Modelling and Simulation of Multilayer Antireflection Coating for Infra-Red light on Silicon Substrate for Nd:YAG solid state lasers

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Abstract- Present work aims at the characterization of ARC films in the visible spectrum, up to five layers antireflection coating film were designed and simulated, optical reflection values were deduced with a Transfer Matrix Method formulation (TMM). Six materials have been selected to investigate the optimum values of the Anti reflection coating (ARC) film for solar cells. The present work has been carried out to investigate the optimum values of reflectance as a function of wavelength in the infra-red region. The reflectance has been reduced from 32% of silicon surface to less than 1% using multilayer ARC film. The three layer ARC film of Cryolite, Silicon Dioxide and Titanium Dioxide has shown a better performance in the infra-red region (800-1100nm) than the Magnesium Fluoride, Cerium fluoride and Zirconium oxide ARC film as its reflectance is almost zero in a broader region of 800-1100nm and is good for Nd:YAG solid state lasers operating at long wave.

Keyword: Antireflection Coating (ARC), Reflectance, Transfer Matrix Method, Double layer ARC, Three Layer ARC, Four Layer ARC, Five Layer ARC, Solar cells.

1. Introduction

Silicon is the best known semiconductor optical material with relatively high refractive index. The most important application of silicon in the visible spectrum is photovoltaic solar panel [1][2]. The conversion of solar energy into other energy form is more effective if the reflectance of the light receiving surface of solar device is minimal in the solar spectrum range [3]. The efficiency of a solar cell and its lifetime can be raised by coating the light sensitive surface of the cell with an Anti Reflection Coating (ARC) [3]. To obtain the AR response at a single wavelength, a single layer or two layers are sufficient. However, when the AR function is broadened to cover a range of wavelengths, the number of layers must also be increased, and the AR structure is a multilayer structure. Many design procedures have been applied to solve this design problem. Most of these procedures address the problem of having a fixed number of refractive indices that are repeated periodically. The optimal length of each layer that satisfies the required specifications is then determined [4][5]. The matrix method [6] is usually employed for calculation of the reflection coefficient. While the well-known single layer quarter-wave film can lead to zero reflection at a single wavelength, broadband ARC is often needed for many applications. In practice coating materials with the required refractive index for the quarter-wave antireflective (AR) film may not be available. To address these issues, a multilayer stack of homogeneous thin films has been investigated extensively for over half a century [7], resulting in the development of a rich variety of multilayer thin film schemes [8] and design methodologies.
The aim of this research is to present a computational process for the numerical design and simulation of antireflection coatings. The optical thickness and refractive index of each layer is adjusted to optimize the reflectance as a function of wavelength.

2. Design Methodology
Transfer Matrix Method is used to calculate the reflection coefficient of a multilayer stack, which consist of series of \( k \) thin film dielectric layers, having a physical thickness \( d_1, d_2, d_3, \ldots, d_k \) and refractive indices \( n_1, n_2, n_3, \ldots, n_k \), respectively, deposited on a substrate of refractive index \( n_s \).

Then for normal indices of light, the reflection (\( R \)) and transmission (\( T \)) of such a stack is given by the following expression:

\[
R = \left( \frac{1 - Y}{1 + Y} \right)^2
\]

And \( T = 1 - R \). (These expressions are true for an absorption-free multilayer stack.) Where \( Y = C/B \) is known as optical admittance of the stack, and

\[
\begin{bmatrix}
B \\
C
\end{bmatrix} =
\begin{bmatrix}
M_{11} & M_{12} \\
M_{21} & M_{22}
\end{bmatrix}
\begin{bmatrix}
1 \\
n_s
\end{bmatrix}
\]

(2)

Where

\[
\begin{bmatrix}
M_{11} & M_{12} \\
M_{21} & M_{22}
\end{bmatrix} = \prod_{r=1}^{K} \begin{bmatrix} 
\cos \delta_r(\lambda) & i \frac{\sin \delta_r(\lambda)}{n_r} \\
\frac{\sin \delta_r(\lambda)}{n_r} & \cos \delta_r(\lambda)
\end{bmatrix}
\]

