

Grain Boundary Effect on Efficiency of Polycrystalline Multilayer (SiNx/ P⁺N/SiOx/SiNx/ PECVD SiOx) Solar Cell

Nisrine Benloucif

Department of electronic, Faculty of science and engineering, Constantine, Algeria

Email address:

Nisrine.benloucif@gmail.com

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Abstract: In this work, we are interested to the study of a solar cell based on polycrystalline silicon and its rear and front passivation using different structures, including the multilayered stack silicon oxide / SiNx / PECVD SiOx and silicon nitride for the front layer. We deduced from the study that the choice of (SiO₂/SiNx/SiO₂) rear passivation layer is optimal. We tried subsequently to optimize the optical gap on the basis of a good agreement between the values of fill factor and the efficiency. In addition, we also proposed a front passivation of the emitter by of silicon nitride layer. We have noted a marked improvement in conversion efficiency for high gas flow ratios $R = \Phi(\text{NH}_3) / \Phi(\text{SiH}_4)$. After we have optimized the parameters of emitter and base layers, we have also contributed in the modeling of grain boundary current density in polysilicon. Electrical simulation shows the influence of grain boundaries surface recombination velocity on grain boundaries current density and the efficiency.

Keywords: Polycrystalline Silicon, Silicon Nitride, Solar Cell, Grain Boundary, Efficiency

1. Introduction

Polycrystalline silicon thin films have been studied extensively in recent years for their photovoltaic applications. Polycrystalline silicon remains the most used material in the solar cells technology. Industries of silicon based on solar cells commonly use silicon nitride as top passivation and antireflecting layer. This material is fabricated as thin film in non-stoichiometric form (SiNx) by Plasma Enhanced Chemical Vapour Deposition (PECVD). So, for photovoltaic conversion, the structure model of our solar cell is simply a PN junction with passivated emitter. This material is deposited by LPCVD from a mixture of Dichlorosilane (DCS), SiH₂Cl₂ and NH₃ Ammonia gases at low pressure [1] and temperatures between 700 °C, 900 °C [1].

Thick thermal oxides of more than 100 nm are commonly used for the production of high-efficiency silicon solar cells from mono-and multicrystalline silicon and have led to the highest conversion efficiencies. This performance of oxides is due to the very good surface passivation by the reduction of the density of interface states. One crucial component of the cell to improve the performance is the rear surface due to

the increasing demands on optical (internal reflection) and electrical quality (surface passivation) [2]. Indeed, the internal reflectivity should be as high as possible to enable a good trapping of photons, prolonging their target and making easily their absorption. The electronic quality of a polycrystalline thin films result from its electrical properties in grain boundaries [3]. The development of the single crystalline silicon solar cells requires the reduction of surface recombination velocity at grain boundary.

2. Problem Formulation

The aim of this work is to study systematically and comprehensively the effect of rear passivation of the efficiency. This paper presents an analytical model of the rear passivation effect to improve the photovoltaic parameters of solar cells with Silicon nitride contact on the front surface. The modelling of the PN solar cell will be made by the calculation of the densities of current in the areas of the cell. In the first, the absorption coefficient values can be found in different literatures. In particular, we took Cody's data [4], where the absorption coefficient is given by:

$$\alpha(\lambda) = \begin{cases} \alpha_{Tauc}(\lambda) = \frac{\beta^2}{E} (E - E_g)^2 \text{ For } E_0 \leq E \leq E_{\max}; \lambda_{\min} \leq \lambda \leq \lambda_c \\ \alpha_{Urbach}(\lambda) = \alpha_0 e^{\frac{E - E_0}{E_0}} \text{ For } E_{\min} \leq E \leq E_0; \lambda_c \leq \lambda \leq \lambda_{\max} \end{cases} \quad (1)$$

α_0 , is obtained by the continuity condition between α_{Tauc} and α_{Urbach} when $E = E_0$; ($\lambda = \lambda_c$).
Gives:

$$\alpha_0 = \frac{B^2}{E_0} (E_0 - E_g)^2$$

The electron-hole pair's generation rate at distance x of the illuminated surface of the cell is given by:

$$G(\lambda, x) = \alpha(\lambda) F(\lambda) (1 - r(\lambda)) e^{-\alpha(\lambda)x} \quad (2)$$

Where the reflection index $r(\lambda)$ is the index reflection of the structure with frontal passivation.

