Solar Energy Materials and Solar Cells 189 (2019) 63–74

Contents lists available at ScienceDirect

Solar Energy Materials and Solar Cells

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

Predictive simulation framework for boron diffused p^+ layer optimization: Sensitivity analysis of boron tube diffusion process parameters of industrial *n*-type silicon wafer solar cells

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ARTICLE INFO

Keywords:
Silicon solar cells
Boron diffusion
Device simulation
N-type Si
Process simulation
Process control
Sensitivity analysis

ABSTRACT

A predictive simulation framework, combining process and device simulation, is developed in order to assist in BBr_3 boron tube furnace diffusion process optimization for *n*-type silicon wafer solar cells. After an appropriate calibration, the influence of the tube diffusion process parameters (drive-in temperature, oxidation temperature, etc) on the final solar cell efficiency can be predicted. The key process parameters of BBr_3 tube furnace diffusion are identified and their sensitivity on the final solar cell efficiency is calculated. An efficiency gain of 0.6% absolute to 20.0% is realized by optimizing only the front-side boron diffused layer of the front and back contacted cells. The efficiency is further improved to 20.9% by introduction of a local back-surface field design. A further optimization potential of up to 0.2% absolute is predicted by modifying the boron diffusion profile.

1. Introduction

N-type crystalline Si solar cells are extensively researched and large-scale commercialization of the technology appears promising. However, the key to the success of a cell concept in production is not only the realized cell efficiency level, but also the understanding and control of the process. This demands a detailed comprehension of how a variation of the process parameters impact on the solar cell's I-V parameters. The optimization of the diffusion process and the resulting doping profiles are an essential part for further increasing the conversion efficiency of silicon wafer solar cells. For n-type Si solar cells, tube furnace diffusion is an industrially feasible technique for the formation of the front-side heavily boron diffused p^+ layer. In order to achieve higher open-circuit voltage (V_{oc}), the dark saturation current density (J_{0e}) of the passivated region has to be as low as possible. To achieve this, the front p^+ layer would preferably be lightly doped with a low surface concentration and a shallow junction. However, at the same time, low specific contact resistance (ρ_c) needs to be ensured for screen-printed metallization [1,2]. To meet this requirement, the surface concentration has to be sufficiently high. Additionally, as shown in several studies [3–10], metal contacts formed by screen printing and firing through dielectrics usually feature metal spikes at the metal-silicon interface which can induce high recombination losses. To reduce metallization induced recombination losses, a deep junction doping profile is required. Thus, in the present work, the focus is on the optimization of the front-side boron diffused p^+ layer of bifacial n-type front-and-back contacted (nFAB) solar cells. The sensitivity of the process parameters is investigated with respect to not only their influence on the doping profiles, but also their impact on the J_{0e}, and most importantly their impact on the solar cell's I-V parameters, meaning the energy conversion efficiency (η), the open-circuit voltage (V_{oc}), the fill factor (FF) and the short-circuit current density (J_{sc}).

2. Experimental details

Four types of samples were prepared in this work: (1) symmetric double side boron diffused samples for electrochemical capacitance voltage (ECV) measurements; (2) symmetric double side boron diffused and plasma-enhanced chemical vapour deposition (PECVD) AlO_x/SiN_x stack passivated p^+np^+ lifetime samples; (3) test samples with a

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https://doi.org/10.1016/j.solmat.2018.09.019
Received 8 April 2018; Received in revised form 10 September 2018; Accepted 15 September 2018

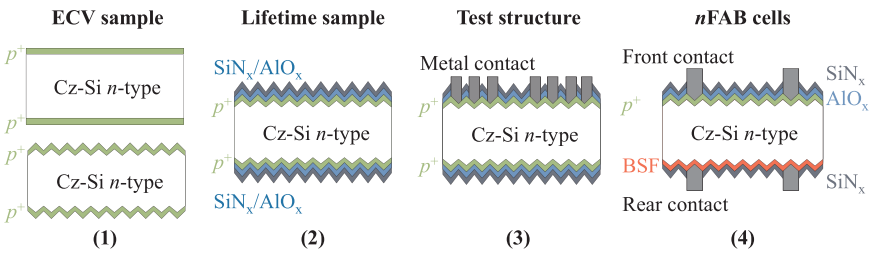

Fig. 1. Schematic illustration of (1) symmetric double-side boron diffused planar (top) and textured (bottom) ECV samples; (2) a symmetric double-side boron diffused and PECVD AlO_x/SiN_x passivated p^+np^+ lifetime sample; (3) a test structure with metal contacts printed on one side; and (4) a n-type front and back contacted (nFAB) solar cell with diffused p^+ layer at the front side.

specially designed metal grid printed on only one side of the wafer in order to extract the metallization induced recombination parameters (J_{01m} and J_{02m}); (4) *n*FAB cell structures. Fig. 1 shows schematic illustrations of the four types of samples prepared in this work.

