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Simulation study of the a-Si:H/nc-Si:H solar cells performance sensitivity to the TCO work function, the band gap and the thickness of i-a-Si:H absorber layer

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Abstract

In this paper, two solar cells n–i–p^+ and n–i–p–p^+ based on hydrogenated amorphous silicon (a-Si:H) and hydrogenated nanocrystalline silicon (nc-Si:H) have been simulated by using *AMPS-1D* (Analysis of Microelectronic and Photonic Structures) simulator. Various factors that affect cell performance have been studied, such as work function of Transparent Conducting Oxide (W_{TCO}), and band gap and thickness of the i-a-Si:H absorber layer. At first the effect of work function W_{TCO} on the performances of both structures was studied. The best cell's external parameters where obtained in the case of n–i–p–p^+ structure. For this latter, the energy band diagram, current–voltage characteristics $J(V)$, the trapped hole density, the distribution of built-in electric field, and the quantum efficiency are calculated and analyzed in depth to understand the effect of W_{TCO}. It is demonstrated that, for high efficiency of solar cell, the W_{TCO} value should be high enough in order to enhance built-in potential, and gives the electric field negative and the front hole barrier height for a neutral (i.e., no band bending) contact at TCO/p^+nc-Si:H interface. Later, band gap and thickness of i-a-Si:H absorber layer are optimized. Simulation results showed that the highest efficiency of 9.35% ($J_{SC} = 13.96$ mA/cm^2; $FF = 71.4\%$; $V_{OC} = 936$ mV) has been obtained in the case of n–i–p–p^+ structure, when values of W_{TCO}, i-a-Si:H band gap and i-a-Si:H layer thickness are 5.45 eV, 1.78 eV, and 550 nm, respectively. A comparison between simulation results and experimental data, showed that the conversion efficiency of n–i–p–p^+ solar cell can be enhanced from 7.44% to 9.35%, by using the optimized values.

Keywords: Solar cell; Work function; a-Si:H; Band gap

1. Introduction

Although significant progress in the conversion efficiency of single p–i–n and n–i–p a-Si:H solar cells, there is still a lot of factors that limit the performance of a solar cell. In addition to the quality of the films that constitute the cell structure, interfaces plays a dominant role in the electric proprieties of a-Si:H based solar cells. The interface between the p-window layer, and the front conducting layer, which is a Transparent Conducting Oxide (TCO) affects strongly the performances of a-Si:H solar cells (Smole et al., 1994; Morales-Acevedo et al., 2012; Bivour et al., 2013). It is known that the work function value of the TCO (W_{TCO}) layer has great impacts on the a-Si:H heterojunction solar cells (Oh et al., 2012; Lee et al., 2013). Despite the fact that TCO layers (SnO_2, ZnO, ZnO:Al, ITO:Zr) exhibit point a good light transmittance

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of the visible light spectrum and a low ohmic resistivity (Smole et al., 1994, 1996; Hussain et al., 2014). Due to the difference in the W_{TCO} and p-window layers, the electric contact at this interface is not a perfect ohmic contact, which causes a band bending. This potential barrier occurs in the p-window layer due to its higher ohmic resistivity (Smole et al., 1994), impedes the collection of photogenerated holes and, thereby, affects the photoelectric properties of the complete solar cell. The TCO films with high work function are used to inject holes carriers in front contact barrier height of HIT solar cells; hence as high as possible values of work function are desired (Hussain et al., 2014; Dao et al., 2010). The film quality and the p/i interface have been improved by applying novel deposition methods that include hydrogen plasma treatment. The a-SiC:H is broadly used as p-window and buffer layer at p/i interface. Nonetheless, the incorporation of carbon atoms into a-SiC:H film induces disordered structural defects and reduces the cell performances (Hu et al., 2006). Other technique which consists the use of hydrogenated nanocrystalline silicon (nc-Si:H), instead of a-SiC:H material, has been developed (Dao et al., 2010). The p-nc-Si:H material is characterized by a higher electrical conductivity and a lower optical absorption (Liu et al., 2011; Yan et al., 2010). However, p-nc-Si:H seems to be an ideal material for the realization of a-Si:H solar cells, with higher interface quality and best performances (Fathi et al., 2011; Wang et al., 2011).

