/crystalline silicon heterojunctions are very promising structures for high efficient solar cells fabricated at low temperature. However, interface defects can enhance the recombination of photogenerated carriers and limit the cell efficiency. In this work, we have investigated the interface defect density of amorphous silicon hydrogenated (a-Si:H) heterojunctions(HJs)based on both n-type and p-type c-Si substrate. We have analyzed the influence of interface defect density on the photovoltaic response of each HJ solar cell using the resources of recognized AMPS-1D simulator by means of inserting an artificial extremely thin layer with a high bulk density of states representing the interface between the amorphous and crystalline silicon interface.

(Received April 17, 2013; accepted June 12, 2013)

Keywords: Interface DOS, Solar cell, heterojunction (HJ), Amorphous silicon,AMPS-1D

1. Introduction

Recent studies on amorphous-crystalline silicon (a-c) heterojunctions have evidenced the potential of these materials to realize low cost, high-efficient solar cells [1]. Despite this, the exact operation of these cells is not fully understood. In particular the transport under illumination and the influence of band discontinuities at the a-c interface have not been completely clarified although this is essential for further optimization of these solar cells [2]. Especially when using a wide bandgap window layer, band discontinuities at the a-c interface could play a significant role in the collection of photogenerated carriers. Up to now, many researchers have focused on the optimization of the fabrication of Si heterojunction solar cells to increase their efficiency.

According to several reports, the control of the interface of a-Si/c-Si to achieve an abrupt interface with a low defect density has been a critical issue, since it is directly related to the open circuit voltage (Voc) [3–4].

A simulation of solar cells based on crystalline and non crystalline materials via AMPS-1D simulator is necessary to study the optimization of the solar cell and the influence of these parameters on the performance in order to obtain a maximum efficiency.

In this work, the AMPS-1D [5](Analysis of Microelectronic and Photonic Structure) simulation program is used to study systematically the effect of a-Si:H(p^+,n^+)/c-Si(n,p) interface layer on illuminated J-V characteristics and therefore the photovoltaic parameters (J_{SC}, η, V_{OC} and FF).

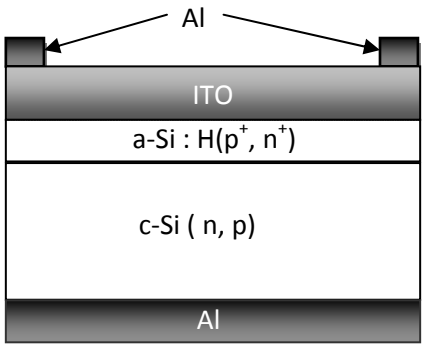

Fig.1. The schematic cross-sectional structure of the a-Si:H (p^+)/c-Si(n) heterojunction solar cells.

2. AMPS-1D model for the simulation

To study the influence of interface defect density in a-Si:H/c-Si heterojunction we have usedAMPS-1D[5]. AMPS can simulate any general semi conductor device structure such as p–n and p–i–n homo- and hetero-junctions, p–i–p and n–i–n structures, multi-junction and Schottky barrier devices. Numerical simulation requires a model for the trap density of states (DOS) in the sample. For the density of localized states in the mobility gap of amorphous silicon it has been assumed that there are both acceptor-like states and donor-like states modeled by exponential band tails (Urbach Tails) and Gaussian mid-gap states (associated to silicon dangling bonds).

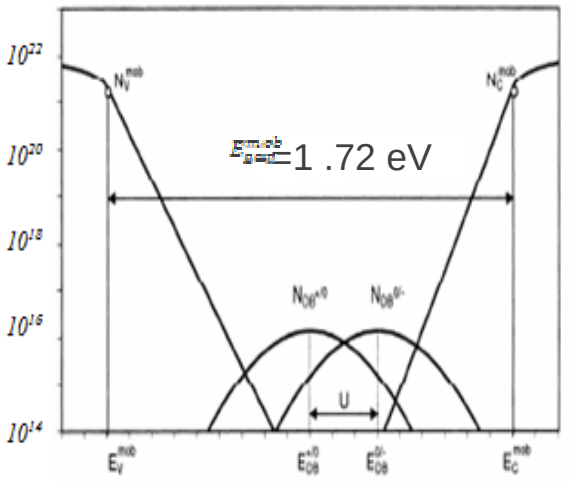

Fig.2. Density of States (DOS) in the gap of the amorphous silicon.

