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# Numerical Modelling of boron diffusion for micro-pyramidal textured N-type silicon

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***Abstract***
*The formation of the emitter is considered as a crucial technological sequence during the manufacture of solar cells the thermal diffusion from a solid source in acylindrical quartz tube constitutes the most widely know and used technique for the formation of the emitter. Indeed, doping of n-type silicon with boron diffusion allows the formation of the p+ emitter. This distribution is often difficult in terms of homogeneity to control and requires adequate detailed understanding of physical phenomena in order to optimize the best profile of dopant diffusion. However, this work is dedicated to the optimization of boron diffusion profile by investigating the effects of temperature and time diffusion on the planar and textured. A comparison with the experimental profile measured by SIMS (Spectroscopy Secondary Ion Mass) was performed. The differences between planar and textured surface are discussed.*

*Keywords: Crystalline silicon solar cells; Boron emitter; Doping profile; N-type silicon; Texturing.*

## 1. Introduction

In the photovoltaic industry, the most widely used material is crystalline silicon. However, the price thereof occurs approximately 40% of the cost of manufacturing modules. The recovery silicon n-type can reduce the cost and solve the problem of shortage of silicon in the solar cell industry. The c-Si materials market is further diversify, as shown in Figure 1, according to the study carried out by International Technology Roadmap for Photovoltaic (ITRPV) in March 2016[1]. It confirms also the predicted shift from p-type to n-type mono-Silicon and this material will dominate the market share after 2020.

The n-type silicon solar cells are promising alternatives with respect to their p-type counterparts because of higher energy potential conversion efficiencies and a large availability of the raw material [2]. Furthermore, the n-type silicon is known to have several advantages over p-type. First, unlike the p-type substrates, n- type one are less sensitive to most metal impurities present in the substrates of solar grade, and that could be introduced in industrial processes to low-cost mass production [2]. Second instead, Czochralski (Cz) n-type substrates do not suffer degradation of SRH lifetime light-induced because of B-O type defects that are commonly found in industrial Cz p-type silicon [3]. As a result, minority carriers lifetime in n-type substrates are generally higher compared to their p-type counterparts [4].

Increasing the efficiency of solar cells requires a multitude of improvements in the different stage of manufacturing. The emitter is the most important element of n-type solar cell. A more promising technology is the direct thermal diffusion of boron

from a boron trichloride (BCl3) or boron tribromide (BBr3) source.

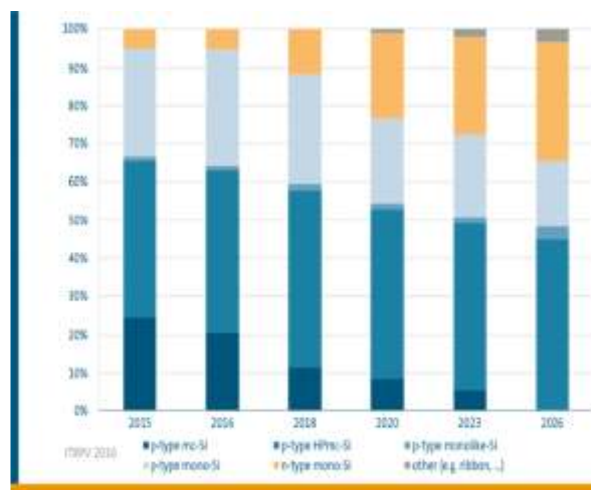


Fig1. Development of different C-Si materials in solar cell fabrication (ITRPV) [1].

Boron doping is a solution extensively investigated today by the scientific community [5, 6]. Boron is also evaluated as a solution to achieve the BSF (Back Surface Field) on the p-type cells [7, 8], but is rarely used commercially because of its long and costly development for this type of application. In literature, boron diffuses mainly through interstitial mechanisms instead of vacancy mechanisms [9]. Theoretical and experimental studies of Bracht [10] and De Salvador [11] proved that the responsible interstitials are $I^0$ and doubly-positive interstitials ($I^{++}$). Since the diffusing species is $BI^0$, they interact with negatively charged substitutional boron ($B_s^-$) and become $BI^0$ by capturing or losing a hole [12].

Process simulation provides an accurate prediction of the resulting doping profiles and provides precious advice in process optimization. In this work, the main motivation is to optimize the emitter, according to the various parameters involved in the diffusion (temperature, time, pressure ...). Using our modeling of boron diffusion, we show that profiles boron can be numerically simulated for planar and textured silicon substrate. The profile measured by the mass of secondary ions Spectroscopy (SIMS) is compared with ones simulated using the Athena Silvaco® Simulator in which several diffusion parameters were modified and used to calibrate boron diffusion simulation. After calibration, the boron profiles on textured samples were obtained by process simulation.

