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Optimization of a-Si:H/c-Si Heterojunction Solar Cells By Numerical Simulation

Melis Bilgic Aksari[a], Aynur Eray[ba*]

[a]*Hacettepe University, New and Clean Energy Research-Application Center, 06800, Beytepe, Ankara/Turkey*
[b]*Hacettepe University, Department of Physics Engineering, 06800, Beytepe, Ankara/Turkey*

Abstract

In this study design and optimization of a-S:H /c-Si heterojunction solar cell was done with AFORS-HET simulation program. Detailed simulation studies of I-V characterization of solar cells have been carried out with TCO/ (n) a-Si:H/ (i) a-Si:H/ (p) c-Si/BSF/Ag structure. Back surface field (BSF) layer created with (p+) a-Si:H layers. Various efforts such as changes in thicknesses, and doping concentrations of all layers, the quality of amorphous layer have been done to achieve higher efficiency. The results of these simulation studies have been obtained to be in a good agreement with the reported studies in the literature, and it is possible to propose some design parameters for HIT cell fabrication.

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Keyword: Heterojnction solar cells; a-Si:H/c-Si; modelling; optimization

1. Introduction

The amorphous silicon/ crystalline silicon heterojunction solar cell is a promising candidate for high efficient solar cells [1-3]. Although the pioneering work of Sanyo group [4-5] showed an efficiency of 23% in heterojunction with intrinsic thin layer (HIT) solar cell, the role of thin a-Si:H intrinsic layer at the a-Si:H/c-Si hetero-interface still remains ambiguous [4-9]. The insertion of a thin intrinsic a-Si:H layer

* Corresponding author. Tel.: +90.312.297.7245; fax: +90 312.299.2037
E-mail address: feray@hacettepe.edu.tr.

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between the doped active layers of the cell is the most widely used technique to achieve defect passivation in heterojunction solar cell. The key factor for defect passivation is the saturation of defect states of the crystalline lattice at the a-Si:H/c-Si interface. Further investigations are still required in understanding of device physics in order to improve conversion efficiency. Simulation studies provide a convenient way to obtain insight in to device physics and to evaluate the role of various parameters in the fabrication process [10-17].

In this study detailed simulation studies of I-V characterization of HIT cells have been carried out with AFORS HET v2.4.1 [10], in order to get more insight into the factors determining the solar cell performance. The most critical part in this cell structure is the preparation and optimization of the a-Si:H emitter and BSF layer. In order to develop a deeper understanding of the physics of this device we carefully analyzed bulk and interface properties of such amorphous layers and studied the variation of the cell parameters. The attention has been focused on the role of the valence band offset at the a-Si:H/c-Si interface on the BSF side for the device performance. After a first attempt of modeling the n-doped a-Si:H emitter properties, simulations results on HJ solar cells will be presented, as a function of the BSF layer properties.

2. Device Simulation and Layer Structures

AFORS-HET (Automat FOR Simulation of HETerostructures) is a numerical simulation tool, which allows to simulate heterojunction semiconductor devices. Our heterojunction solar cells consist of the n-doped a-Si:H emitter layer, the p-doped c-Si absorber layer, the intrinsic a-Si:H layer buffer layer and the p^+-doped a-Si:H BSF layer. For the simulation of the density of localized states in amorphous layers, it has been assumed that there are both acceptor like states (in the upper half of the gap) and donor like states (in the lower half of the gap). Both of these acceptor and donor like states consist of exponential band tail states and Gaussian mid-gap states. For the crystalline silicon, defect density is chosen as single defect at 0.56eV with a concentration of $1.10^{10}cm^{-3}$. Surface recombination velocities of the electrons and holes were set as 1.10^7cm/s. The set of parameters used in this study are given in Table 1. The TCO front contact and the Ag back contact were optically simulated by taking into account the material absorption coefficients and refractive indexes as given in the default values in AFORS-HET. Simulation data presented in this study deals with AM1.5 solar spectrum and at room temperature.