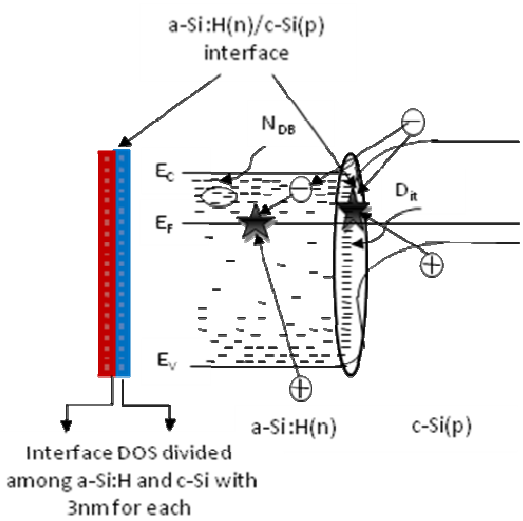

Fig.3. Band structure at the a-Si:H/c-Si hetero-junction. Defect states (D_{it})at the a- Si:H/c-Si interface and in the a-Si:H bulk are indicated by dashes. The interface and bulk recombination pathways for photogenerated carriers are indicated by arrows.

3. Recombination at the a-Si:H/c-Si interface

For a-Si:H/c-Si heterojunction cells, the key to high cell efficiency is the recombination at the a-Si:H/c-Si interfaces: The a-Si:H layers not only induce a band bending but also passivate both the front and the rear surfaces of the c-Si by saturation of dangling bonds [7].

High defect densities $D_{it}(cm^{-2})$ or $N_{dbi}(cm^{-3})$at the a-Si:H/c-Si interfaces,above10^{18} cm^{-3}, lead to apronounced decrease in Voc and a concomitant decrease of the efficiency η. Two recombination pathways can contribute to the recombination at the interface, cf. Fig. 3: (a) Charge carriers generated in the c-Si absorber can recombine via dangling bond states at the c-Si surface, if the passivation by the a-Si:H network is insufficient. (b) if the charge carriers can overcome the a-Si:H/c-Si barrier either via thermionic emission or by tunneling into the a-Si:H band tail states, they see a very efficient recombination pathway via dangling bond defects in the a-Si:H. Instead of discussing interface states, it would therefore be more precise to discuss defects at an effective interface which consists of the unsaturated Si-Si dangling bonds as well as the a-Si:H defects close to the a-Si:H/c-Si interface, within the tunnel length of charges coming from the c-Si.

4. Simulation results and discussion

For the AMPS-1D simulation we need an initial set of parameters for all the properties of the amorphous and crystalline silicon materials (like bandgap, electronic affinity, doping concentration, mobilities, gap-defect states distribution in the bulk and at interfaces layers, etc.).

In Table 1 we summarize the values used in our simulations and the a-Si:H(n^+)/c-Si(p) has the same values. For a-Si:H we obtained data from the AMPS-1D parameter compendium and from the available literature. For simulation under illumination we used the AM 1.5 spectrum normalized to 100 mW/cm^2.

Fig. 4 shows the effect of changing the interface density states (N_{dbi})on the photovoltaic parameters (J_{SC}, η, FF, V_{OC}) on an interfacial layer divided between the c-Si (3nm) and a-Si:H (3nm) when the volumic equivalent interface states density N_{dbi} take the values of $10^{19}cm^{-3}$ and more.

Table 1. Parameter set for the simulation of hetero-junction solar cells with AMPS-1D.

Parameters and units	a-Si:H(p+)	a-Si:H(p+) interface	c-Si(n) interface	c-Si(n)
Thickness (nm)	5	3	3	300000
Electron affinity (eV)	3.8	3.8	4.05	4.05
Band gap (eV)	1.72	1.72	1.12	1.12
Effective conduction band density (cm^{-3})	2.5×10^{20}	2.5×10^{20}	2.8×10^{19}	2.8×10^{19}
Effective valence band density (cm^{-3})	2.5×10^{20}	2.5×10^{20}	1.04×10^{19}	1.04×10^{19}
Electron mobility($cm^2V^{-1}s^{-1}$)	10	10	1076	1076
Hole mobility($cm^2V^{-1}s^{-1}$)	1	1	460.9	460.9
Acceptor concentration(cm^{-3})	10^{19}	10^{19}	0	0
Donor concentration(cm^{-3})	0	0	10^{16}	10^{16}
Band tail density of states ($cm^{-3}eV^{-1}$)	10^{21}	10^{21}	10^{19} - 10^{21}	1
Characteristic energy (eV) for donors, acceptors	0.05- 0.03	0.05- 0.03	0.05- 0.03	0.05- 0.03
Capture cross-section for donor states, e, h (cm^2)	10^{-15} - 10^{-17}	10^{-15} - 10^{-17}	10^{-15} - 10^{-17}	10^{-15} - 10^{-17}
Capture cross-section for acceptor states, e, h (cm^2)	10^{-17} - 10^{-15}	10^{-17} - 10^{-15}	10^{-17} - 10^{-15}	10^{-17}- 10^{-15}
Gaussian density of states N_{DB} (cm^{-3})	5×10^{18}	10^{17}- 10^{20}	10^{17}- 10^{20}	
Gaussian peak energy (eV) donors, acceptors	1.12-1.02	1.12-1.02	0.6 - 0.5	
Standard deviation (eV)	0.15	0.05 - 0.5	0.05- 0.5	
Capture cross section for donor states, e, h (cm^2)	10^{-14} -10^{-15}	10^{-14} - 10^{-15}	10^{-14} - 10^{-15}	
Capture cross-section for acceptor states, e, h (cm^2)	10^{-15} - 10^{-14}	10^{-15} - 10^{-14}	10^{-15} - 10^{-14}	
Switch-over energy (eV)		0.86	0.56	0.56
Capture cross-section for donor states, e, h (cm^2) Capture cross-section for acceptor states, e, h (cm^2)		10^{-15} - 10^{-17} 10^{-17} -10^{-15}	10^{-15} - 10^{-17} 10^{-17} - 10^{-15}	10^{-15} - 10^{-17} 10^{-17} - 10^{-15}

