Simulations of Implantation Temperature Impact on Three-dimensional Texturing in Silicon Solar Cells

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**Abstract:** Recently new advance texturing is one of the candidates for enhancing optical absorption in mono-crystalline thin film solar cells and making low cost solar cell. Silicon has relatively large reflection in UV-Visible spectral region, also absorbs strongly in this region; however, its near IR absorption is weak. The absorption enhancement can occur through diffractive scattering from surface with feature dimension larger than \(\lambda/n\), where \(n\) is silicon refractive index. For surface feature with size smaller than \(\lambda/n\), surface is behaving like a gradient index film. By creating three-dimensional surface with sub wavelength textures on front and sidewalls, it may be possible to enhance absorption beyond the \(4n^2\) statistical limit. There is an idea that says implantation process during fabrication process affect solar cell efficiency because of p-n junction dependence to temperature. This maybe complicated the efficiency prediction. Since, because of difficulty of laboratory test and fabrication the simulation of implantation temperature method is considered for a well known three dimensional texturing at first. Simulations in first step are done for an ideal three dimensional surface texturing with 21\(\mu\)m depth and an ideal p-n junction below 1\(\mu\)m under frontal surface. In this simulation the p-n junction has a constant depth all over the solar cell. Then by using implantation modeling tries to predict the p-n junction place by varying the temperature all over the surface. It is shown that the p-n junction position and its shape completely depend on the temperature that causes a variety of efficiency for a well known advanced texture. In this case the p-n junction shows a discontinuity at 700 \(^\circ\)C that case an efficiency drop for 21% to 10%. These simulations confirm the impact of implantation temperature on optical simulation. Results are shown to find out the best design for advance three-dimensional texturing need to predict discontinuity temperature in fabrication process. Simulations also show the dependence of efficiency with geometrical surface features and how discontinuity temperature change by shape and size of the periodic texture pattern. Results show there is a limitation in final performance of mono-crystalline solar cell with periodic texture pattern.

**Keywords:** Renewable energy, solar cells, thin film, surface texturing.

**Nomenclature**

- \(d\) grating period .......................... \(\mu\)m
- \(n\) refractive index ..............................
- \(\lambda\) wavelength ................................. nm
- \(\theta_c\) critical angle ..............................
- \(\theta_{n,i}\) diffraction order angle ..............
- \(\Phi\) ion dose per square centimeter ...........
- \(\eta_{i,j}\) coupling efficiency ...............
- \(R_p\) projected range ......................... cm

**1. Introduction**

Silicon has relatively high reflectance in UV-Visible spectral region, however it also absorbs strongly in this region [1]. In near IR (800-1100 nm) spectral region, particularly near the band edge, absorption is weak, i.e., absorption depth is \(~100\ \mu\)m at \(\lambda\sim1\ \mu\)m. This weak absorption fundamentally limits the efficiency of Si solar cells: in thin films due to incomplete optical absorption, and in thick films due to bulk recombination losses. Light trapping schemes based on geometrical optics considerations have been extensively investigated in conventional [2]. Maskless, random, pyramidal texturing with feature sizes \(>>\lambda\) on the front surface not only helps randomize scattering within the substrate, but also takes advantage of
the high refractive index of Si leading to total internal reflection of light rays outside the narrow cone defined by the critical angle \( \theta_c = \sin^{-1}(1/n) \).

