Solar Energy 170 (2018) 780–787

Contents lists available at ScienceDirect

Solar Energy

journal homepage: www.elsevier.com/locate/solener

Computational analysis of a high-efficiency tunnel oxide passivated contact (TOPCon) solar cell with a low-work-function electron-selective-collection layer

Cheng Quan[a,b,*,1], Yuheng Zeng[b,1], Dan Wang[b], Mingdun Liao[b], Hui Tong[b,c], Zhenhai Yang[b], Zhizhong Yuan[a], Pingqi Gao[b], Baojie Yan[b], Kangmin Chen[a], Jichun Ye[b]

[a] School of Material Science & Engineering, Jiangsu University, Zhenjiang City 212013, PR China
[b] Ningbo Institute of Material Technology and Engineering, Chinese Academy of Sciences (CAS), Ningbo City 315201, PR China
[c] University of Chinese Academy of Sciences, Beijing City 100049, PR China

ARTICLE INFO

Keywords:
Passivated contact
Low work-function metal
Tunnel oxide
Silicon solar cell

ABSTRACT

In this work, the tunnel oxide passivated contact (TOPCon) with a low-work-function electron-selective-collection (ESC) layer is studied using a numerical simulation method. An exhaustive comparison between the low-work-function ESC TOPCon and the heavily-doped-Si TOPCon solar cell is carried out to find out the differences between these two kinds of devices. The work function modulated ESC TOPCon with a work function of typically < 3.6 eV and a low defect-density oxide layer of 1.2–1.4 nm displays an maximum implied open circuit voltage (iV_{oc}) of 742 mV and a superior fill factor (*FF*) of 86%, which is competitive with a regular heavily-doped-Si ESC TOPCon solar cell. Noted that a defective transition layer (DTL) between the low-work-function layer and the oxide layer is studied herein, in which enhanced recombination decays not only the surface passivation but also the carrier transport. Also, the practical problems that might impede the development of a high-efficiency low-work-function ESC TOPCon solar cell are discussed. In summary, this work presents an overall computational analysis of the low-work-function ESC layer, tunnel oxide, defective transition layer and their combined effects on device performances, which provides a pathway towards fabricating a high-efficiency low-work-function ESC TOPCon solar cell.

1. Introduction

Silicon heterojunction solar cell with the interdigitated back-contacted structure has created the new world's record of 26.6% (Yoshikawa et al., 2017a, 2017b). Inspired by the concept of silicon heterojunction solar cell, to develop high-efficiency silicon heterojunction solar cells with new materials for carrier-selection collection has become a hot topic in the photovoltaic field. In general, various new materials with a low or high work function (metal, metal oxide, or metal fluoride) can play as the role for carrier-selective collection, exhibiting the potential to compete with the traditional heavily-doped Si layer. Some pioneering works have proved that the new-concept solar cells with various carrier-selective collection layers exhibit excellent performances with the power conversion efficiency approaching 20% (Allen et al., 2017, Wan et al., 2016a, 2016b, Allen et al., 2016, Yang et al., 2016a, 2016b, Wan et al., 2016a, 2016b, Bullock et al., 2016).

Noted that in the existing publications, most work used the intrinsic hydrogenated amorphous Si as the tunnel layer to passivate contact. However, to deposit an intrinsic hydrogenated amorphous Si film needs a high-quality plasma-enhanced chemical-vaper-deposition system that is typically expensive. To overcome this issue, using SiO_2 to replace hydrogenated amorphous Si as the tunnel layer to passivate contact is a possible option, as its growth is much simpler and cheaper (Asuha et al., 2003, Moldovan et al., 2014, Barnett et al., 2003) due to the avoidance of the plasma-enhanced chemical-vaper-deposition system. More important, an optimized SiO_2 layer has exhibited excellent passivation and tunnel properties in high-efficiency tunnel oxide passivated contact (TOPCon) solar cells (Richter et al., 2017, Feldmann et al., 2014a, 2014b, Tao et al., 2016, Yan et al., 2015). Using tunnel oxide with a low-work-function capping layer is a promising option for the electron-selective-collection (ESC) structure, because the electron tunnel barrier (~3.05 eV) is much lower than the hole barrier (~4.73 eV) in oxide.