(3)

The phase thickness of the \( r \)^{th} layer is given by \( \delta_r(\lambda) = \frac{2\pi n_r d_r}{\lambda} \) for the normal incidence of light of wavelength \( \lambda \). For symmetrical multilayer stack \( M_{11} = M_{22} \), and if \( M_{11} \neq M_{22} \) the multilayer is called an unsymmetrical multilayer stack. The matrix involved in the equation (3) is called characteristics matrix and its determinant is unity \([4]\). The process of finding the \( R, T \) involves essentially computation of the optical admittance \( Y \) of the stack by matrix multiplication method provide that refractive index as a function of \( \lambda \) and the physical thickness of each layer is known. Therefore, the necessary and sufficient conditions to produce zero reflectance are calculated based on equations 4-7 \([10]\).

For a double layer

\[
n_1^4 = n_0^3 n_{sl} \quad ; \quad n_2^4 = n_0 n_{sl}^3
\]

(4)

For a three layer

\[
n_1^8 = n_0^7 n_{sl} \quad ; \quad n_2^8 = n_0^4 n_{sl}^4 \quad ; \quad n_3^8 = n_0 n_{sl}^7
\]

(5)

For a four layer

\[
n_1^{16} = n_0^{15} n_{sl} \quad ; \quad n_2^{16} = n_0^{11} n_{sl}^5 \quad ; \quad n_3^{16} = n_0^5 n_{sl}^{11} \quad ; \quad n_4^{16} = n_0 n_{sl}^{15}
\]

(6)
For a five layer
\[ n_1^{32} = n_0^{31} n_{st} ; \quad n_2^{32} = n_0^{26} n_{st}^6 ; \quad n_3^{32} = n_0^{16} n_{st}^{16} ; \quad n_4^{32} = n_0^6 n_{st}^{26} ; \quad n_5^{32} = n_0 n_{st}^{31} \]  
(7)

3. Reflectance Spectrum Analysis

The simulation of the reflection has been done using Matlab software, and the reflectivity of the silicon has been simulated with two, three, four and five layers of antireflection coatings. The program is optimized at \( \lambda_0 = 940 \text{ nm} \) central wavelength in order to make it suitable for Nd:YAG solid state lasers applications, in the infra-red region. The parameters like optical thickness and refractive index for each layer coating are optimized. The materials selected have low wave absorption, homogeneity, high packing density, good adhesion, low stress, hardness and ability to survive in different environments.

3.1. Double Layer Antireflection Coating

The refractive index \( n_{si} \) of silicon in the spectral region 700-1200 nm is 3.5 and when the surrounding medium is air (\( n_{a} = 1 \)) the refractive index of the first layer should be 2.5 and of the second layer should be 1.3 so the three different combinations of dielectric materials (Silicon Dioxide with Zinc Sulphide), (Cryolite with Titanium Dioxide) and (Magnesium Fluoride with Cerium Oxide) were selected as given in figure 1. The reflectance spectra of double layer coating of the above three combinations of dielectric materials, with varying optical thickness were analyzed.

\[
\begin{array}{ccc}
\text{Normal Incidence of Light} & \text{Normal Incidence of Light} & \text{Normal Incidence of Light} \\
\downarrow & \downarrow & \downarrow \\
 n_1(1.46) & n_1(1.35) & n_1(1.38) \\
n_2(2.32) & n_2(2.40) & n_2(2.20) \\
n_5(3.5) & n_5(3.5) & n_5(3.5) \\
\end{array}
\]

**Figure 1.** Schematic of double layer, optical thickness \( n_id_i \) and wavelength \( \lambda_0 \) for normal incidence of light.