N-type 6-in. large area Cz-Si wafers with bulk resistivity of 2–5 Ω cm were used for the study. First, the raw wafers were laser marked at the top right corner and then dipped into 20% KOH solution for 9 min for saw damage etching (SDE). Then, the wafers were textured in KOH/IPA/potassium silicate solution at 80 °C for 12 min. After texturing, the wafers were subjected to full Radio Corporation of America (RCA) cleaning. For planar samples, the samples were subjected to a full RCA cleaning right after the SDE process. The boron diffusion process was realized in an industrial quartz tube furnace (Tempress, TS81004). The boron diffusion profiles were varied in the following way: two baseline boron diffusion recipes (2-step diffusion) with sheet resistance (R_{sheet}) of 60 and 40 Ohm/sq. were optimized by including an in-situ oxidation process (3-step diffusion). The R_{sheet} of the boron diffused p^+ layers were adjusted to yield 90 and 65 Ohm/sq., respectively. The ECV samples were obtained with a short dip in 10% hot HF (50 °C) for 2 min after tube diffusion to remove the borosilicate glass (BSG) layer. The lifetime samples and the test structure samples received deposition of PECVD (Meyer Burger) AlO_x/SiN_x stacks on both sides with thicknesses of 20 nm AlO_x and 60 nm SiN_x. A specially designed test structure (see Fig. 2) was printed with an industrial screen printing tool (DEK, PVD1200IR).

The test structure includes 8 different mini-cells with metal fraction ranging from 0% to 29%. The varying metal fraction was realized by increasing the metal finger width from 0 to 380 μm. In addition to the 8 mini-cells, five fingers were additionally printed for finger resistance measurement with a metal pad connected at each end. Both the printed samples and the carrier lifetime samples were fired at a peak temperature of 750 °C in a fast firing belt furnace (BTU International, SinTerra) with the four zones set as 425, 500, 600 and 725 °C. For the cell fabrication, boron diffusions were only applied at the front side.

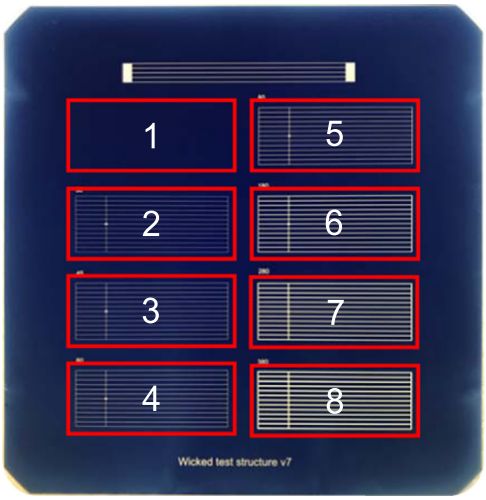

Fig. 2. Photo of the test pattern formed by screen printing of Ag/Al paste on one side of the test sample.

The rear side receives a $POCl_3$ diffusion with R_{sheet} aiming at 50 Ohm/square. The same PECVD stack (20 nm AlO_x and 60 nm SiN_x) of the lifetime samples is applied on the front side of the solar cell, while its rear surface is passivated with a 75 nm SiN_x layer. A commercial Ag/Al paste is used for the front side metal grid and a commercial Ag paste is used for the rear side metal grid. The 5-busbar (BB) configuration is used for both the front side and the rear side. A floating BB configuration, where the BB only contacts the metal fingers but does not contact the heavily diffused Si layer, is applied at the rear side.

The active boron doping profiles were measured with ECV (WEP, CVP21) profiling. The sheet resistance R_{sheet} was measured at 49 points equally spaced over the wafer surface, using a four-point probe (CMT-SR2000N-PV). The lifetime samples were characterized with a Sinton lifetime tester (Sinton, WCT-120). The total saturation current density of the diffused layer (J_{0e}) of the sample was extracted using the Kane-Swanson method [11] at an injection level of 1×10^{16} cm^{-3}. The metallization induced recombination parameters (J_{01m} and J_{02m}) were extracted with intensity dependent photoluminescence (PL) imaging (BT Imaging, LIS-R2) and image processing with the SERIS developed software Griddler AI [12] from the screen printed test samples. The ρ_c is measured with the transfer length method (TLM, IVT-Solar). A commercial *I-V* tester (SINU220, Wavelabs) is used to measure the *I-V* characteristics of the solar cells.

3. Simulation approach

Three levels of simulations are involved in this work: process simulation, test structure simulation and solar cell simulation. First, process simulations were performed with Sentaurus TCAD [13] to see how the doping profile and the corresponding R_{sheet} value change with variation on six of the key process parameters (deposition temperature $T_{deposition}$, drive-in temperature $T_{drive\text{-}in}$, oxidation temperature $T_{oxidation}$, deposition duration $t_{deposition}$, drive-in duration $t_{drive\text{-}in}$, and oxidation duration $t_{oxidation}$). Please note currently other factors, such as the gas ratio between O_2 and N_2 (which may also alter the shape of the doping profiles though), are not discussed in the present work (also, the setting of BBr_3 flow generally follows the safety instructions from the vendor, and is rarely changed). However, the mechanisms involved in the process, such as oxidation and segregation are well incorporated in the presented model [14].

Then, the test structure simulations include a carrier lifetime simulation of symmetrically diffused and AlO_x/SiN_x passivated lifetime samples, and a PL image simulation of a test structure with a screen printed contact being applied on one side of the lifetime sample. The lifetime simulation is performed with EDNA [15,16], provided online by PV Lighthouse [17]. The simulated diffusion profiles (obtained from the process simulation) were imported into EDNA [15,16] to see how J_{0e} changes upon variation of the boron diffusion process parameters. An auto-fitting procedure by Griddler AI, a finite-element simulation program [12], was used to simulate and “best-match” the measured intensity-dependent PL images, thereby enabling us to extract the metallization induced recombination parameters J_{01m} and J_{02m} for several given (measured) diffusion profiles [10]. Currently, there is no simulation program available that is able to predict the J_{01m} and J_{02m} values as a function of the doping profile. Thus, a graphical linear