Light Trapping in Thin Film Polycrystalline Silicon Solar Cell using Diffractive Gratings

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Abstract

We report on an investigation of a periodic diffractive Si grating structure used to enhance the absorption in thin film Si cells with an active layer 2 μm by modelling. The media of the grating can be air (n=1.0) with detached back reflector or coated with a layer of dielectric material, SiO₂ (n=1.4) as a buffering layer. Gratings with periods of 500, 800 and 1200 nm were located on the rear side of the cell, with depths from 150 nm to 300 nm. The reason to use a shallow grating depth is to ensure smallest material loss. The influence of the grating period, depth and surrounding media on the short circuit was investigated and the optimal grating parameters were obtained. A structure which has a 500 nm period, 150 nm depth, in air media gives the best light trapping, with 76.5% enhancement of short current density (Jsc).

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Selection and peer-review under responsibility of Solar Energy Research Institute of Singapore (SERIS) – National University of Singapore (NUS). The PV Asia Pacific Conference 2012 was jointly organised by SERIS and the Asian Photovoltaic Industry Association (APVIA)

Keywords: Diffraction; silicon thin-film solar cells; light-trapping; gratings

1. Introduction

Thin film solar cells are promising candidates for future generations of photovoltaics because they offer cost effectiveness and possibility of deposition on flexible substrates. However, reduced film thickness also leads to weaker absorption which fundamentally limits the performance of thin film Si solar cells. Therefore, effective light trapping over the sun spectrum is essential for efficient thin film
solar cells with an active silicon layer in the micrometer range of ~1-20μm [1-2]. The basic principle of light trapping is to prevent light that has entered the solar cell from leaving it again and thus increasing the probability of it being absorbed. These can be realised by two effects simultaneously, including 1) diffraction or scattering by surface textures which can change the direction of the incident light in such a way that as much of it as possible travels at higher angles and longer pass length within the cells and 2) coupling the incident light with the guided mode in the active solar cell which can effectively confine the light within cells. Numerous schemes and structures have been developed to achieve the light trapping, such as random or periodic pyramids [3, 4], gratings [5-7], plasmonic nanoparticles [8-10], thin silicon on insulator (SOI) waveguides [11], and photonic crystals [12-14]. Among of them, diffractive gratings exhibit great potential in this application because the use of gratings either to diffract the light at higher angles to travel in the material or to couple the light in the form of a guided wave [15-16]. The choice of the grating period with respect to the wavelengths allows selecting diffraction or guided wave configurations.

Diffractive gratings for an application in thin film solar cells were first suggested by Ping Sheng et al. as early as 1983 [17]. Recently, different gratings materials have been used, such as metallic gratings [18], which have the tendency to increase parasitic optical absorption loss due to the metal. In this paper, we investigate Si binary gratings located on the rear surface of thin polycrystalline silicon solar cells. Comparing with the front side located gratings, positioning the gratings on the rear surface can avoid the unwanted loss for short wavelength because the light with short wavelength can be completely absorbed before it is diffracted by the grating. One of the advantages of using Si gratings is that the high refractive index of Si can results in strong diffraction effect with a shallow grating modulation length. Secondly, the light absorbed in the grating pillar can directly contribute to the overall cell light absorption. An optimised grating will diffract as much light as possible into higher angle directions, namely high diffraction efficiency in higher diffracted orders. If the light is incident from the substrate side, the grating should also possess higher refracted diffraction ($R_m$) than the transmitted diffraction ($T_m$, m is the diffraction order) because the refracted light is directly diffracted back to the Si but the transmitted light may suffer loss due to the absorption of the back reflector before it reaches the Si layer again.

The grating parameters are of great importance in determining grating performance. The period $p$ controls the spectral position of the different orders of diffractions and controls the pass length of light. The refractive index of the surrounding media $n$ can affect both diffracted angles and the efficiency. A more profound discussion of these grating parameters is found in [19]. In this paper, we use a FDTD simulation method to optimise the gratings parameters to maximise the cell performance. We closely investigate the effect of grating period, depth and refractive index of the surrounding dielectric media on the light absorption and therefore the Jsc enhancement. The power profile was captured to understand the phenomenon of light tapping due to the diffraction.