![Reflectance Spectrum Analysis](image1)

(a) quarter-quarter optical thickness

![Reflectance Spectrum Analysis](image2)

(b) quarter-half optical thickness
Figure 2 shows a comparison of reflectance of three different (dual layer) ARC films with that of without ARC film. In figure 2 (a), the reflectance graph of all the three ARC films of quarter-quarter optical thickness is shown. As per the graph, Cryolite with Titanium Dioxide has shown better performance. A minimum reflectance of 0.04% is achieved at 1125 nm which is close to the central wavelength (940 nm). The layer of Cryolite with Titanium Dioxide reduces the average reflection from 32% to less than 1% in between 800-1200 nm and has the average reflectance of 0.24%. This particular form of broadband ARC film may be suitable for use in antireflection film for infra-red radiations.

By increasing the optical thickness of the inner layer from quarter to half wavelength, figure 2 (b), the average reflectance of all the three ARC films are increased. As per the graph, Silicon Dioxide with Zinc Sulphide has the lowest value of average reflectance (8.7%), among all the three layers, in the infra-red region. A minimum reflectance of 5.9% is achieved at 940 nm. The Silicon Dioxide with Zinc Sulphide layer has a narrowband antireflection region in the range of 900-1000 nm but there is no zero reflection point and as the average reflectance is also higher than 5% so this layer cannot be an effective ARC film with low reflectance in infra-red optoelectronic devices.

In figure 2 (c), the reflectance graph of all the three ARC films for half-quarter optical thickness is shown. As per the graph, Magnesium Fluoride with Cerium Oxide has the lowest value of average reflectance (6.33%) and has a minimum reflectance of 2.58% at 940 nm which is better than the other two ARC films. As this layer has a minimum reflectance at 940 nm it may be suitable for Nd:YAG solid state lasers applications and as an ARC film in the narrowband (900-100nm) of infra-red spectrum. The simulated results of minimum and average reflectance of double layer ARC films are tabulated in table 1.
Table 1. Reflectance of double layer ARC films

<table>
<thead>
<tr>
<th>Thickness</th>
<th>Types of ARC Film</th>
<th>Wave Length(nm)</th>
<th>Minimum Reflectance (%)</th>
<th>Avg. Reflectance (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\lambda/4$ &amp; $\lambda/4$</td>
<td>SiO$_2$ +ZnS</td>
<td>725</td>
<td>0.0197</td>
<td>1.52</td>
</tr>
<tr>
<td></td>
<td>Na$_3$AlF$_6$ + TiO$_2$</td>
<td>1125</td>
<td>0.041</td>
<td>0.24</td>
</tr>
<tr>
<td></td>
<td>Mg$_3$F$_2$ + CeO$_2$</td>
<td>735</td>
<td>0.32</td>
<td>1.56</td>
</tr>
<tr>
<td>$\lambda/4$ &amp; $\lambda/2$</td>
<td>SiO$_2$ +ZnS</td>
<td>940</td>
<td>5.90</td>
<td>8.70</td>
</tr>
<tr>
<td></td>
<td>Na$_3$AlF$_6$ + TiO$_2$</td>
<td>700</td>
<td>9.27</td>
<td>10.70</td>
</tr>
<tr>
<td></td>
<td>Mg$_3$F$_2$ + CeO$_2$</td>
<td>940</td>
<td>8.71</td>
<td>10.59</td>
</tr>
<tr>
<td>$\lambda/2$ &amp; $\lambda/4$</td>
<td>SiO$_2$ +ZnS</td>
<td>940</td>
<td>4.49</td>
<td>7.72</td>
</tr>
<tr>
<td></td>
<td>Na$_3$AlF$_6$ + TiO$_2$</td>
<td>940</td>
<td>5.95</td>
<td>7.88</td>
</tr>
<tr>
<td></td>
<td>Mg$_3$F$_2$ + CeO$_2$</td>
<td>940</td>
<td>2.58</td>
<td>6.33</td>
</tr>
</tbody>
</table>