In reducing reflection using sub-wavelength structures, defined either by lithography or random masking methods, light incident on the Si substrates generates no diffraction orders, and preferably only obliquely propagating orders inside the Si substrate [3-5]. For lithographically-defined surface, the period is chosen such that there are no diffraction orders in air, i.e., \( \lambda/d > 1 \). Inside the semiconductor, first and second diffraction orders are propagating due to its higher refractive index \( n \), i.e., \( 2 \times \lambda/(n \times d) < 1 \). For the case of a randomly textured surface, incident light will support a large number of diffraction orders since it is a composite of several periodic structures[6]. The total optical path length neglecting back surface reflection for sake of simplicity is give by

\[
\text{optical \ - \ path \ - \ length} = \sum_{i,j} \eta_{i,j} T_{i,j},
\]

where the summation index \( i \) corresponds to grating period \( d_i \) of the random surface, and the summation index \( j \) corresponds to diffraction orders of the period \( d_i \), and \( \eta_{i,j} \) represents the coupling efficiency of the transmitted intensity \( T_{i,j} \). The optical paths of each of the diffraction order is enhanced by \( 1/\cos(\theta_{m,i}) \), where \( \theta_{m,i} \) is the diffraction order angle with surface normal defined earlier. In this manner, frequency space inside the Si substrate can be effectively populated. Finally, for the third case, where features are smaller than the wavelength inside Si, no diffraction orders are propagate inside the Si substrate, which is similar to a gradient-index anti-reflection film, and is not conductive to enhanced solar cell performance.

In case of three-dimensional texturing, the trench sidewalls are also randomly textured with sub-wavelength features as described in Fig. 1.d. In such a case, each transmitted diffraction order on incidence at sidewalls, generates multiple beams, therefore, creating several more light paths than would have existed within textured/planar sheet [7]. Such an approach can potentially exceed \( 4n^2 \) optical enhancement limit predicted by Yablonovitch [8].

![Fig. 1. Grating texture with (a) one dimension repetition (b) two dimension repetition (c) three dimension repetition. One dimension and two dimension use for solar cell application.](image)

2. Mathematical implantation models

2.1. Gaussian Implant Model

There are several ways to construct 1D profile. The simplest way is using the Gaussian
distribution, which is specified by:

\[ C(x) = \frac{\phi}{\sqrt{2\pi}\Delta R_p} \exp\left(-\frac{(x - R_p)^2}{2\Delta R_p^2}\right) \]  \hspace{1cm} (1)

where \( \Phi \) is the ion dose per square centimeter specified by the dose parameter. \( R_p \) is the projected range. \( \Delta R_p \) is the projected range straggling or standard deviation.

### 2.2. Pearson Implant Model

Generally, the Gaussian distribution is inadequate because real profiles are asymmetrical in most cases. The simplest and most widely approved method for calculation of asymmetrical ion-implantation profiles is the Pearson distribution. The Pearson function refers to a family of distribution curves that result as a consequence of solving the following differential equation:

\[ \frac{df(x)}{dx} = \frac{(x - a)f(x)}{b_0 + b_1x + b_2x^2} \]  \hspace{1cm} (2)

in which \( f(x) \) is the frequency function. The constants \( a, b0, b1 \) and \( b2 \) are related to the moments of \( f(x) \) by:

\[ a = -\frac{\Delta R_p\gamma(\beta + 3)}{A} \]  \hspace{1cm} (3)

\[ b_0 = -\frac{\Delta R_p^2(4\beta - 3\gamma^2)}{A} \]  \hspace{1cm} (4)

\[ b_1 = a \]  \hspace{1cm} (5)

\[ b_2 = -\frac{2\beta - \gamma^2 - 6}{A} \]  \hspace{1cm} (6)

where \( A = 10\beta - 12\gamma^2 - 18 \); \( \gamma \) and \( \beta \) are the skew-ness and kurtosis respectively.

### 2.3. Dual Pearson Model

To extend the applicability of the analytical approach toward profiles heavily affected by channeling, the dual (or Double) Pearson was suggested method. With this method, the implant concentration is calculated as a linear combination of two Pearson functions:

\[ C(x) = \Phi_1f_1(x) + \Phi_2f_2(x) \]  \hspace{1cm} (7)

where the dose is represented by each Pearson function \( f1, f2(x) \). \( f1(x) \) and \( f2(x) \) are both normalized, each with its own set of moments. The first Pearson function represents the random scattering part (around the peak of the profile) and the second function represents the channeling tail region. Equation (7) can be restated as:
\[ C(x) = \Phi \left[ \mathcal{R} f_1(x) + (1 - \mathcal{R}) f_2(x) \right] \]  

(8)

where \( \Phi = \Phi_1 + \Phi_2 \) is the total implantation dose and \( \mathcal{R} = \frac{\Phi_1}{\Phi} \).