2. Simulation

A finite difference time domain (FDTD) method was used to analyse the wave propagation in solar cells. FDTD numerically solve the differential form of Maxwell’s equations, so that complex device designs can be modelled and optimised device parameters can be obtained. Figure 1 shows the sketch of the investigated solar cell configuration with a layer of Si layer on the rear surface of the bulk active layer and the basic parameters relevant for the simulations. The solar cell has a flat front surface covered with an antireflection coating of 100nm SiNx. The solar cell itself consists of a 2 μm layer of silicon bulk
material which is etched down with certain depth to form the diffractive gratings. The grating is characterised by its period $p$, width $w$ and its modulation depth $d$. These parameters play a central role in optimising the performance of the gratings. At the rear side of the structure, a back reflector (150 nm Ag, in this simulation) is situated 250 nm away from the grating surface. The gap between the back reflector and the grating is either air or a layer of SiO$_2$ which can be used a buffer layer as well. A normally incident source was used to illuminate through the glass substrate side, with a spectral region 300-1000 nm. The arrows represent a schematic light path in the cell. Different colours show the diffraction or reflection at different interfaces. The labels $R_0$, $R_{-1}$, $R_{+1}$ and $T_0$, $T_{-1}$ and $T_{+1}$ are the $0^{th}$ (specular) and $1^{st}$ refraction orders and transmitted orders, respectively. The simulated grating parameters are shown in Table 1.

![Schematic diagram of the solar cell configuration](image)

Fig. 1. Sketch of the investigated solar cell configuration with a layer of Si layer on the rear surface of the bulk active layer and the basic parameters relevant for the simulations. The arrows represent a schematic light path in the cell. Different colours show the diffraction or reflection at different interfaces. The labels $R_0$, $R_{-1}$, $R_{+1}$ and $T_0$, $T_{-1}$ and $T_{+1}$ are the $0^{th}$ (specular) and $1^{st}$ refraction orders and transmitted orders, respectively.

Table 1. Simulated grating parameters

<table>
<thead>
<tr>
<th>Period p nm</th>
<th>Depth d nm</th>
<th>Media refractive index n</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>500</td>
<td>150</td>
</tr>
<tr>
<td>2</td>
<td>800</td>
<td>200</td>
</tr>
<tr>
<td>3</td>
<td>1200</td>
<td>300</td>
</tr>
</tbody>
</table>

Simulations were performed for the square array of the gratings by applying periodic boundary conditions. We also ran a reference simulation for a plain Si solar cell and the results are used as a reference to investigate the influence of the gratings on the optical properties of thin film Si cell. The power absorbed in Si ($P_{ab}$) is calculated based on the two monitors positioned on top of Si grating surface ($M_t$) and bottom of the bulk Si layer ($M_b$):

$$P_{ab}(\lambda) = 100\% \times \text{Power}(M_t) - \text{Power}(M_b)$$  \hspace{1cm} (1)

Based on the $P_{ab}$, we could further calculate the quantum efficiency of a solar cell, $QE(\lambda)$ is defined by

$$QE(\lambda) = \frac{P_{ab}(\lambda)}{P_{in}(\lambda)}$$  \hspace{1cm} (2)
where $P_{\text{in}}(\lambda)$ is the incident light. Using the quantum efficiency and with the assumption that all electron-hole pair contributes to photocurrent, the most of important characteristic to define the cell performance, the short circuit current density $J_{\text{sc}}$ is given by

$$J_{\text{sc}} = e \int \frac{\hat{A}}{hc} QE(\lambda) I_{\text{AM1.5}} d\lambda$$

Constant $c$ is the speed of light in the free space and $I_{\text{AM1.5}}$ is AM 1.5 solar spectrums. The optimised grating designs were obtained to maximise the short circuit current.

3. Results and discussion

3.1. Absorption enhancement due to gratings

Figure 2a shows the schematic cross section of a plain silicon thin film solar cell set up in the simulation. This structure is consistent with the standard polycrystalline silicon thin film solar cell process developed by the SPREE, UNSW. Figures 2b and c shows the power profile within the structure at a wavelength of 400 and 700 nm. It can be seen that light with a short wavelength (400 nm) is absorbed within the first few hundreds of nanometers of the solar cell, since the silicon exhibits a high absorption coefficient for shorter wavelengths. However, for light with a longer wavelength (>700 nm), it can propagate through the silicon layer and this part of light cannot contribute to the $J_{\text{sc}}$ of the cell without any additional structure help. From Fig. 2c we can also see that, for a plain cell, the power absorption in the silicon layer is dominated by the constructive and destructive interferences of the forward and backward propagating waves and therefore, a clear fringe pattern can be observed.

![Figure 2a](image)

(a) The schematic cross section of a plain silicon thin film solar cell; (b) and (c) corresponding simulated power profile at the wavelength of 400 and 700 nm respectively.