The effect of internal reflectivity of the rear layer passivation r_r is presented as:

$$G(\lambda, x) = \alpha(\lambda) F(\lambda) (1 - r(\lambda)) e^{-\alpha x} + \alpha(\lambda) F(\lambda) (1 - r(\lambda)) e^{-\alpha H} r_r e^{\alpha(H-x)} \quad (3)$$

We obtain:

$$G(\lambda, x) = F(\lambda) \alpha(\lambda) (1 - r(\lambda)) e^{-\alpha x} (1 + r_r(\lambda))$$

Knowing that the determination of the distribution of the electric field in these areas is based on the resolution of the Poisson equation:

$$\overrightarrow{\text{div}}(E) = \frac{dE(x)}{dx} = \frac{\rho(x)}{\epsilon} \quad (4)$$

We obtain:

$$E(x) = \begin{cases} E_p(x) = \frac{-ep_i}{\epsilon} (x - x_m) \\ E_i(x) = \frac{-en_i}{\epsilon} (x_{ip} - x_{in}) = \text{constante} \\ E_n(x) = \frac{en_i}{\epsilon} (x - x_{ip}) \end{cases} \quad (5)$$

$E_p(x), E_i(x), E_n(x)$ represent the field in the areas P, N and (I) intrinsic layer.

The current density in the N region is written:

$$J_N(\lambda) = J_N(x, \lambda) \Big|_{x=x_N} = qp\mu_p E_N(x) - qD_p \frac{dp}{dx} \Big|_{x=x_N} \quad (6)$$

Starting from the continuity equation in the N area in

order to calculate the current density in this extrinsic area:

$$\frac{dp}{dt} = G_p - U_p - p\mu_p \frac{dE_N}{dx} - \mu_p E_N \frac{dp}{dx} + D_p \frac{d^2 p}{dx^2} \quad (7)$$

In regime permanent $\frac{dp}{dt} = 0$, we obtain a second-order equation with coefficients depending on x.

The first boundary condition is the continuity of current density at the surface where $x = H$, characterized by the surface recombination velocities S_p [4].

$$S_p \Delta p = -D_p \frac{dp}{dx} \Big|_{x=H}$$

H is the total thickness of the cell.

The second condition is the continuity of the minority carriers' density, obtained as a relaxation of the continuity of pseudo-Fermi levels [4].

The application of this requirement to $x = x_N$ gives: x_N is the beginning of the N area.

$$p = p_0 = \frac{n_i^2}{N_d} \Big|_{x=x_N}$$

n_i^2 : Is the intrinsic concentration.

By using a numerical resolution method of a differential equation of order, 2, with variable coefficients, we get a system of linear equations with tridiagonal matrix. Gauss method is used for a numerical resolution.

The structure is under the grain boundaries current density effect of this region. The current of minority at the grain boundaries is expressed by [5]:

$$J_{gb}(x) = qD_n \frac{\partial(p_n - p_{n_0})}{\partial x} = qS_{gb} (p_n - p_{n_0}) \quad (8)$$

Where S_{gb} is the recombination velocity at grain boundaries.

At the emitter region, we have indeed the boundary condition imposed by the continuity of the current density given by:

$$S_{gb} \Delta p = D_p \frac{dp}{dx} \Big|_{x=\pm d}$$

Where d is the limit of the space charge region around the grain boundary.

In our work we assume the presence of the grain boundary at $x = x_n$ of the base region so we can write:

$$J_{gb} = qS_{gb} \left(\frac{n_i^2}{Nd} - p_k \right) \quad (9)$$

Where $\frac{n_i^2}{Nd}$ is the concentration of minority carriers at the point $x = x_n$ in the N region of the cell.

