DOUBLE LAYER ANTI-REFLECTIVE COATINGS FOR SILICON SOLAR CELLS

Daniel N. Wright, Erik S. Marstein and Arve Holt

Section for Renewable Energy, Institute for Energy Technology, P.O.Box 40 Kjeller, NO-2027, NORWAY

ABSTRACT

In this paper simulated single and double layer anti-reflective coatings based on the refractive index limits of silicon nitride (SiN) and silicon oxide (SiO2) are presented. The best structure combines SiN and SiO2, resulting in a reflectance of 0.044 based on the AM1.5 photon flux from 300-1150nm. PC1D solar cell simulations show that an increase in short circuit current density of 6.4% was possible by replacing an optimised single SiN layer with the abovementioned double layer.

INTRODUCTION

A good anti-reflective coating (ARC) is vital for solar cell performance as it ensures a high photocurrent by minimising reflectance. Unlike many other optoelectronic devices, solar cells operate at a range of wavelengths, from 300 - 1200nm, which means they need a broadband ARC. In industrial multi-crystalline silicon solar cell manufacture this is done by a single layer ARC. As discussed later, these do not minimise reflectance over a large range of wavelengths although they reduce reflection dramatically compared to a bare silicon surface.

Studies on double layer ARCs have been reported. The most stable configuration with respect to variations in film thicknesses have been found to be designs with a high refractive index (n) on the substrate and a low n towards the ambient [1].

Both magnesium fluoride/zinc sulphide (MgF2/ZnS) double layers deposited by electron beam sputtering [2] and titanium oxide (TiO2) double layers deposited by Atmospheric Pressure Chemical Vapour Deposition [3] show very low reflectance over a broad wavelength range. However, both techniques require a separately thermally grown silicon oxide (SiO2) layer for surface passivation.

A different approach is to implement a SiO2/SiN stack deposited by Plasma Enhanced Chemical Vapour Deposition (PECVD) [4]. This approach solves the abovementioned passivation issue and is the technique which most resembles the work described in this paper.

PECVD allows for tuning of both SiN and SiO2 films by adjusting deposition parameters, where the most used is the gas flow ratio of the precursor gases. SiN has been deposited with n varying from 1.8 to 3.2 (at 632.8nm) using a SiH4/NH3 gas mixture [5,6]. By changing the precursor gases to SiH4 and N2O, SiO2 with n varying from 1.46 to 2.05 has been shown [7,8]. Although SiN and SiO2 films deposited by PECVD contain hydrogen and are not stochiometric, they will be referred to as SiN and SiO2 for convenience.

EXPERIMENTAL

In this work we have used The Essential MacLeod software from Thin Films Center Inc. [9] to simulate ARC structures and calculate their reflectance spectra. The ARC structures were simulated on 550µm thick polished crystalline Si wafers as these are used in our laboratory characterisation of PECVD SiN. The thickness (d) is of importance to the back surface reflection at long wavelengths.

The wavelength dependent n and extinction coefficient (k) data for SiN has been taken from Philipp [10], whose values are measured on thermally grown stochiometric SiN (SiN4). For silicon they have been derived from reflectance and transmittance data from Virginia Semiconductors [11]. SiO2 data has been taken from the Essential MacLeod software material database. Reflection spectra were simulated for wavelengths from 300 to 1150nm and at an incidence angle of 9°. These parameters were chosen because they equal the specifications of our reflection measurement equipment.

Total reflectance was calculated from the reflection spectra by

\[
\text{Reflectance} = \frac{\int_{300}^{1150} \frac{R(\lambda)S(\lambda)}{E(\lambda)} d\lambda}{\int_{300}^{1150} \frac{S(\lambda)}{E(\lambda)} d\lambda}
\]

where S(\lambda) is the spectral irradiance based on the AM1.5 reference [12], R(\lambda) is the simulated reflection, E(\lambda) is the photon energy and d\lambda is 1nm. The denominator calculates a total photon flux of 2.78x10^{21} (photons s \(^{-1} \) m\(^{-2}\)), corresponding to a possible short circuit current density of 44.60 mA cm\(^{-2}\) at an internal quantum efficiency of 1 and reflectance of 0.

Optimisation of the ARC/Si stack was done by the a refinement method known as Simplex. It works by first changing a parameter in the design and then simulating the reflection spectrum of the design. A Figure of Merit is then calculated, which in our case was set to be the numerator in Eqn. 1. Refinement stops when the Figure of Merit has reached a local minimum.

