AMPS MODELING OF NANOCRYSTALLINE SI P-LAYER IN A-SI NIP SOLAR CELLS

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ABSTRACT

This paper reports numerical simulations for the impact of a wide bandgap p-type hydrogenated nanocrystalline silicon (nc-Si:H) on the performances of a-Si based component solar cells, using Analysis of Microelectronic and Photonic Structures (AMPS) computer model developed at Penn State University. The effects of band offset and potential barrier formed at the interfaces of p-layer with i-layer and ITO front contact were also investigated. The simulated results show that 1) with increasing bandgap of p-nc-Si:H (E_{gp}), the V_{oc} increases beyond 1 V, then decreases, due to the band offset at the p/i interface, which also leads to an anomalous illuminated I-V characteristics with a bending close to the open circuit point; and 2) the front contact barrier plays a similar role to hinder the hole collection and may cause the illuminated I-V curve to bend seriously.

INTRODUCTION

In order to provide guidance for the optimization of triple-junction amorphous silicon based solar cell fabrication, we carried out numerical simulations using AMPS model developed at Penn State University [1]. The modeling is geared toward understanding of 1) the impact of the wide bandgap p-μc-Si:H layer on V_{oc} for the top cells, and 2) the influence of band offsets between p-μc-Si:H and i-a-SiGe on the illuminated I-V characteristics for the middle and bottom component cells of a triple-junction a-Si solar cell

MODELING AND RESULTS

It is well known that proper selection of the basic parameters of the material concerned is very important for modeling research. In this study, the chosen parameters for AMPS modeling, as listed in Table 1, include: the basic energy band parameters of the bandgap E_g, effective densities of states N_c and N_v for the conduction band and valence band, and the electron affinity χ_e; the parameters describing the defect densities of the characteristic energy E_o of the Urbach band tail, the Gaussian defect density N_{gap} in the mid gap; the acceptor concentration N_A for the p-layer and the mobility μ_e and μ_h for electrons and holes.

For i-layer of the top cells, we chose E_g=1.84eV, as measured and reported in our previous work [2]. We chose N_c and N_v to be the same as that of crystalline silicon. For the p-layer, we assumed two kinds of them: p-type hydrogenated microcrystalline silicon (p-μc-Si:H) and p-type hydrogenated nanocrystalline silicon (p-nc-Si:H). The former is thought to be simply composed of microcrystallites, and the volume fraction of the interface phase between the microcrystallites could be ignored. However the latter is thought to consist of nanometer-sized crystallites embedded in wide bandgap interface phase, having in fact a two phase structure. We do not yet have enough information on them, so we tentatively differ them by different Urbach band tail E_o and mobility μ. For the pure p-μc-Si:H, we assumed E_o= 0.01 eV and 0.02 eV for conduction band and valence band, respective, and μ= 5 and 0.5 $cm^2/s \cdot V$ for electrons and holes, respectively. For the p-nc-Si:H, the Urbach band tails become larger with E_o= 0.06 and 0.1 eV for conduction and valence bands, respectively, and the carrier mobilities decrease to μ= 2 and 0.2 $cm^2/s \cdot V$ for electrons and holes, respectively.

As for the electron affinity χ_e, we assumed it to be equal to that of c-Si. This means that the band offsets at p/i interface mostly occur at the valence band edge. Another sensitive parameter for the simulation is the barrier height ϕ_{B0} at the front ITO/p-layer interface, which should be dependent on both the work function difference and the interface states. In order to demonstrate the influences of the p-layer bandgap E_{gp} on the performances of solar cells, we first chose ϕ_{B0} = 1.28eV, as an example, to pin the E_F at somewhere below E_c by an interfacial layer.

The simulated photovoltaic parameters of V_{oc} and FF, obtained from AMPS, are shown in Table 2 as a function of the p-layer bandgap E_{gp} varying from 1.5 to 2.0eV. As we can see, for the p-nc-Si:H, V_{oc} increases from 0.805V to 1.026V with increasing E_{gp} from 1.5 to 1.8V, then decreases with further increasing E_{gp}. The reason for the decline of V_{oc} is because the valence-band offset at the p/i interface forms a barrier for photogenerated holes drifting across the p/i interface to the p-layer. For the pure μc-Si p-layer, the dependence of V_{oc} on E_{gp} is similar to the case of p-nc-Si:H, except that rather higher V_{oc} (1.155V) could be reached, which, as of today, has not yet been achieved experimentally. It is noticed that the calculated results are very sensitive to the choice of E_0, for instance, when E_0 is decreased by a slight 0.01eV from the case of the p-nc-

Si:H, it will lead to V_{oc}=1.054V and FF=0.757, which are close to what we have observed in our top cells.