3.2. Three Layer Antireflection Coating

Here three layer antireflection coating is considered for simulation. Figure 3 gives schematic of three layers of optical thickness $n_1d_1$ and wavelength $\lambda_0$ for normal incidence of light. In figure 4, the reflectance graph two ARC films of quarter-quarter-quarter and quarter-half-quarter optical thickness are shown. Figure 4 (a) shows that the Magnesium Fluoride, Cerium fluoride and Zirconium oxide has shown better performance in the range of 900-1000nm as compared to other three layer ARC film comprising of Cryolite, Silicon Dioxide and Titanium Dioxide. Almost zero reflectance (0.002%) is achieved at 941nm with average reflectance of 3.47%. This layer can be an effective ARC film with high efficiency and low reflectance in the 900-1000nm infra-red region. In figure 4 (b), the optical thickness of the middle layer is changed from quarter to half wavelength and as a result the reflectance of Cryolite, Silicon Dioxide and Titanium Dioxide, three layer ARC film, becomes almost zero in a broader region of 800-1100nm. This combination has an average reflectance of 1.81% throughout the infra-red spectrum. The simulated results of minimum and average reflectance of three layer ARC films are tabulated in table 2.

```
Normal Incidence of Light
↓

<table>
<thead>
<tr>
<th>$n_1$ (1.35)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$n_2$ (1.46)</td>
</tr>
<tr>
<td>$n_3$ (2.4)</td>
</tr>
<tr>
<td>$n_5$ (3.5)</td>
</tr>
</tbody>
</table>

Normal Incidence of Light
↓

<table>
<thead>
<tr>
<th>$n_1$ (1.38)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$n_2$ (1.63)</td>
</tr>
<tr>
<td>$n_3$ (2.2)</td>
</tr>
<tr>
<td>$n_5$ (3.5)</td>
</tr>
</tbody>
</table>
```
Figure 3. Schematic of three layers, optical thickness $n_id_i$ and wavelength $\lambda_0$ for normal incidence of light.

![Figure 3](image)

(a) quarter-quarter-quarter optical thickness  
(b) for quarter-half-quarter optical thickness

Figure 4. (a, b) Reflectance spectra of Triple layer antireflection coating on silicon.

Table 2. Reflectance of triple layer ARC films

<table>
<thead>
<tr>
<th>Thickness</th>
<th>Types of ARC Film</th>
<th>Wave Length (nm)</th>
<th>Minimum Reflectance (%)</th>
<th>Avg. Reflectance (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\lambda/4$ &amp; $\lambda/4$ &amp; $\lambda/4$</td>
<td>Na$_3$AlF$_6$+SiO$_2$+TiO$_2$</td>
<td>941</td>
<td>2.86</td>
<td>4.89</td>
</tr>
<tr>
<td>&amp; MgF$_2$+CeF$_3$+ZrO$_2$</td>
<td></td>
<td>941</td>
<td>0.002</td>
<td>3.47</td>
</tr>
<tr>
<td>$\lambda/4$ &amp; $\lambda/2$ &amp; $\lambda/4$</td>
<td>Na$_3$AlF$_6$+SiO$_2$+TiO$_2$</td>
<td>873</td>
<td>0.13</td>
<td>1.81</td>
</tr>
<tr>
<td>&amp; MgF$_2$+CeF$_3$+ZrO$_2$</td>
<td></td>
<td>1120</td>
<td>0.08</td>
<td>1.71</td>
</tr>
</tbody>
</table>

3.3. Four Layer Antireflection Coating

Figure 5 shows schematic of four layers of optical thickness $n_id_i$ and wavelength $\lambda_0$ for normal incidence of light. In figure 6 (a), the reflectance graph of two different ARC films for the quarter-quarter-quarter-quarter optical thickness is shown. As per the graph, Cryolite, Silicon Dioxide, Cerium Fluoride and Titanium Dioxide layer has shown a lower value of average reflectance (1.52%) throughout the infra-red spectrum and two almost zero reflectance points at 800 and 1140nm which is good for the optoelectronic devices which operate at these wavelengths in the infra-red spectrum. It can be seen from the figure that if Cerium fluoride is replaced by Magnesium Fluoride, the ARC film shows almost zero reflectance (0.002%) at 940nm and has a zero narrowband antireflection region in between 900 and 1000nm. This form of ARC film can be suitable for use in Nd:YAG solid state lasers. In figure 6 (b), the optical thickness of second outer layer is changed from quarter to half wavelength and the graph shows that the Cryolite, Silicon Dioxide, Cerium Fluoride and Titanium Dioxide layer becomes better, with two almost zero reflectance points at 715nm and 940nm and a lower value of average reflectance (1.96%). This form of three layer ARC film may be suitable for the lasers or other optoelectronic devices which require zero reflectance at these two different wavelengths. The simulated results of minimum and average reflectance of four layer ARC films are tabulated in table 3.