## 2. EXPERIMENT

The Boron diffusion is briefly discussed here. The process of diffusion of boron was performed in an industrial furnace quartz tube and subjected to low pressure about 200-600 mbar. The gases are introduced by means of two different injectors positioned at the rear of the tube. $N_2$ is considered the carrier gas from the dopant source through a bubbler. Oxygen gas $O_2$ is introduced into the diffusion tube to ensure the oxidation of silicon at high temperatures. The diffusion process is achieved in two steps: a pre-deposition step which forms a borosilicate glass (BSG) and a layer in situ drive-in in which boron atoms diffuse deeper in the silicon substrate at highest temperature. In the pre-deposition step, Boron reacts with oxygen and forms a layer of $B_2O_3$ which is located inside the borosilicate Glass (BSG for Boron Silicate Glass). Subsequently $B_2O_3$ reacts with Si and forms $SiO_2$ and boron. The reaction can be written as

$$2B_2O_3 + 3Si \longrightarrow 4B + 3SiO_2 \qquad (1)$$

This reaction can be limited by Si oxidation:

$$Si + O_2 \longrightarrow SiO_2 \qquad (2)$$

The deposition of BSG has similar temperature dependence as the growth of phosphosilicate glass (PSG) [13]. At the involved temperatures, boron

diffuses into silicon matrix forming the p-n junction with the n-type base initially doped at $5e^{15}$ $cm^{-3}$ with a bulk resistivity of 1Ω.cm. All the wafers have a thickness of 200µm.

## 3. SIMULATION APPROACH

Process simulations were carried out to reproduce the 1D boron depth profiles measured on planar sample using TCAD simulator software (SILVACO, the Athena module) [14]. As boron diffuses entirely via the interstitial mechanisms, the vacancy diffusion mechanisms were turned off in the simulations. Both neutral state interstitial $I^0$ and doubly positively charged interstitial $I^{++}$ were considered to contribute to the boron diffusion process similar as the approach taken by De Salvador and al [11]. The boron diffusion profile has a strong impact on the recombination activity in the emitter region via Auger and surface recombination. It is recommended to optimize the boron diffusion profile in order to minimize Auger and surface recombination while maintaining a reasonably low contact resistance. Boron profile optimization is typically achieved by tuning diffusion process. The Figure2 shows the experimental profile of boron doping ($BCl_3$) during the emitter formation in n-type mc-Si obtained by Secondary Ion Mass Spectroscopy SIMS analysis. By considering a tolerable error range, good agreement with the experimental doping profile confirms the validity of the simulation model and the parameters that have been adopted. As expected, the profile presents a relatively high surface concentration for a depth of 0.3µm.

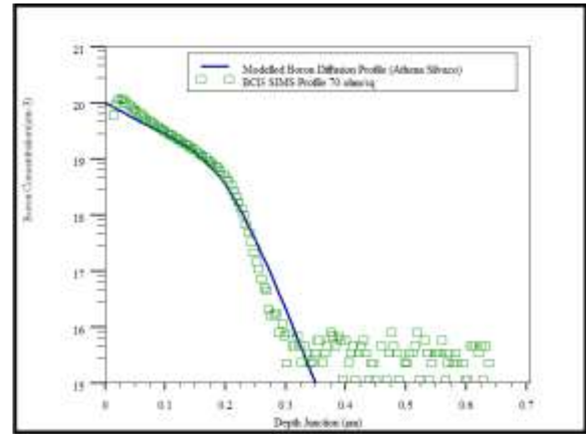

Fig.2. Modelling of the SIMS experimental boron diffusion profile.

## 4. RESULTS

### *4.1. Process simulation on planar samples*

#### *4.1.1 Effect of diffusion temperature*

The temperature variation is the simplest way to obtain different sheet resistance emitters. In figure 2, the variation of boron profile versus temperature is showed for a diffusion constant time. The sheet resistance has been measured by using a four probe method. As the temperature increases, the formed junctions are deeper and the sheet resistance decrease. These results were then compared with experimental data in order to be validated [15]. An increase of deposition temperature shows a strong influence on the boron dopant profile. This behaviour is explained by variation of the diffusion coefficient with temperature. For this reason, the process temperature to achieve the required junction depth has proven to be rather delicate. The advantage of this model is to determine the amount of boron be injected during the process for emitter concentration and desired depth.