3. Simulation

Changing the period and depth of groove would affect efficiency. The goal is to find the best design with maximum efficiency. In modeling, physically-based process simulation predicts the structures that result from specified process sequences. In a complete simulation usually we need doing three stages; 1- process simulation 2- device simulation and 3- circuit simulation. SILVACO International provides an opto-electronic software product that models the behavior of semiconductor materials, devices, and circuits using finite element techniques. In fact it is “Virtual Wafer Fab” which can determine electrical characteristics of that device based conditions are inputted. There are different models that must take into account based on; drift and diffusion current, position dependent doping, optical carrier generation, and so on. The most important tools for solar cell simulation are ATLAS, ATHENA and Luminous which have been recently used [7]. Fig.2. shows typical solar cell simulations to find implantation impact on texturing effect.

By using etching process in different time it is possible to make rectangular texture in various depths and periods. In this investigation we consider phosphorous atom to implantation on a p-type Si substrate which heat up to 900K. By using Dual Pearson model we find there are some discontinuities in p-n junction which it appears in deep groove. Fig. 3 shows simulation results in some period and depths.

![Simulation of solar cell by using SILVACO software’s, 1D grating structure with 10-µm period and 3-µm depth](image)

Fig. 2 Simulation of solar cell by using SILVACO software’s, 1D grating structure with 10-µm period and 3-µm depth

4. Results

Table (1) and its related graphs (Fig. 4) shows output efficiency for different rectangular 2-D texturing. In all of those cases the temperature and time of doping consider constant with
700K and 30 minute respectively. The data shown in actual fabrication there is another limitation for efficiency boosting by implantation process. It is found out beside optimization of grove depth and period according to optical absorption by using wave optics, p-n junction discontinuity due to fabrication process might be considered as another parameter.

Table 1. Modeling results for solar cell efficiency due to variation in period and depth groove in 3D texturing

<table>
<thead>
<tr>
<th>Depth (µm)</th>
<th>η(%) period 5 (µm)</th>
<th>η(%) period 10 (µm)</th>
<th>η(%) period 20 (µm)</th>
</tr>
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<tbody>
<tr>
<td>50</td>
<td>0.76</td>
<td>6.17</td>
<td>9.4</td>
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<tr>
<td>40</td>
<td>1.24</td>
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</tr>
<tr>
<td>5</td>
<td>9.6</td>
<td>9.5</td>
<td>9.53</td>
</tr>
</tbody>
</table>

Fig. 3 Simulation of solar cell by using SILVACO software’s, (a) 2D grating structure with 20-µm period and 10-µm depth, and (b) 2D grating structure with 20-µm period and 40-µm depth. The discontinuity happened for the last at 20-µm.

5. Conclusion

Although rectangular grating on solar cell increase the efficiency but implantation impact during fabrication could affect on efficiency boosting. P-N junction discontinuing make a lost in thin monocrystalline solar cell. Simulation shows maximum relative efficiency is in the period range of 10-15 micrometer and 10-20 groove depth for phosphorus doping with 900K in 30 minutes. This result helps to design optimum configuration for solar cell texturing. It is shown that the p-n junction position and its shape completely depend on the temperatures that cause a variety of efficiency for a well known advanced texture. In this case the p-n junction shows a discontinuity at 700 ºC that case an efficiency drop for 21% to 10% (figure 4).
Fig. 4. Implantation period impact on solar cell efficiency. (a) Maximum relative efficiency was happened in 10-15 micrometer period. (b) Maximum relative efficiency was happened in 10-20 micrometer groove depth

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References