Several important scientific issues have to be classified before the application of the tunnel oxide/low-work-function ESC structure in

* Corresponding author at: School of Material Science & Engineering, Jiangsu University, Zhenjiang City 212013, PR China.
E-mail addresses: quancheng@nimte.ac.cn (C. Quan), kmchen@ujs.edu.cn (K. Chen), jichun.ye@nimte.ac.cn (J. Ye).
[1] Represent as co-first authors.

https://doi.org/10.1016/j.solener.2018.06.008
Received 10 November 2017; Received in revised form 7 May 2018; Accepted 1 June 2018

TOPCon solar cells. First, it is suggested that a highly defective transitional layer (DTL) would be generated between the low-work-function material and SiO_2 because of the high-energy atom bombardment during the physics vapor deposition, such as the electron-beam evaporation or the magnetron sputtering. However, the effects of this highly defective transitional layer on device performances are still unrevealed. Second, because of the different passivation mechanism in comparison with the heavily-doped Si film, the effects of work function on the field passivation and on electron-tunnel efficiency have to be understood before fabricating a well optimized device. Third, because of the damage of oxide by the high-energy physics vapor deposition, the effects of oxide defects on passivation need to be demonstrated before achieving a well optimized SiO_2/low-work function ESC structure.

Aiming to answer the above science issues, the numerical tool, AFORS-HET is used to explore the effects of work function, defective transitional layer and tunnel oxide on the performances of the low-work-function ESC TOPCon solar cell. After answering the above concerns, the computational analysis come to the inference that the tunnel SiO_2/low-work-function layer is a promising structure for a high-efficiency silicon heterojunction solar cell with both excellent surface passivation and carrier collection. Also, an exhaustive comparison between the low-work-function ESC TOPCon and the heavily-doped-Si ESC TOPCon solar cells is carried out to find out the differences between these two kinds of devices. In general, the work provides an overall view to understand the design of a high-efficiency TOPCon solar cell with the low-work function ESC contact.

2. Model and simulation

The AFORS-HET developed by Hahn-Meitner-Institute Berlin is a professional and powerful 1-D numerical simulation tool for heterojunction solar cells (AFORS-HET). The principle of this software is presented as following. To describe a semiconductor device numerically, the AFORS-HET solves the one dimensional semiconductor equations, including Poissoń equation and the transport equation for electrons and holes, with the help of finite differences under different conditions, i.e.: (a) equilibrium mode (b) steady-state mode, (c) steady-state mode with small additional sinusoidal perturbations, (d) simple transient mode, that is switching external quantities instantaneously on/off, (e) general transient mode, that is allowing for an arbitrary change of external quantities. Furthermore, the physical processes of a Si solar cell, including generation, recombination, transportation, and contact, are all considered by this software. The generation of electron/hole pairs can be described by taking incoherent/coherent internal multiple reflections into account or by Lambert-Beer absorption. The carrier recombination mechanisms (radiative band to band recombination, Auger recombination and Shockley-Read-Hall recombination) are considered. Interface currents are modelled to be driven either by drift diffusion or by thermionic emission. The metallic contacts can be modelled as Schottky or Schottky-Bardeen metal/semiconductor contacts or as metal/insulator/semiconductor contacts.

Thus, the internal cell characteristics, such as band diagrams, local generation/recombination rates, carrier densities, cell currents, voltage, quasi steady-state surface photovoltage, and phase shifts can be calculated. In summary, the AFORS-HET becomes a widely accepted tool to understand a Si heterojunction solar cell, through which a number of simulation papers have been published (AFORS-HET).