It is evident that the presence of the c-Si interface layer affects drastically the photovoltaic performance in particular (η, V_{OC} and FF) in the case (a).We note no effect of this interface density on short circuit current J_{SC}. Moreover, the simulation results show a slight dispersion of PV parameters in the both HJ cells.

However, in the case (b) with an additional a-Si:H interface layer, we find again a degradation of the PV parameters only in a-Si:H(p^+)/c-Si(n) HJ solar cell. Whereas, the a-Si:H(n^+)/c-Si(p) HJ solar cell presents a very low photovoltaic response.

In Fig. 5,we present the effect of changing the standard deviation ($W_{DG,}$ W_{AG}) of donor and acceptor dangling bonds DOS on the photovoltaic parameters (J_{SC}, η, FF, V_{OC}) on the c-Si and a-Si:H interface layer respectively.

We can see that when $W_{DG,\ AG}$ increases, all the PV parameters also increase. This is explained by the overlapping of the donor and acceptor dangling bond distribution which attenuate the efficiency of the trapping and consequently an improvement of conversion efficiency and fill factor, slightly of open circuit voltage and no variation of J_{SC}. The same behavior was observed for the a-Si:H(n^+)/c-Si(p) HJ solar cell i.e low output parameters.

The fig.6 represents the current voltage characteristics for the three samples a-Si:H(P^+)/c-Si(N), with c-Si artificial interface layer and added a-Si:H artificial interface layer. We observe the voltage decreases when we added an interface from 0.658 V to 0.395V but the short circuit current remains around 32 mA/cm^2.

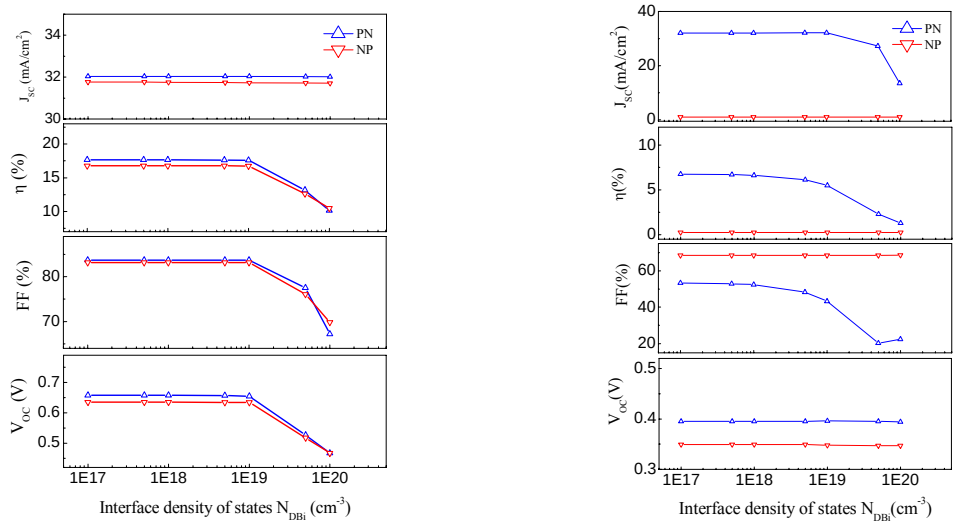

Fig. 4.Photovoltaic parameters (J_{SC},η, FF and V_{OC}) as function of the interface DOS of dangling bond N_{DBi} in the both a-Si:H/c-Si HJ with 3nm of artificial c-Si interface layer (a), added with 3nm of artificial a-Si:H interface layer (b).