3. Simulation Results and Discussions

As a first step of simulation studies, we have performed the systematic simulations to obtain the optimized n doped a-Si:H emitter-layer with outstanding quality, aiming to track their contribution to solar cell output parameters (J_{sc}, V_{oc}, and η). During these studies, the mid gap defect densities and the doping concentration in the n-layer were kept constant. The dependence of the cell parameters on the thickness of the emitter layer is presented in Fig. 1a. Reduction of the thickness of the emitter layer results in an increase of the short circuit current (J_{sc}) and the conversion efficiency (η) of the cells, although the open circuit voltage (V_{oc}) remains nearly constant. Our simulated spectral response measurements show that a decrease in the short circuit current is due to the increase of optical absorption a-Si:H (n^+) layer and their extreme low contribution to the photocurrent. Insertion of an intrinsic a-Si:H buffer layer with a thickness of 5 nm between the crystalline silicon absorber and the n-doped emitter layer results in a further increase of the η (see Fig. 1). The carrier recombination at the a-Si:H/c-Si is one of the most important factor to determine the device open circuit voltage and as a consequence the device

performance. Since most of the photovoltaic effects have taken place in the interface layer, it has been very sensitive to the defect states distribution at the interface. During the optimization the c-Si absorber layer, defect density of c-Si has been reduced to $10^{10}cm^{-3}$. The resistivity of crystalline silicon is also another important parameter that strongly affects the solar cell characteristics. In the commercial wafers, the resistivity changes in the range of 1-10 Ωcm. In the literature, a resistivity of 0.1Ωcm and of 0.5 Ωcm are given as best choice by several groups [12, 16]. For that purpose, by changing the doping density of c-Si layer in the range of 1.10^{16} cm^{-3} and $1.10^{17}cm^{-3}$, it has been tried to optimize the solar cell parameters. According to the increase of I_{sc}, V_{oc} and FF, the efficiency increases from 14.97% ($1.10^{16}cm^{-3}$) to 18.55% ($1.10^{17}cm^{-3}$). As a result of this observation, the doping concentration of c-Si (p) layer has been chosen as 1.10^{17} cm^{-3} .

Table 1. Parameter details of different layers used in this simulation

Parameters	(p) a-Si:H	(i) a-Si:H	(n) a-Si:H	(p) c-Si
Layer thickness (nm)	5-70	5/3	5	3.10^{5}
Electron affinity (eV)	variable	3.9	3.9	4.05
Mobility gap (eV)	variable	1.72	1.75	1.12
Effective density of states N_c / N_v (cm^{-3})	$1.10^{20}/1.10^{20}$	$1.10^{20}/1.10^{20}$	$1.10^{20}/1.10^{20}$	$2.810^{19}/1.110^{19}$
Doping concentration (cm^{-3})	1.10^{20}	-	1.10^{20}	1.10^{17}
Electron mobility / Hole mobility (cm^2 /Vs)	variable	20/5	20/5	Variable
Total DOS in Gaussian states (cm^{-3})	10^{19}	10^{16}	10^{19}	-
Standard deviation in Gaussian states (eV)	0.2	0.2	0.2	-
Position of donor-like Gaussian states (eV)	1.05	0.9	0.45	-
Position of acceptor-like Gaussian states(eV)	1.2	1.1	0.7	-
Energy slope donor-like band tail (meV)	90	50	50	-
Energy slope acceptor-like band tail (meV)	30	60	40	-
DOS in tail states (cm^{-3})	10^{21}	10^{18}	10^{21}	-

