Design of Broadband Anti Reflecting Thin Film Filters using Silicon-Compatible Materials

Faridah¹, Nopriadi²
Jurusan Teknik Fisika, Fakultas Teknik, UGM
Jl. Grafika No. 2 Yogyakarta 55281

Abstract

Design of antireflection (AR) thin film filters using only Si-compatible materials is extremely important for any electronic photodetector fabricated using standard semiconductor processing.

The objective of the research is to design a broadband AR thin film filters using Silicon Compatible Materials. The research was conducted in two steps. The first step was the developing theoretical design and the second one was computer optimization.

The design method is based on the main properties of symmetrical multilayer periods developed by Nenkov and Pancheva (1997). The materials used were limited only to those practically employed in a microelectronic cleanroom environment. The optimization of the design result was done using a special computer software in order to improve the coating performance.

The result of design provides a low reflectance (<10 % within the passband) for a Si substrate in the wavelength range of 380 to 780 nm.

Keywords: Thin Film Filter, Anti Reflection Coating (ARC), Silicon Compatible Materials, Symmetrical Multilayer, TF Calc

1. Introduction

Thin film technology is the current technology of choice for the fabrication of most of the optical filters, because of its clear technical advantages, its passive nature that offers simple system integration, and its flexibility and modularity. It has been widely applied to many optical devices (e.g., lenses, computer monitors, eye glasses, window panes, light bulbs, mirrors, solar cells, detectors, laser gyroscopes, television cameras, prisms, WDM and DWDM filters, VCSEL lasers, etc.), and was field-proven to be reliable.

Antireflection (AR) thin film filters design has been developed strongly and matured over the decades (Lockhart and King, 1947; Young, 1961; Berning, 1985; Southwell, 1985; Baumeister, 1986; Nagendra, 1988; Thelen, 1989; Cojocaru, 1992; Nenkov and Pancheva, 1997). The primary emphasis in the design of such interference multilayer coatings is to control the reflected or transmitted light at wavelengths ranging from X-rays to far infrared (IR). More specifically, a coating's effect is determined by how its layers control the interference and absorption of light.

The research is to design of a broadband antireflection (AR) thin film filter. The broadband AR was designed for Si substrates (not glass, as is the target in the majority of literature source) and realized using only Si-compatible materials. It is extremely important for any electronic photodetectors fabricated using standard semiconductor processing. Therefore, result of the research is an important contribution of the project for the future development and implementation of real-life optical detector which must use only thin film filters constructed with Si-compatible materials.
2. Fundamental Theory: Anti Reflection Coatings Based on Symmetrical Multilayer Periods Properties

The main properties of a multilayer symmetrical period may be described by its characteristic matrix $M$ obtained as a product of Abeles’ characteristic matrices of separate layers (Nenkov and Pancheva, 1997; Thelen, 1989):

$$ M = \begin{bmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{bmatrix} $$

(1)

For matrices of every symmetrical combination of dielectric nonabsorbing layers, $M_{11} = M_{22}$. This relation allows the characteristic matrix of a symmetrical period to be replaced by the characteristic matrix $M$ of an equivalent single layer,

$$ M = \begin{bmatrix} \cos \Gamma & j \sin \Gamma \\ jN \cos \Gamma & \cos \Gamma \end{bmatrix}, \quad j^2 = -1 $$

(2)

with equivalent phase thickness $\Gamma$ and equivalent refractive index $N$ defined as

$$ \Gamma = \arccos(M_{11}) $$

(3)

$$ N = \sqrt{\frac{M_{21}}{M_{12}}} $$

(4)

The characteristic matrix of a multilayer stack from $p$ identical successive symmetrical periods is described by the matrix:

$$ M = \begin{bmatrix} \cos p\Gamma & j \sin p\Gamma \\ jN \cos p\Gamma & \cos p\Gamma \end{bmatrix} $$

(5)

which corresponds to an equivalent single layer with the same refractive index $N$ and the phase thickness $p\Gamma$.

This formal analogy is not valid for an arbitrary wavelength $\lambda$. For every symmetrical period, there are spectral regions for which $M_{11} < -1$ and $M_{11} > 1$. These are the spectral regions in which both $N$ and $\Gamma$ are imaginary and where a strong increase of reflectance occurs when the number of symmetrical periods in a multilayer is increased, i.e. a stopband appears. Boundary conditions for these zones follow from $M_{11} = -1$ and $M_{11} = 1$.

The main properties of a coating made up of symmetrical dielectric periods may be summarized as follows (Nenkov and Pancheva, 1997):

- A multilayer stack with a number of identical successive symmetrical periods may posses high reflectance in spectral regions near the following wavelength and corresponding values of relative wavenumber $g = \lambda_0 / \lambda$.

$$ \lambda = \frac{\lambda_0}{g}, \frac{\lambda_0}{2}, \frac{\lambda_0}{3}, ..., \frac{\lambda_0}{k} $$

(6)

i.e. $g = 1, 2, 3, ..., k$ where $\lambda_0 = 2\sum n_i d_i$ is the optical thickness of the $i$th layer in the period, and $k$ is an integer positive number ($k = 1, 2, 3, ...$) that is called the stop-band order.