Knowing that n_i^2 / N_d and p_N is the $y(x)$ solution of carrier mobility at x_{N+1} and x_n abscises in N region.

The behavior of grain boundaries under illumination is explained by the fact that the interface states adjust their load by hall capture (N), and this reduces the potential at the grain boundary. From the expression of minority concentration $p(d)$ at the grain boundaries [3]:

$$p(d) = p_0 \exp \frac{q\phi_b}{kT}$$

We obtain:

$$J_{gb} = qS_{gb}p_0 \left(\exp \frac{q\phi_b}{kT} - 1 \right) \quad (10)$$

This last expression allows us to estimate the value of the height barrier at the grain boundary, knowing the value J_{gb} .

Finally, the expression of total current generated in the cell, taking into account the influence of the grain boundaries in the emitter and in the base will be written as:

$$J_{ph\ total} = J_{ph} - (J_{gbe} + J_{gbb})$$

$$J_{ph\ total} = J_{ph} - J_{gb} \quad (11)$$

The real output characteristic (current - voltage) is given by:

$$J = J_{ph} - J_s \left(e^{\frac{V+R_s J}{R_{sh} J_s}} - 1 \right) - \frac{V + R_s J}{R_{sh}} \quad (12)$$

R_s : Series resistance, R_{sh} : Shunt resistance

J_s : Saturation current density.

3. Results and Discussions

In this paper we will study the electrical characteristics of the cell with the rear passivation layer, trying to optimize the physical parameters in order to obtain the best performance. After obtained this optimization, the study will be completed by the influence of a front passivation layer on the efficiency of solar cell. The aim of this work is the evaluation of recombination current density grain boundaries effect on the output characteristics of this polycrystalline solar cell structure.

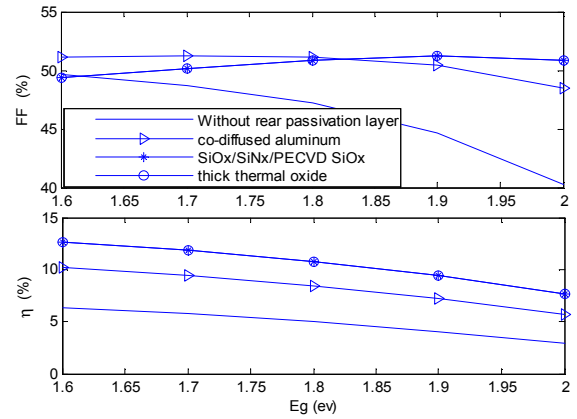


Fig.1. Fill Factor and efficiency variation with optical gap under the rear passivation layers effect

Figure (1) illustrates the evolution of the fill factor depending on the gap energy. The variation of fill factor of the cell under the influence of the back passivation versus gap energy, allowed us to see that from the gap value of 1.8 eV, the variation of fill factor follows the variation of the efficiency, showing that a better effect of rear passivation is for SiO₂ and SiO_x / SiN_x / SiO_x layers, fill factor values reaches 52%, this result is confirmed by the literature [6]. We can deduce that the value of 1.8 eV of the gap should be optimal.

The conversion efficiency was evaluated at 9.70 % using co-diffused aluminium, BSF structure ($r=0.5\%$, $Sp=1800\text{cm/s}$), increase until to reach 10.46 % for the best system of thermal oxide [2] with ($r=0.9\%$, $Sp=200\text{cm/s}$). The optimum efficiency is obtained by using thin oxide/silicon nitride/SiO_xPECVD ($r=0.9\%$, $Sp=300\text{ cm/s}$). The last results show that the internal reflectivity should be as high as possible to obtain a good efficiency in co-operation with well passivated surface properties [2]. Figure (2) shows the different output characteristics of the cell, the short circuit current J_{sc} , the open circuit voltage V_{oc} , the form factor FF, and efficiency η as a function of the thickness w_n of base region, using as variable doping parameter N_d .