![Figure 4](image)

![Table 2](image)
Normal Incidence of Light

\[
\begin{array}{|c|}
\hline
n_1 (1.35) \\
\hline
n_2 (1.46) \\
\hline
n_3 (1.63) \\
\hline
n_4 (2.4) \\
\hline
n_5 (3.5) \\
\hline
\end{array}
\]

Normal Incidence of Light

\[
\begin{array}{|c|}
\hline
n_1 (1.35) \\
\hline
n_2 (1.46) \\
\hline
n_3 (1.38) \\
\hline
n_4 (2.4) \\
\hline
n_5 (3.5) \\
\hline
\end{array}
\]

**Figure 5.** Schematic of four layers, optical thickness \( n_i d_i \) and wavelength \( \lambda_0 \) for normal incidence of light.

(a) quarter-quarter-quarter-quarter optical thickness

(b) quarter-half-quarter-quarter optical thickness

**Figure 6.** (a,b) Reflectance spectra of four layer antireflection coating on silicon

**Table 3.** Reflectance of four layer ARC films

<table>
<thead>
<tr>
<th>Thickness</th>
<th>Types of ARC Film</th>
<th>Wave Length (nm)</th>
<th>Minimum Reflectance (%)</th>
<th>Avg. Reflectance (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \lambda/4 &amp; \lambda/4 &amp; \lambda/4 &amp; \lambda/4 )</td>
<td>( \text{Na}_3\text{AlF}_6+\text{SiO}_2+\text{CeF}_3+\text{TiO}_2 )</td>
<td>800</td>
<td>0.21</td>
<td>1.52</td>
</tr>
<tr>
<td></td>
<td>( \text{Na}_3\text{AlF}_6+\text{SiO}_2+\text{MgF}_2+\text{TiO}_2 )</td>
<td>940</td>
<td>0.002</td>
<td>2.84</td>
</tr>
<tr>
<td>( \lambda/4 &amp; \lambda/2 &amp; \lambda/4 &amp; \lambda/4 )</td>
<td>( \text{Na}_3\text{AlF}_6+\text{SiO}_2+\text{CeF}_3+\text{TiO}_2 )</td>
<td>715</td>
<td>0.002</td>
<td>1.96</td>
</tr>
<tr>
<td></td>
<td>( \text{Na}_3\text{AlF}_6+\text{SiO}_2+\text{MgF}_2+\text{TiO}_2 )</td>
<td>735</td>
<td>1.41</td>
<td>4.29</td>
</tr>
</tbody>
</table>
3.4. **Five Layer Antireflection Coating**

Now finally the five layer ARC has been considered as shown in figure 6, which shows the schematic having optical thickness $n_1d_1$ and wavelength $\lambda_0$ for normal incidence of light. It can be seen in figure 8 (a) that by addition of a fifth layer of low index and selecting the Low High Low High formation of outer four layers and the fifth layer of index close to that of substrate, a five layer ARC of Cryolite, Silicon Dioxide, Cryolite, Silicon Dioxide and Titanium Dioxide is formed. The graph depicts that the broadening effect is achieved and as a result an average reflectance of 1.41% is achieved in the infra-red region (700-1200 nm). By changing the optical thickness of fourth layer from quarter to half wavelength the average reflectance of both formations has been increased slightly but the improved results can be seen in between 900-1000nm as there is almost zero reflectance in this narrowband, as shown in figure 8 (b), and this type of ARC film may be suitable for narrowband (900-1000nm) optoelectronic devices and not for the solar cell applications in the entire infra-red spectrum. The simulated results of minimum and average reflectance of five layer ARC films are tabulated in table 4.