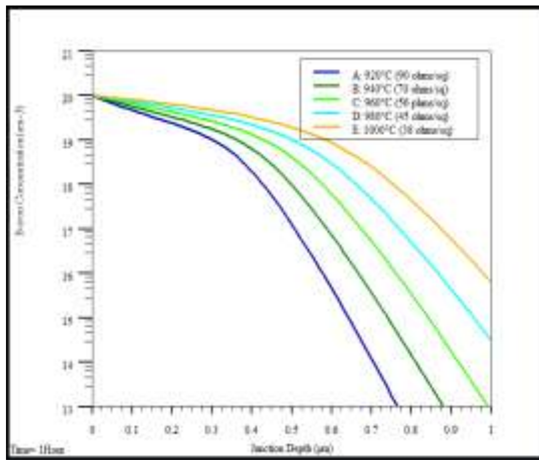

Fig.3. Boron diffusion profiles in silicon obtained with various diffusion temperatures for 1hour diffusion time

#### *4.1.2 Effect of diffusion time*

Time is a very important parameter in the boron diffusion. Penetration of the boron atoms in the silicon controls also the desired junction depth. The time of the drive-in step, permit to give the monitoring of the junction depth. Indeed, BSG introduced in the pre-deposition step, acts as a constant dopant source in a time period at constant temperature. All these results confirm that the diffusion of boron in silicon is strongly affected by tube furnace conditions.

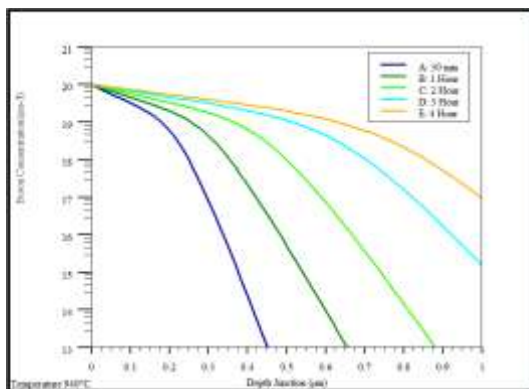

Fig.4. Boron diffusion profiles in silicon obtained with various diffusion times at 940°C.

### *4.2. Process simulation for pyramidal textured samples*

1D boron profile has been successfully reproduced in the numerical simulation of the process. After optimizing the diffusion parameters on a planar surface, we proceeded to simulate 2D boron profiles. Characterization of boron distribution under textured surfaces is a challenging task. For textured surfaces we use the same thermal parameters profiles B and C (Figure.3), both the pre-deposition and drive-in steps contribute to these profiles. The width of the simulated inverted micro-pyramids is 3.5(μm). Figure 5 shows the effect of the temperature diffusion on emitter junction depth. For profile C the junction depth is deeper compared to the one of profile B, the junction depth is 0.4μm and 0.3μm, respectively. The results of simulated 2D boron profile also show that the emitter junction depths differ considerably for the temperature diffusion.

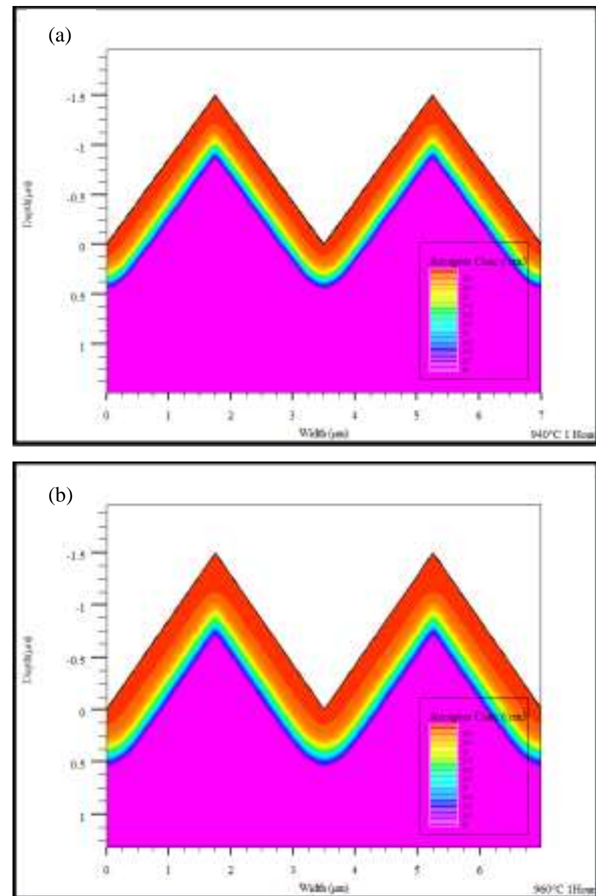


Fig.5. Simulated 2D boron profiles for two profiles: profile B (a) and profile C (b) on pyramidal textured surface.