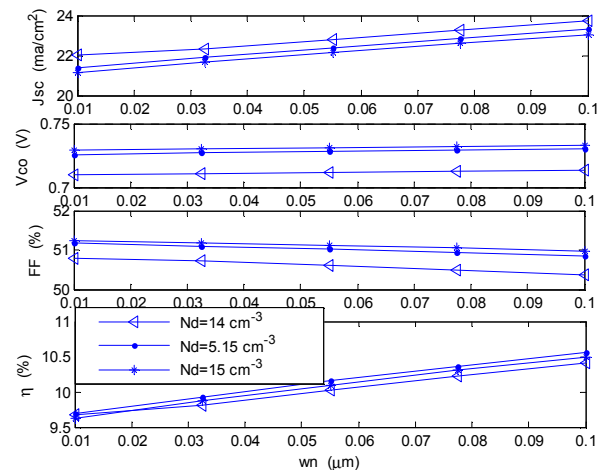


Fig.2. Output characteristics versus doping and thickness of the base area

This figure clearly indicates an increase in short circuit current with the enlargement of the base thickness from 0.01 microns to 0.1 microns. The open circuit voltage is almost constant over this range thickness, while fill factor decrease. The efficiency follows the short-circuit current variation, showing a marked increase. This result indicates that the optimum thickness of the base region should be the widest possible. The variation of efficiency versus doping shows clearly that the base area doping should be as low as possible. The conversion efficiency reaches its maximum for a very thin thicknesses of the emitter ($W_p=0.01 \mu m$). This is not inconsistent with the literature, or the P emitter layer should be as thin as possible [7]. Our simulation results permit us the optimization of the doping concentration of polycrystalline emitter at 10^{19} cm^{-3} (Fig.3), giving an optimum efficiency 10.57%.

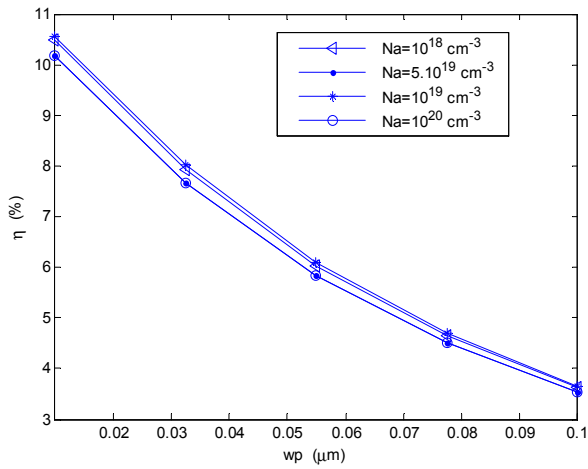


Fig.3. Efficiency versus doping and thickness of emitter

In this study we present silicon nitride gas flow ratio $\Phi (\text{NH}_3) / \Phi (\text{SiH}_4)$ influence on the efficiency. In this application, silicon nitride films front passivation layers are considered to be more ideally suited.

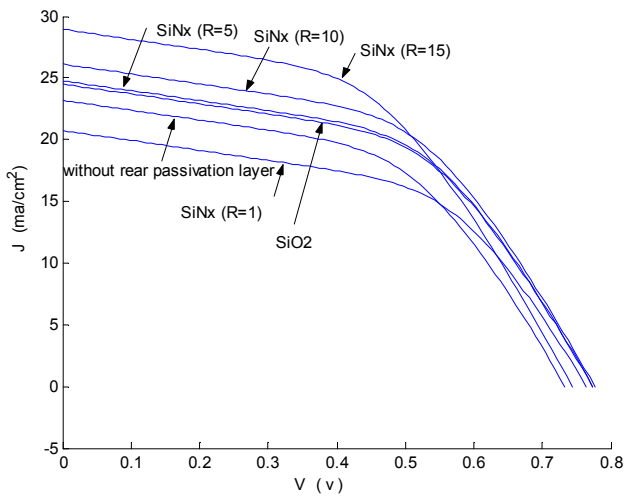


Fig.4. Front passivation effect on characteristic (current-voltage) of the cell

The conversion efficiency is estimated at 11.91% with the use of silicon oxide. Increase with silicon nitride and this is for high flow gas ratio. It ranges from 12.02% for $R = 5$ until reaching 12.88% for $R = 15$. This is in good agreement with the literature [8].