Both d and n were changed in the process within specified limits taken from the literature mentioned in the introduction. Adjustment of n was done by a scaling
factor, the packing density, which scaled equally at all wavelengths.

RESULTS AND DISCUSSION

Three designs were refined: a single and double layer based on SiN and a mixed double layer combining SiN and SiO₂. In the following, optimisation results and subsequent analysis from PC1D simulations will be presented.

Single layer coating

For a single layer of SiN the reflectance was mapped with respect to n and d of the film, resulting in a contour plot (see Fig. 1). A minimum reflectance of 0.104 can be reached with a n=1.95 and d=81nm. This is a fairly high value for reflectance and would be lower for a textured silicon solar cell. Assuming an internal quantum efficiency (IQE) of 1 at all wavelengths, the potential JSC (J_PSC) for this ARC would be 39.94 mA cm⁻².

The optimised reflectance spectrum was simulated and correlated with the incident and reflected photon flux (see Fig. 2). The minimum at 640nm corresponds to the wavelength at which the d and n of the film causes a phase shift of π on the light which is reflected off the SiN/Si interface. This interferes destructively with the light reflected off the air/SiN interface. For a single layer coating, this wavelength can be found by

\[ \lambda_{\text{min}} = 4 \times n_{\text{SiN}} \times d_{\text{SiN}} \]  

(2)

where \( \lambda_{\text{min}} \) is the wavelength at minimum [13]. The minimum will also have a zero reflectance if refractive index at the minimum coincides with

\[ n_{\text{SiN}} = \sqrt{n_{\text{Air}} n_{\text{Si}}} \]  

(3)

Double layer coating

Double layer anti-reflective coatings work on the principle of creating two reflectance minima fairly close together and keeping the interconnecting maximum as low as possible. Explanations of minima and maxima in double layers are more complex than for single layers and will not be discussed in detail.

Double layer SiN

For a double layer containing only silicon nitride the lowest reflectance was reached with a structure \( n_{\text{bottom}}=2.99, \ n_{\text{top}}=1.82 \) and \( d_{\text{bottom}}=42\text{nm}, \ d_{\text{top}}=87\text{nm} \). The reflectance spectrum is shown as a solid line in Fig. 3 and results in a total reflectance of 0.055.
The resulting structure had a topmost layer which corresponded to the lower limit for the $n$ of PECVD SiN, thus indicating that one might obtain lower reflectance if the top layer could have a lower $n$. In addition, the practicality of making such a double SiN layer is inhibited by the fact that it incorporates layers on both extremes of what a PECVD system can deliver.

**Double layer SiN and SiO$_2$**

A solution to the abovementioned problem would be to use PECVD SiO$_2$ films as these have tuneable $n$ lower than that of SiN. The resulting refinement created a structure in with $n_{\text{bottom}}=2.67$, $n_{\text{top}}=1.55$ and $d_{\text{bottom}}=49\text{nm}$, $d_{\text{top}}=94\text{nm}$. Neither of these $n$ are difficult to obtain in PECVD systems. Compared to the single layer ARC, the reflectance at wavelengths shorter and longer than 640nm was reduced by 70% and 47%, respectively, resulting in a reflectance of 0.044 (see Fig. 3). This is 0.007 (absolute) lower than a simulation using the structure of Chen et al. [2].

**PC1D results**

The reflectance spectra were used in PC1D simulations to compare the effect on the short circuit current density, $J_{\text{SC}}$, for two solar cell structures which were both based on the standard PC1D template for a low cost material silicon solar cell. The material was set to p-type with resistivity of 1.2 $\Omega \cdot \text{cm}$ and a diffused emitter with error function distribution and 50 $\Omega / \text{sq}$ emitter sheet resistance. Front texturing was enabled, the base contact had a resistance of 0.015 $\Omega$ and the cell had an internal shunt of 0.3 Siemens. The bulk lifetime was set to 7.03$\mu$s and back Surface Recombination velocity to $10^5 \text{ cm s}^{-1}$.

It was desirable to study the effect of the reduced reflectance on two cells with different blue response and the easiest way to do this was to set two values for the front surface recombination velocity ($S_f$). A $S_f$ of $10^3 \text{ cm s}^{-1}$ was chosen for a poor blue response and a $S_f$ of $10^6 \text{ cm s}^{-1}$ for a good one.