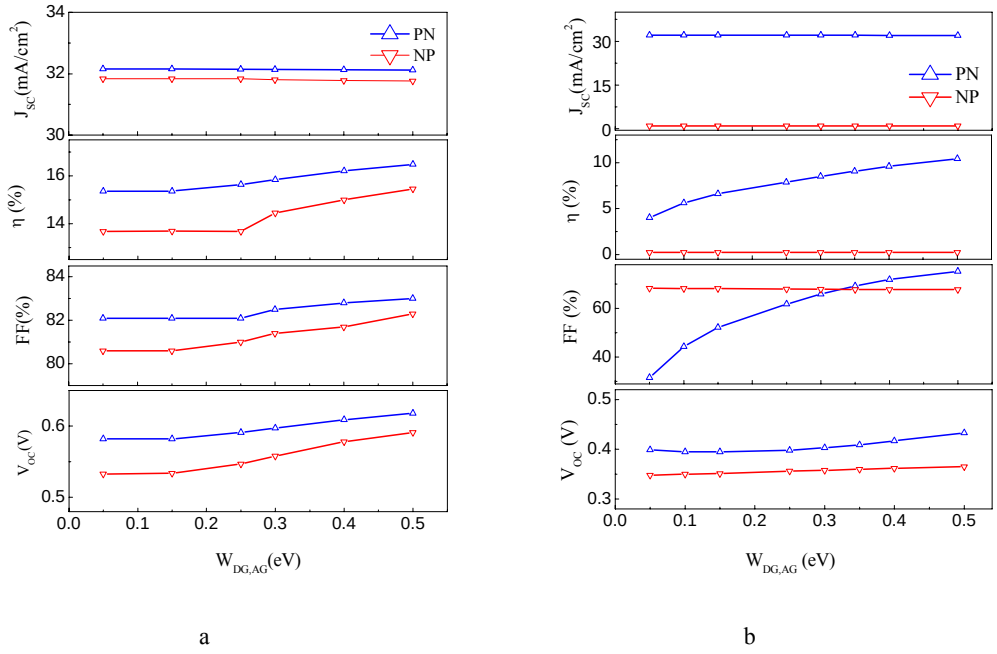

Fig. 5.Photovoltaic parameters (J_{SC},η, FF and V_{OC}) as function of the standard deviation of interface DOS of dangling bond $W_{DG,AG}$in the both a-Si:H/c-Si HJ with 3nm of artificial c-Si interface layer (a), added with 3nm of artificial a-Si:H interface layer(b).

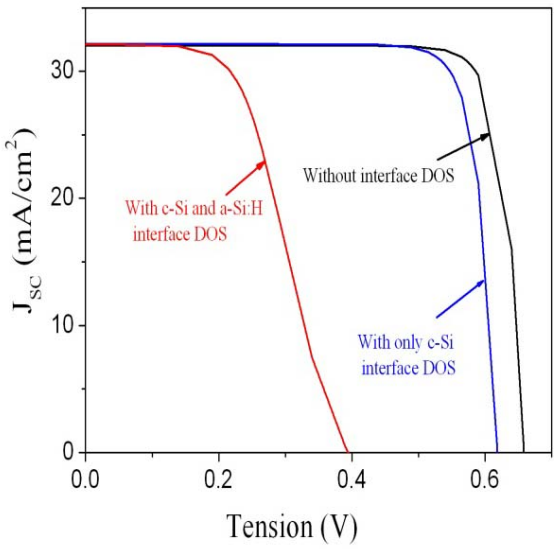

Fig.6. Current–voltage characteristics under AM1.5 illumination for the three samples.

5. Conclusion

We have used a simulation of solar cells based on crystalline and non-crystalline materials via AMPS-1D program based on the one-dimensional numerical resolution of transport equations governing the electrical behavior of semiconductor devices which are: the Poisson equation and both continuity equations of electrons and holes. The interest of the AMPS-1D is the inclusion of density of states (DOS) typically of the CVD deposition techniques that consists of band tails and dangling bonds.

We have analyzed the influence of interface layer on the photovoltaic parameters PV (J_{SC}, V_{CO} η and FF) in the both a-Si: H(n^+, p^+)/c-Si(p, n) of HJ solar cells. The results of our simulations have shown that:

- High defect of dangling bonds density D_{it} (N_{DBi}) at the a-Si:H/c-Si interfaces layer,above10^{12}cm^{-2}relating to 10^{19} cm^{-3}, lead to pronounced decrease in Voc and a concomitant decrease of the efficiency η.
- The photovoltaic parameters are influenced by the artificial a-Si;H layer more than by the artificial c-Si layer especially for a-Si: H(n^+)/c-Si(p) solar cell.
- The best photovoltaic output are reached for an a-Si:H(p^+)/c-Si(n)solar cell as those found experimentally. The determination and control of interface properties are a major step in the development of a-Si:H/c-Si heterojunction devices. Alternatively, Sanyo Ltd. has developed a silicon solar cell called Hetero-junction with intrinsic thin layer (HIT) cell, with the purpose of reducing the carrier recombination and defect density state at the interface.

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