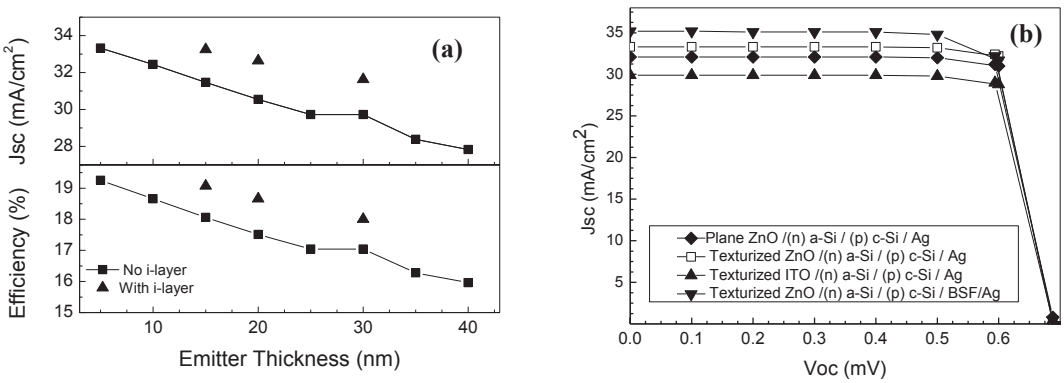

Fig. 1. (a) The change of solar cell parameters (J_{sc}, and η) as a function of the emitter layer thickness. (b) simulated I-V curves with different TCO layers.

After optimization of emitter layer, and absorber layer, some simulation studies have been performed to search the influence of front contact. Due to the low conductivity and low thickness of the amorphous emitter layer, the use of a highly conductive transparent layer is necessary to transfer the carriers to the metal contact. In Fig. 1b, the simulated I-V curves are plotted to show the influence of plane or textured TCO layers obtained by ZnO and ITO. Significant improvement in device behavior was achieved when a ZnO front layer was used with textured structure.

To analyze the influence of BSF p^+ -doped a-Si:H layer has been added at the back of the cell. An increase in the thickness of p doped layer results in a further increase of η. By setting the thickness of p-layer to 70nm, several simulation studies have been performed by changing the band offset. Our simulation studies show that the band offset values are very important in optimization of BSF layer. A sharp decrease has been seen in the fill factor and the efficiency, with the increasing of valence band offset (ΔE_v) at the a-Si:H/c-Si interface on the BSF side. As seen in Table 2, this effect is more pronounced with the decreasing of the doping level of (p) a-Si:H layer. As the valance offset (ΔE_v) increases, a large barrier occurs for majority carriers (hole) to transfer through the back contact. This observation can be explained as impeding the hole collection and therefore holes are accumulated on the c-Si side of the interface and repel the approaching holes resulting an improved photo generated electron back diffusion. As a result of this pile-up, an increased recombination has been occurred and BSF is screened from the rest of the device. This observation is in agreement with those of the reported in the literature [7, 17].

Table 2. Variation of solar cell output parameters with valence band offset

Eact (eV)	ΔEv (eV)	Voc (mV)	Jsc (mA/cm^2)	FF (%)	η (%)
0.33	0.38	691.4	38.88	83.49	19.50
0.45	0.41	691.4	33.49	66.62	16.35
0.45	0.58	313.3	21.33	60.13	9.25
0.46	0.63	186.7	8.74	30.96	5.05

4. Conclusion

The influence of various parameters of emitter layer and BSF layer on HIT solar cell performance was investigated using AFORS-HET simulation program. In order to have a realistic set of parameters that characterize our cells, several experimental results in the literature [1-9, 11] have been modeled. The resistivity of crystalline silicon is an important parameter that strongly affects the solar cell characteristics, which should be taken into account in the realistic simulations. In order to reach the best performance, the n doped emitter layer should be low enough and heavily doped p type BSF layer should be thick enough. Our result is that the optimum emitter thickness is close to d = 5 nm. For the back surface field the valance band offset should be as low as possible. Our simulated structure reproduces the experimental device structures in the literature [1-9]. The highest efficiency of 19.50% was reached with texturized ZnO/ (n) a-Si:H / (i) a-Si:H / (p) c-Si / (p) a-Si:H / Ag structure.

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