Table 1 Parameters used in AMPS modeling

Layer	E_g (eV)	N_c (cm^{-3})	N_v (cm^{-3})	E_0 (C/V) (eV)	N_A (cm^{-3})	N_{gap} (cm^{-3})	μ_e/μ_h ($cm^2/V\cdot s$)	χ_e (eV)
i-layer	1.84	2.80E+19	1.04E+19	0.03/0.05		5.00E+15	5/0.5	4.05
p-μc-Si layer	1.5*	2.80E+19	1.04E+19	0.01/0.02	1.04E+19	1.04E+18	5/0.5	4.05
p-nc-Si layer	1.5*	2.80E+19	1.04E+19	0.06/0.1	1.04E+19	1.04E+18	2/0.2	4.05

* denotes the variable for this study

Table 2 AMPS simulation results for the top cells with different E_{gp}

	Wide bandgap p-layer		PV for p-nc-Si		PV for pure p-μc-Si	
	E_{gp} (eV)	L (nm)	Voc (V)	FF	Voc (V)	FF
1	1.5	10.9	0.805	0.752	1.005	0.766
2	1.6	8.6	0.899	0.761	1.094	0.782
3	1.7	7.1	0.989	0.76	1.152	0.793
4	1.8	6.1	1.026	0.748	1.155	0.767
5	1.9	5.3	1.008	0.735	1.084	0.74
6	2	4.7	0.947	0.706	0.988	0.724

QUANTUM CONFINEMENT EFFECTS AND P-NC-SI:H

There are usually two ways of achieving wide bandgap p-μc-Si:H, either by alloying, e.g. SiC_x, SiN_x, or by decreasing the size of Si clusters to a nanometer range. In our case the H content inside the Si microcrystalltes is believed to be small, so any cause for larger bandgap of p-μc-Si:H could be mainly due to the quantum size confinement effects, rather than the alloy effects. It was reported that the effective bandgap widening ΔEg of Si clusters is proportional to $1/L^{\Upsilon}$, where L is the size of Si clusters and Υ = 1 to 2 depending on the theoretical models used. For example, for the effective mass approach [3], Υ = 2 and for the density-function approach [4], Υ = 1. Based on the density-function approach, we estimated the sizes of Si clusters in the range of 10.9 to 4.7nm for the p-μc-Si:H or p-nc-Si:H with E_{gp} = 1.5 to 2.0e V, as also listed in Table 2.

However, these theoretical calculations were performed only for isolated nanocrystals, which could be approximately applied to Si clusters embedded in a dielectric matrix (e.g., SiO_x, SiN_x), forming relatively deep quantum-dot system. In our case, the dielectric matrix could be only the wide bandgap SiH_x complex, surrounding the Si clusters and forming an interface phase. Therefore, the wide bandgap p-layer is actually a two-phase structure of nc-Si and SiH_x, and the volume fraction of the interface phase could not be ignored. As an example, we consider a p-layer composed of Si crystallites of 7nm. The volume fraction of the interface phase in this case should be in the range of ~0.33 to 0.52, if the thickness of the interface phase is in the range of ~1 to 2nm, the minimum value needed for isolating the clusters. Therefore, for the wide bandgap p-layer we used the term “p-nc-Si:H”, instead of p-μc-Si:H, as it comprises nanometer-sized Si crystallites and the surrounded SiH_x interface matrix.

Experimentally, the deposition conditions for p-nc-Si:H mainly employ a high H-dilution, a high rf power and a low substrate temperature, likely leading to the formation of crystalline phase with nanometer-sized grains (nano-crystalline phase) and surrounding SiH_x interface matrix (amorphous phase). It was also reported that using well deposited μc-Si:H with high volume fraction of microcrystallinity as the p-layer one obtains a lower V_{oc} [5]. This is because the mobility gap of p-μc-Si:H could be limited to around 1.12eV, i.e., the bandgap of single crystal Si.