Figure 3a shows the cross-section of a unit cell of the grating structured Si cell and Figs. 3b-c shows the simulated power profile for an incident wavelength of 700 nm with grating modulation depths of 150 and 200 nm. The grating period is 500 nm. By comparing the power profiles with Fig. 2c, it can be seen that most of the power is effectively trapped within the Si layer and the light pass through the cell is significantly reduced and therefore, the power absorbed in the silicon layer is increased for both grating depths. The perfect fringe pattern in the plain cell was disturbed due to the scattering and diffraction introduced by the gratings. These two factors contribute to the enhancement of the effective path length of light inside the silicon layer and a consequence, the absorption is increased. From both Figs. 3b and 3c we see with a modulation depth 150 nm, the light intensity trapped in the Si layer is higher than that of the depth 200 nm.
The influence of the grating structure on the absorption for different wavelengths was studied by calculating the power absorbed in the active layer based on Eq. 3. Figure 4 shows the calculated absorbed power as a function of the wavelength with active Si layer: plain cell, cell with a grating structure with a height of 150 nm and periods of 500 nm and 1200 nm. From this figure, it shows that the introduction of a grating leads an increase in the absorption at a wavelength larger than 500 nm and the influence of the gratings becomes more significant as wavelength increases. Additionally, we see that, for a small period of 500 nm, a significant increase and more sharp peaks are observed, whereas for 1200 nm, the absorption enhancement is reduced which means the diffraction effect is much weaker.

3.2. Influence of grating parameters

In order to find out the influence of the grating parameters on the cell performance, we calculate the short circuit current for wavelengths from 400 to 1000 nm using Eq. 5. Figure 5 shows the short circuit as a function of the period for different depths in air media. With increasing period, a drop of the short circuit current can be observed for both depths. The observation can be explained by using the grating equations [20]:

\[ \sin \theta = \frac{n \lambda}{d} \]

where n is the refractive index of the medium, \( \lambda \) is the wavelength of the light, and d is the period of the grating.
\[ p n \sin (\theta_m) = m \lambda \] (4)

Where \( n \) denotes the refractive index of the propagating media after diffraction, in our case, it can be air or \( \text{SiO}_2 \); \( m \) specifies the diffraction order and \( \theta_m \) being the diffraction. As the period increases, the diffraction angle for an integrated grating is reduced. Consequently, the effective thickness of the solar cell is reduced which reduce the absorption enhancement and therefore the \( J_{sc} \) in the cell. The grating depth controls the diffraction efficiencies of each order.

![Figure 5](image1.png)

Fig. 5. Comparison of short circuit current for structured cell as a function of the period for different depth

![Figure 6](image2.png)

Fig. 6. Comparison of short circuit current for cell with (a) a grating period 500 nm and (b) 1200 nm with different grating depth in air and \( \text{SiO}_2 \) media

Figure 6 shows the short circuit current for a grating period 500 and 1200 nm with different grating depths in air and \( \text{SiO}_2 \) (\( n=1.4 \)) medium. This figure can tell how depth and the surrounding medium affect the \( J_{sc} \) together. Similar trend was observed for both periods. With a shallow depth, \( J_{sc} \) is higher in air than in \( \text{SiO}_2 \) media. As the depth increases, this trend goes to the opposite direction. For 300 nm depth, \( J_{sc} \) with a \( \text{SiO}_2 \) media is slightly higher than that of air media. Cathopole and Green [21] reported that for solar cells with periodic gratings, the power absorbed is maximised, if the phase shift of the grating modes is equal to 180 or its odd multiples. The phase shift of a grating is defined as

\[ \Delta \varphi = \frac{2 \pi d \Delta n}{\lambda} \] (5)
Where $\Delta n$ is the refractive index difference between grating material and the surrounding medium and $\lambda$ is the incident wavelength. From Eq. 2, we can see that the depth and refractive index of the media works together in determining a certain phase shift and therefore the power absorption in silicon. The highest Jsc 38.83 mA/cm$^2$ was achieved for a depth 150 nm in air media, which is enhanced by 76.5% comparing with the plain cell 22 mA/cm$^2$.

4. Conclusions

In summary, we have demonstrated by FDTD simulations that high absorption and therefore Jsc enhancement can be achieved with a shallow grating layer on the rear surface of thin film Si solar cell. These gratings allow the higher diffraction orders reflect back to the silicon. The diffraction efficiency and the diffracted angle which ultimately affect the Jsc enhancement depend on the modulation depth, surrounding media and the grating period. The period of the diffraction grating should be small, so that the light is diffracted at larger diffraction angles. However, if the grating period is too small, high orders diffraction modes cannot propagate. The short circuit current is maximised as a grating period of 500 nm and a grating depth 150 nm in air media. The total Jsc is increased from 22 to 38.8 mA/cm$^2$, which gives an enhancement of 76.5%.

Acknowledgements

J R acknowledges the receipt at of a Vice-Chancellor research fellowship, University of New South Wales.

References