In this paper, we concentrate on the influence of the interfacial work function at the TCO/p^+ window layer on the performances of n–i–p^+ and n–i–p–p^+ solar cells by using simulations. The calculations were conducted using a software program called *AMPS-1D* to examine how the values of TCO work function affects the performances of hetero-junction a-Si:H/nc-Si:H devices. We also discuss the band gap and the thickness of i-a-Si:H absorber layer effect on the performance of n–i–p–p^+ solar cell. We analyze the reasons for the high performance of this kind of hetero-junction solar cells in terms of band structure diagram, $J(V)$ characteristics, trapped holes density, electric field and quantum efficiency (QE).

2. Structure of a-Si:H/nc-Si:H heterojunction solar cell and simulation model

In this study, we simulated tow experiment solar cells based on hydrogenated amorphous silicon (a-Si:H) and hydrogenated nanocrystalline silicon (nc-Si:H). These structures were realized by Liu et al. by using the radio frequency plasma enhanced chemical vapor deposition method (Liu et al., 2011). In detail, numerical device simulations are performed for the TCO(ITO)/p^+nc-Si:H(15 nm)/i-a-Si:H(300)/n-a-Si:H(25 nm)/staineless steel (*SS*) and TCO (ITO)/p^+nc-Si:H(15 nm)/p-nc-Si:H(10 nm)/i-a-Si:H(300 nm)/n-a-Si:H(25 nm)/staineless steel (*SS*). The second device was fabricated by incorporating, a 10 nm thick of p-nc-Si:H buffer layer in the first structure, between the active layer (i-Si:H) and the p^+window layer. The two cells were grown on stainless steel (*SS*) substrate which plays the role of back contact. The Indium Tin Oxide (*ITO*) electrodes were deposited at 100 °C, on the p^+ side, as front contact by using the *RF* sputtering technique.

The influence of TCO work function (W_{TCO}) at TCO/p^+window interface, the band gap and thickness of the i-a-Si:H absorber layer, on the performances of solar cells, were not studied by Liu et al. (Liu et al., 2011). In this work, *AMPS-1D* (one-dimensional Analysis of Microelectronic and Photonic Structures) program was used for optimizing the effect of these parameters on the performances of n–i–p^+ and n–i–p–p^+ solar cells. The calculations carried out for the analysis were based on Poisson's equation and electron and hole continuity equations approach to analyze the transport behavior of semiconductor electronic and optoelectronic device structure including solar cells. *AMPS-1D* has two pictures, namely, the Lifetime and Density of State (*DOS*) pictures. In the *DOS* picture the details of recombination traffics, trapping and the charge state of the defects are fully explained (McElheny et al., 1988; Zhu et al., 1999). The *DOS* picture, hence, has been employed to simulate the a-Si:H/nc-Si:H hetero-junction solar cells. The typical parameters characterizing the different layers constituting the structures and used in the simulation were based on various measurement results and references (Liu et al., 2011; Belfar and Aït-kaci, 2012; Morales-Acevedo et al., 2012; Hernandez-Como and Morales-Acevedo, 2010). All the other input parameter values used in this work and which gives a best agreement between our simulation results and experimental data of (Liu et al., 2011) can be found in our previous work (Belfar and Aït-kaci, 2012).

In this calculation, we assumed that the surface recombination speeds of electrons and holes were both 10^7 cm/s. The barrier height at back contact φ_{bL} (n layer/SS) was taken constant and equal to 0.2 eV, by against the barrier height φ_{bo} at front contact (ITO/p^+ window layer) was varied with variation the work function values of TCO (W_{TCO}). The light reflection at the front contact (*RF*) was set to 0.2. Since there is no back reflector in the simulation structures we assumed that the back contact (stainless steel) has a reflection coefficient (*RB*) of 0. For the illumination, we used the *AM 1.5* spectrum normalized to 100 mW/cm^2. Values of 2 eV, 1.88 eV, and 1.72 eV were used as band gap energies, for the p^+nc-Si:H window, p-nc-Si:H buffer, and n-a-Si :H layers, respectively. For the intrinsic layer, the band gap energy (*Eg*) was varied from 1.70 eV to 1.86 eV.

3. Simulation results and discussion

3.1. Effect of TCO work function on the performance of n–i–p^+ and n–i–p–p^+ solar cells

The work function of Transparent Conductive Oxide (W_{TCO}) as the window materials has a great impacts on