BAND OFFSET AT P/I INTERFACE

We mentioned above that the decrease of V_{oc} with further increasing E_{gp} (see Table 2) is due to the band discontinuity at the p/i interface occurring at the valence band edge. This occurs when we assume that χ_e = 4.05eV, which is equal to the value of c-Si, no matter how the p- and i-layer changes. The influences of the band discontinuity on the cell performances should be more serious when we use the wide bandgap p-nc-Si:H layer for

the mid and narrow bandgap a-SiGe cells. Figure 1 shows the I-V characteristics of two mid-gap a-SiGe solar cells deposited under similar conditions except the p-nc-Si layer, lower substrate temperature T_s for GD554 and higher T_s for GD572. The low T_s for GD554 probably leads to smaller size for the crystallites and wider bandgap due to quantum confinement. From Fig. 1 one can see that GD554 not only has low FF but also an anomalous illuminated I-V curve, with a bending close to the open circuit point. It should be noted here that the same low-temperature deposited p-layer, used in GD554, is ideal for wide bandgap (1.8 eV) a-Si:H top cell that has V_{oc} of 1.04V and FF of 73% without any bending in I-V curve near the open circuit point.

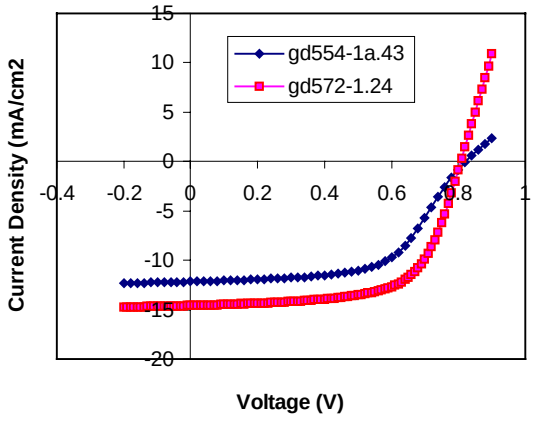

Figure 1. I-V curves of a-SiGe middle cells with p-layer deposited at different temperatures, $T_s(p)$=70 ^oC for GD554 and $T_s(p)$=140 ^oC for GD572.

In order to better understand this issue we also carried out numerical simulations for mid bandgap a-SiGe cells (Eg=1.6eV) using AMPS model. The variable in the calculation is also the bandgap E_{gp} of the p-layer, while keeping χ_e unchanged (4.05eV). The simulated results are shown in Fig. 2a (E_{gp}=1.8eV) and 2b (E_{gp}=1.6eV). It can be seen from Fig. 2a that there is an anomalous rollover behavior in the IV characteristics at forward bias close to the V_{oc}, similar to the experimental observation on that of GD554. But when the p-layer bandgap E_{gp} is decreased down to 1.6eV, the same value as that of the intrinsic layer, the rollover behavior in the IV characteristics disappears, and the FF increases, as shown in Fig. 2b.

The underlying reason responsible for this phenomenon could be more clearly seen from their band diagrams under thermodynamic equilibrium, as illustrated in Fig. 3. The EF, Eca (Ecb) and Eva (Evb) denote the Fermi level, conduction band edge and valence band edge, respectively. For the p-nc-Si:H layer of 1.8 eV, the band offset of 0.2 eV in the valence band edge at the p/i interface induces a barrier at the p/i interface for the photogenerated holes to get collected to the p-layer. Especially when the built-in potential is much weakened when the forward bias is near V_{oc}, the hindered action of the extra barrier on the hole drifting across the interface will be more significant, leading to the rollover behavior in the I-V characteristics.

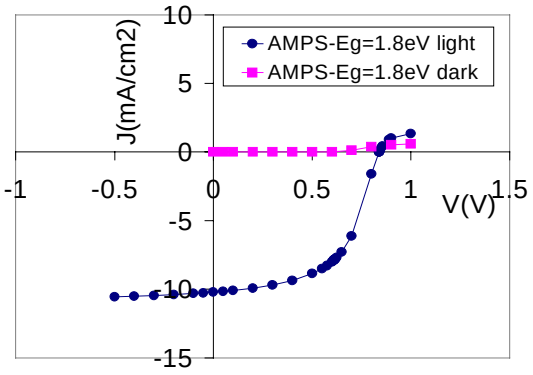

Fig. 2a The calculated dark and illuminated J-V characteristics for mid bandgap cells with E_{pg} = 1.8eV

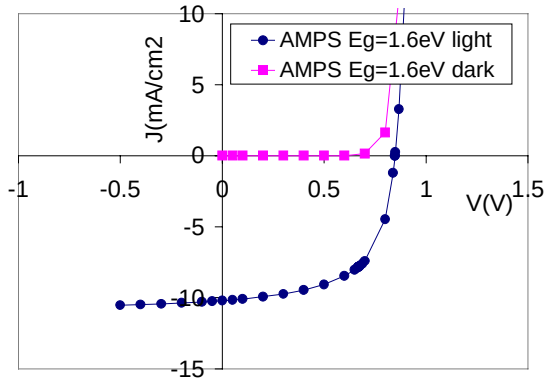

Fig. 2b The calculated dark and illuminated J-V characteristics for mid bandgap cells with E_{pg} = 1.6eV.