In this work, the solar cell featuring of the rear tunnel oxide and a low-work-function capping layer is studied exhaustively using the AFORS-HET. The device structure is given as the following: front electrode /SiN_x (front pyramid-textured) /p^+-Si emitter /n-Si wafer /SiO_2 /defective transition layer /low-work function capping electrode. Graphic representation and energy band structure of the simulated device structure and the detailed parameters are given in Fig. 1(a), (b) and Table 1, respectively. The default parameters of the electrical and optical layers are generally referred to the existing reports (Feldmann et al., 2014a, 2014b). Multiple reflections and a coherence model is used to describe the optical absorption. The thermionic-emission and thermionic-field model and the tunneling model are used to describe carrier transport through the SiO_2 dielectric layer. The band gap narrowing effect is already considered in AFORS-HET.

Herein, a defective transitional layer with high-density bulk defect was considered to be formed between the SiO_2 and the low-work-function layer because of the high-energy atom bombardments during the physical-vaper deposition. In practice, the defective transitional layer might be various kinds of metal oxides. For simplification, it is assumed that the defective transition layer is weak n-type material (the default parameters are referred to Si) with a donor concentration of 1×10^{10} cm^{-3} and with a bulk-defect density of more than 1×10^{18} cm^{-3}/eV.

Two fundamental parameters of tunnel oxide, the interface-states density (D_{it}) and the pinhole density through the oxide (D_{ph}), are considered in the simulation. Herein, it needs to classify that the pinhole is essentially a micro-hole or a micro-channel through tunnel oxide, due to the destruction of oxide integrity by impurity diffusion during the high-temperature anneal (Lancaster et al., 2016). Through pinhole, the bulk carriers will leak and be recombinated at interface, which decays the performance of solar cell. Mathematically, a pinhole density can be considered as a proportion of carrier leaking through the oxide layer, which turns the 2D physics issue to a 1D mathematics manipulation.

where t is the thickness, N_a and N_d the acceptor concentration and donor concentration, Chi the electron affinity energy, E_g the band gap, dk the relative dielectric constant, m_e and m_h the relative effective mass of electron and hole, D_{it} interface-state density, D_{ph} pinhole density through the insulator layer (dimensionless unit), and w/o means without.

3. Results and discussion

3.1. Passivation optimization

Note that implied V_{oc} (iV_{oc}), derived from implicit current–voltage characteristic curves of quasi-steady-state photo-conductance is an essential parameter to evaluate the overall performance of a Si solar cell, as it reflects the quality of surface passivation and the lifetime bulk carrier (Sinton and cuevas, 1996). The implied open circuit voltage (iV_{oc}) of the double-sides symmetrical passivation structure, low-work-function layer /defective transitional layer (DTL) /SiO_2 /n-type Si /SiO_2 /DTL /low-work-function layer, is studied exhaustively to estimate surface passivation of the low-work-function ESC structure. The iV_{oc} can be described using Eq. (1):

$$iV_{oc} = \frac{kT}{q} Ln\left(\Delta n\left(\frac{\Delta n + N_{dop}}{n_i^2}\right)\right) \quad (1)$$

where Δn is the excess carrier density at one sun, k the Boltzmann constant, T the temperature, q the elementary charge, N_{dop} the bulk doping density, and n_i the intrinsic carrier concentration. N_{dop} and t of the wafer used for the calculation are 5×10^{15} cm^{-3} and 200 μm respectively.

The effects of the thickness of the tunnel oxide and the work function of the ESC layer on surface passivation are investigated, as shown in Fig. 2. To understand the field passivation of low-work-function ESC layer, the passivation of the regular TOPCon solar cell with a heavily-doped Si ESC layer ($N_d = 1 \times 10^{21}$ cm^{-3}) is also given for comparison.

First, inserting a thin and crystalline-perfect oxide layer (without D_{it} and D_{ph}) is crucial to improve iV_{oc}, which is similar to the case of the heavily-doped Si ESC TOPCon structure (Zeng et al., 2017). The ESC layer with a work function of 4.2 eV is taken as the example to explain this phenomenon, i.e. the iV_{oc} increases from 520 to 740 mV with the increment of oxide thickness from 0 to 1.2 nm. Second, covering with a