<table>
<thead>
<tr>
<th>Normal Incidence of Light</th>
<th>Normal Incidence of Light</th>
</tr>
</thead>
<tbody>
<tr>
<td>$n_1$ (1.35)</td>
<td>$n_1$ (1.35)</td>
</tr>
<tr>
<td>$n_2$ (1.46)</td>
<td>$n_2$ (1.46)</td>
</tr>
<tr>
<td>$n_3$ (1.35)</td>
<td>$n_3$ (1.38)</td>
</tr>
<tr>
<td>$n_4$ (1.46)</td>
<td>$n_4$ (1.63)</td>
</tr>
<tr>
<td>$n_5$ (2.4)</td>
<td>$n_5$ (2.4)</td>
</tr>
<tr>
<td>$n_6$ (3.5)</td>
<td>$n_6$ (3.5)</td>
</tr>
</tbody>
</table>

**Figure 7.** Schematic of five layers, optical thickness $n_1d_1$ and wavelength $\lambda_0$ for normal incidence of light.
Figure 8. Reflectance spectra of five layer antireflection coating on silicon.

Table 4. Reflectance of five layer ARC films

<table>
<thead>
<tr>
<th>Thickness</th>
<th>Types of ARC Film</th>
<th>Wave Length(nm)</th>
<th>Minimum Reflectance (%)</th>
<th>Avg. Reflectance (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>λ/4 &amp; λ/4 &amp; λ/4</td>
<td>Na₃AlF₆+SiO₂+Na₃AlF₆+SiO₂+TiO₂</td>
<td>735</td>
<td>0.014</td>
<td>1.41</td>
</tr>
<tr>
<td>&amp; λ/4 &amp; λ/4</td>
<td>Na₃AlF₆+SiO₂+MgF₂+CeF₃+TiO₂</td>
<td>940</td>
<td>0.0018</td>
<td>1.75</td>
</tr>
<tr>
<td>λ/4 &amp; λ/4 &amp; λ/4</td>
<td>Na₃AlF₆+SiO₂+Na₃AlF₆+SiO₂+TiO₂</td>
<td>940</td>
<td>0.07</td>
<td>4.48</td>
</tr>
<tr>
<td>&amp; λ/2 &amp; λ/4</td>
<td>Na₃AlF₆+SiO₂+MgF₂+CeF₃+TiO₂</td>
<td>940</td>
<td>0.002</td>
<td>4.40</td>
</tr>
</tbody>
</table>

4. Conclusion

The surface of silicon reflects huge part of the incident light radiation in the whole spectral range between 700-1200 nm as its refractive index is relatively high. A double layer can be a better solution of antireflection coating in the range between 700-1200 nm. But double layer ARC does not minimize this high reflectance over a broad range of wavelength although it reduces reflection drastically compared to a plain silicon surface. The layer of Cryolite with Titanium Dioxide reduces the average reflection from 32% to less than 1% in between 800-1200 nm and has the average reflectance of 0.24%. This particular form of broadband ARC film may be suitable for use in antireflection film for broadband infra-red devices. The three layer ARC film of Cryolite, Silicon Dioxide and Titanium Dioxide has shown a better performance in the infra-red band (800-1100nm) than the other forms of ARC films as its reflectance is almost zero in a broader region of 800-1100nm and is good for Nd:YAG solid state lasers operating at long wave. The further increment in the number of layers like four layer and five layer ARC films resulted in the higher value of the average reflectance as compared to double and three layer ARC films but these forms have shown zero reflectance points at specific wavelengths and also in narrow bands which may be more useful for devices that operates at a single wavelength or narrow band. The double layer of Cryolite with Titanium Dioxide has shown better performance among all the material formations with a minimum reflectance of 0.04% and the average reflectance of 0.24%.

REFERENCES