Following this thought, we decreased experimentally the bandgap of the p-layer by using a higher substrate temperature that presumably leads to larger nc-Si particle size and less quantum-confinement induced increase of bandgap. The increase in the p-layer temperature resulted in much improved performances of the mid and narrow bandgap solar cells, as shown in Fig. 1 for device GD572. This result also suggests that the major band edge discontinuity occurs at the valence band.

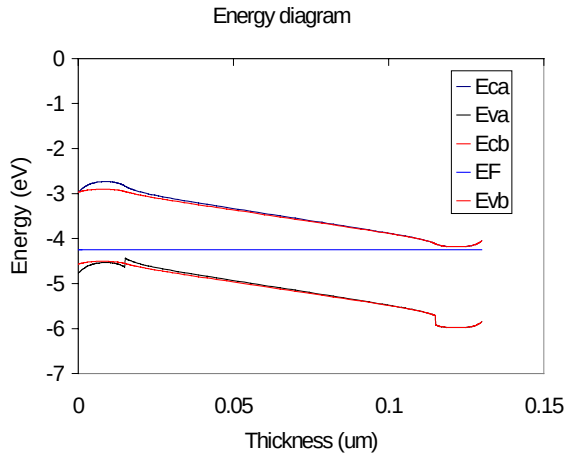

Fig. 3 The calculated thermodynamic equilibrium energy diagrams for the mid cell p-i-n structures shown in Fig. 2a and 2b. The p-layer is on the left hand side.

BARRIER AT ITO/P INTERFACE

The above discussion on the band offset at p/i interface is based on a fixed barrier height ϕ_{B0} = 1.28eV at the front ITO/p-layer interface. Now we address the influences of ϕ_{B0} on the photovoltaic performances of e.g. mid bandgap a-SiGe cells (E_g=1.6eV) under the condition of zero band offset at the p/i interface (E_{pg}=1.6eV).

The results of numerical simulations using AMPS model are given in Fig. 4, showing the calculated light I-V characteristics under AM1.5 as a function of ϕ_{B0}.

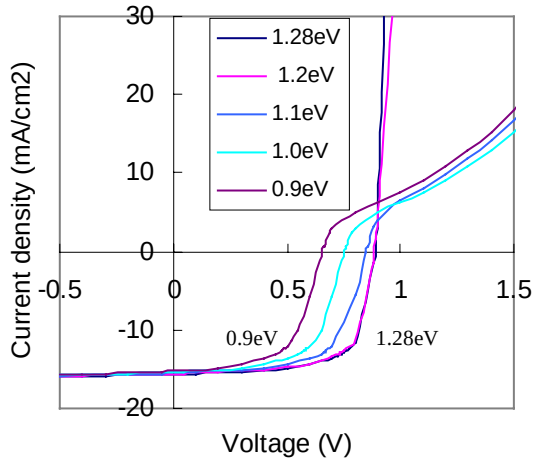

Fig. 4 The simulated light I-V characteristics for mid cells with different ϕ_{B0}.

It is seen that with the barrier height ϕ_{B0} decreases to 1.1eV or less, the photovoltaic parameters become obviously worse. Furthermore, an anomalous rollover behavior appears on the corresponding illuminated I-V curves. This is because in the case of ϕ_{B0} < 1.1eV, a hole potential barrier larger than ~0.2 eV is formed at the ITO/p-layer interface, which may block the collection of the photogenerated holes. Of course if this potential barrier for holes coexists with the valence-band offset at the p-interface, its influence on cell performances is more serious.

SUMMARY

We have carried out AMPS modeling for the impacts of the bandgap of p-nc-Si:H and its interfaces with both the i-layer and ITO front contact on the performances of a-Si based component solar cells. The simulated results show that 1) with increasing E_{gp} from 1.5 to 2.0 V, the V_{oc} increases first beyond 1 V, then decreases; 2) the reason for the V_{oc} decrease may be due to the valence-band offset at the p/i interface, which also leads to an anomalous rollover behavior in the illuminated I-V characteristics near the open circuit point; 3) the front contact barrier at p/ITO interface plays a similar role to hinder the hole collection and may cause the illuminated I-V curve to bend more seriously.

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