A poor blue response is characterised by low internal quantum efficiency (IQE) below wavelengths of 400nm (see Fig. 4, right). $J_{\text{SC}}$ increased with use of the double layered ARCs as expected (see Table 1.). By defining a relative quantum efficiency as

$$RQE = \frac{J_{\text{SC}}}{J_{\text{PSC}}}$$ (4)

it can be seen that this value decreases for both double layered ARCs. A characteristic for these layers is the large reduction of reflectance between 400 and 520nm, while there is an increase between 530 and 700nm due to the local maxima (see Fig. 3). In this case, the reduction appears at wavelengths with low IQE and the increase at wavelengths with high IQE.

As the refinement process does not change extinction coefficient of the design, further work on the subject should be based on incremental ranges of $n$ with representative wavelength dependent extinction coefficient.

### Table 1. PC1D output parameters listed with respect to chosen anti-reflective coating.

<table>
<thead>
<tr>
<th>Reflectance</th>
<th>J$_{\text{SC}}$, $S_f=10^3$</th>
<th>J$_{\text{SC}}$, $S_f=10^6$</th>
<th>Potential J$_{\text{SC}}$</th>
<th>RQE, $S_f=10^3$</th>
<th>RQE, $S_f=10^6$</th>
</tr>
</thead>
<tbody>
<tr>
<td>unit</td>
<td>Single</td>
<td>Double</td>
<td>Mixed</td>
<td>%</td>
<td>%</td>
</tr>
<tr>
<td>Reflectance</td>
<td>0.104</td>
<td>0.055</td>
<td>0.044</td>
<td>81.5</td>
<td>80.9</td>
</tr>
<tr>
<td>J$_{\text{SC}}$, $S_f=10^3$</td>
<td>32.56</td>
<td>34.08</td>
<td>34.53</td>
<td>84.0</td>
<td>83.8</td>
</tr>
<tr>
<td>J$_{\text{SC}}$, $S_f=10^6$</td>
<td>33.56</td>
<td>35.52</td>
<td>35.81</td>
<td>84.0</td>
<td>84.0</td>
</tr>
<tr>
<td>Potential J$_{\text{SC}}$</td>
<td>39.94</td>
<td>42.13</td>
<td>42.64</td>
<td></td>
<td></td>
</tr>
<tr>
<td>RQE, $S_f=10^3$</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>RQE, $S_f=10^6$</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**Absorption**

The structures reported in this paper have been assumed to be non-absorbing, an assumption that may hold for the low refractive index films, albeit somewhat optimistic for the high refractive index films. Chen et al. [2] found that their SiO$_2$/SiN structure had higher absorption at short wavelengths than a MgF$_2$/ZnS structure and although the surface passivation of the former was superior, it was unable to counter balance the effect of the absorption. Both double layer structures presented in this paper have $n$ above that of Chen et al. and can hence be expected to have high absorption at short wavelengths.

As the refinement process does not change extinction coefficient of the design, further work on the subject should be based on incremental ranges of $n$ with representative wavelength dependent extinction coefficient.

**Passivation**

Aside from having very good optical properties, the anti-reflective coating needs to passivate the surface of the solar cell. PECVD SiN contains between 15 to 20 atomic percent hydrogen [14,15] due to the high hydrogen content in the precursor gases. Upon the high
temperature process of contact firing, the hydrogen will be released from the silicon nitride and diffuse into the silicon and passivate recombination sites in the bulk [16]. Several studies have been conducted into the relationship between passivation quality and the refractive index of PECVD SiN [6,17-18] and from these studies it is unclear whether the high refractive index of the SIN bottom layer would be advantageous with respect to bulk and surface passivation.

CONCLUSION

In this paper we have presented simulated single and double layer anti-reflective coatings (ARCs) on polished crystalline silicon wafers, based on silicon nitride and silicon oxide thin films. The refractive indexes of the films have been varied within the possible limits for PECVD found in the literature. While the single layer SiN ARC managed a minimum reflectance of 0.104, the combination of SiN and SiO₂ reflected as little as 0.044, based on the AM1.5 photon flux from 300-1150nm. Assuming non-absorbing films, this increased the short circuit current density of a non-optimised PC1D simulated cell by 6.0% with a poor blue response and 6.7% with a good one. However, SiN films with high refractive index are known to absorb at short wavelengths and hence these figures might be exaggerated.

REFERENCES