Boron diffusivity is dependent on temperature, but also on the concentration of silicon self-interstitials [16]. Figure 6 shows the junction depth formed in top and bottom region to pyramid. For both profiles B and C, the junction depth is deeper at the top region of the pyramid than in the bottom region and sidewalls. Because of the pyramids geometry, concentration of silicon self-interstitials is dense in the top regions and is less dense in the bottom. This is a result of the geometry of the pyramids on the textured surface, which causes the unevenness of the emitter region.

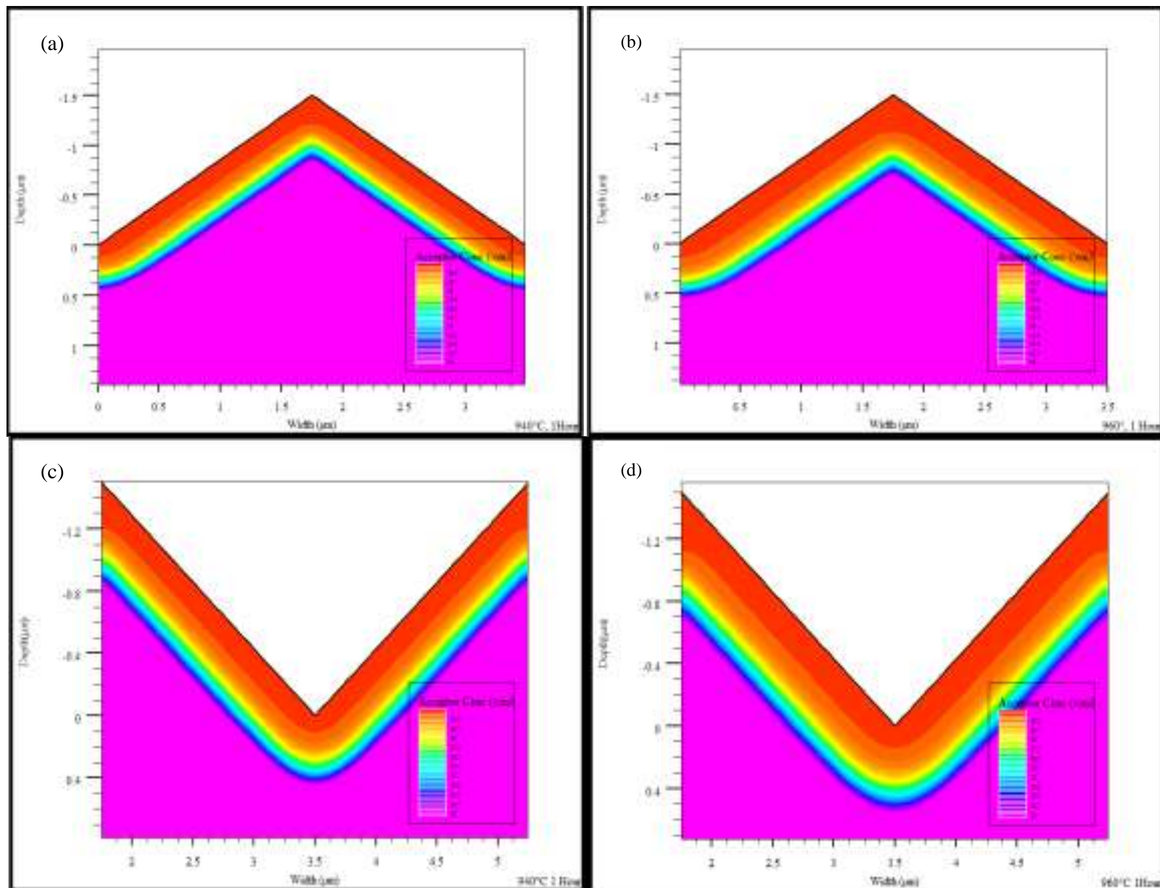


Fig.6. Cross-sectional image of emitter junction from SILVACO, Athena module. Profile B in (a) top pyramid, (c) bottom pyramid. Profile C in (b) top pyramid, (d) bottom pyramid.

## 5. CONCLUSION

For the N-type solar cell with the potential to improve its efficiency and reliability, the boron diffusion mechanism underlying the formation of $p^+$ layers has been studied for planar and textured surfaces. A suitable 2D numerical simulation of the boron diffusion profile for pyramidal textured samples is presented in this work. Simulated 1D depth profiles agree very well with measured profile. We have seen that the temperature and time of diffusion can control the junction depth and quality emitter formed to planar and textured. Our simulation results showed that deeper and shallower junctions were formed near the top and bottom regions in the textured Si surface, respectively. We propose that the nonuniform distribution of Si self-interstitials caused by the geometry of the pyramid texture leads to the enhancement or retardation of B diffusion, which is responsible for the formation of uneveness junction profiles in the p+ emitter of textured Si solar cells

## 6. ACKNOWLEDGEMENTS

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