In this work, we will calculate the grain boundaries current density in the emitter heavily doped 10^{19} cm^{-3} and this is carried out for different surface recombination velocity at grain boundaries [3].

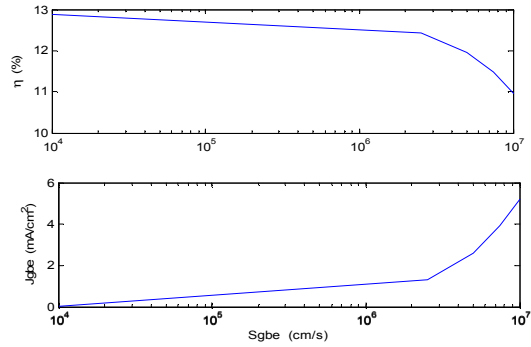


Fig.5. Current density at grain boundaries and efficiency variation versus emitter grain boundaries surface recombination velocity

Figure 5 illustrates current density at grain boundaries and conversion efficiency variation with grain boundaries surface recombination velocity in the emitter. The evolution of current density at grain boundaries with the increasing of recombination velocity at the grain boundaries is remarkable. The conversion efficiency reaches a minimum value of 10.95% at a surface recombination velocity of about $10^7 \text{ cm} / \text{s}$.

However, the optimal value of the recombination velocity at the grain boundaries ($10^4 \text{ cm} / \text{s}$) gives the optimum performance 12.88%.

In order to understand the phenomenon of conduction through the grain boundary, we will study the grain boundaries surface recombination velocity in the base region slightly doped influence on the conversion efficiency. We are going to put evidently the relation between the surface recombination velocity and the efficiency. Figure 6 shows clearly that the reduce of the grain boundaries surface recombination velocity decreases the current density at grain boundaries and increases the performance of the cell.

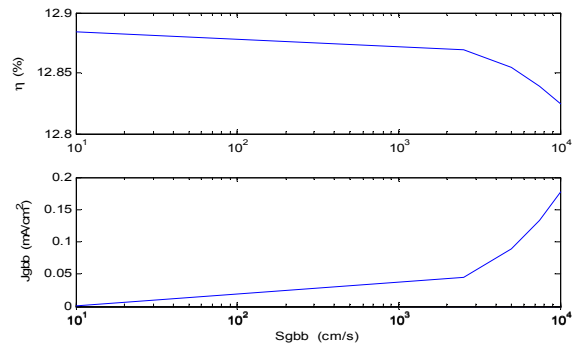


Fig.6. Current density at grain boundaries and efficiency variation versus base grain boundaries surface recombination velocity

4. Conclusion

In this study, we were interested to the rear passivation system, particularly (thin oxide / SiN_x / PECVD-SiO_x) structure. This paper presents a simulation of the characteristics of the polycrystalline silicon real solar cell. The variation in the conversion efficiency as a function of gap energy presents its maximum at $E_g=1.8$ eV. The effect of the rear passivation is studied we have seen an improvement in the efficiency, the optimum efficiency is obtained using thin oxide/ silicon nitride/ silicon oxide PECVD as rear passivation structure. After that, we have optimized the parameters of the base area slightly doped and the passivated emitter layer, heavily doped. The silicon nitride thin-layer has proven its effectiveness for passivation defects. We found that the gas ratio $\Phi(\text{NH}_3) / \Phi(\text{SiH}_4)$ precisely control the conversion efficiency. This last increases with high ratio ($R=10$), we obtain 12.88% for $R = 15$.

In this paper, we have shown that the performances of polycrystalline solar cell are closely related to the current density at grain boundaries. The calculation of the grain boundaries current density allowed us to achieve the following results:

The reduce of the grain boundaries surface recombination velocity increases the performance of the cell.

An optimum emitter grain boundary surface recombination velocity value 10^4 cm/s. In the base, the optimum surface recombination velocity is found to 10 cm / s.

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