- In the spectral region between two neighboring stopbands, a symmetrical period can be formally replaced by a single layer with equivalent index $N$ and phase thickness $\Gamma$ of values which depend on the period structure. If the multilayer coating consists of $p$ identical successive symmetrical ABA periods, it will be equivalent to a single layer with the same refractive index $N$ and phase thickness $\Gamma$.

The ARC design method based on the main properties of symmetrical multilayer periods developed by Nenkov and Pancheva (1997). The desired corresponding bandwidth can be achieved by suppressing various orders (one or two order) of stopbands and selecting appropriately the design wavelength.

3. Methodology

There were two steps in the research. The first step was the developing theoretical design and the second one was computer optimization to get desired design performance.

Developing theoretical design

In this step, the desired filter was design theoretically based on well-established mathema-
tical formulae. The design algorithm was developed based on the main properties of symmetrical multilayer periods developed by Nenkov and Pancheva (1997). The desired corresponding bandwidth could be achieved by suppressing various orders (one or two order) of stopbands and selecting appropriately the design wavelength. The materials used were limited only to those practically employed in a microelectronic clean environment. It was assumed that all the materials were homogeneous, isotropic and non-absorbing.

Computer optimization

There are some factors contribute to the deviation of the practical performances of a real coating from the theoretical ones. The first factor is due to the limited of number of practically available materials. The ideal AR coating is an inhomogeneous layer with a continuous transition of the refractive index from one massive medium to the other one or, as an approximation, a set of very thin homogenous layers with refractive indices increasing in small steps from the low-index massive medium to the high-index medium (Thelen, 1989).

This coating is however of no practical value since the choices of materials are limited and mixing two materials to generate intermediate refractive indices is very difficult.

The second factor is the inherent dispersion of any real material. Moreover, an increased thickness of any layer increases the dispersion of the entire coating. Therefore, the final result will be far from the ideal characteristic.

Based on the two mentioned factors above, computer optimization of the theoretical design is necessary. Computer simulations of the optical multilayer structures, designed in the research, and their corresponding characteristics were performed using the professional software package TFCALC. All these computer simulation took into account the dependence of wavelength (i.e. dispersion) of the optical properties of the available materials.

However, it must be underlined that there are various optimization approaches. In some case the optimization was achieved by varying the thickness of the layers, but in other cases by varying only the refractive indices of some layers, while in other cases both parameter values were changed starting from the values provided by the initial design. Furthermore, the optimization were not limited at only changing $d$ or $n$: whenever required, new layers were added and/or initial layers decreased in thickness until deleted or replaced by other layers. Therefore, the final design after computer optimization might be very different from the initial design.

Another practical limitation is given by the fact that monocrystalline silicon should not be in direct contact with silicon nitride or air (Poenar, 1996). This is not desirable as the density of surface states could be quite large and variable in time, compromising the operation of the devices realized in the substrate. In order to avoid this problem, one can introduce a ‘buffer’ oxide layer between the designed multilayer coating and the underlying Si substrate. In order to improve the surface properties of the substrate without altering its optical characteristics, the oxide thickness of this ‘buffer’ should be as thin as possible as it is shown in Figure 1. It is clear that even for the non-ideal case, the 100 Å SiO$_2$ film still is a much better alternative, as it offers only a negligible deviation from the optical behavior of bare Si.

Consequently, in order to avoid any undesirable surface properties of the substrate, if the first layer of the coating does not result from the calculations to be an oxide film, then it will always be automatically assumed that the Si substrate is covered with a 100 Å thermal oxide layer.

4. Result and Discussion

The design of AR filter follows a few key underlying ideas:

1) The AR filter should provide a low reflectance ($<10\%$ within the passband) for a Si substrate (not glass, as is the target in the majority of literature sources) in the wavelength range of 380 to 780 nm;
2) Only Si-compatible materials should be used in order to enable its usage for electric photodetectors fabricated using standard (e.g. CMOS) semiconductor processing. This means that only Si (monocrystalline, polycrystalline or amorphous), $\text{SiO}_2$ ($n=1.46$) and $\text{Si}_3\text{N}_4$ ($n=2$) can be used.

However, oxynitride (a Si-compatible material with properties intermediate between oxide and nitride) could also be used. The refractive index of this material is in the range of 1.46 to 2.0.

Finally, other Si-compatible materials which can also be used are doped oxide glasses, like PSG/BSG/BPSG (the presence of the dopant modifies to some extent their optical properties), and low stress nitride (a Si-rich nitride with an average refractive index $n \approx 2.2$ and with some notable absorption in the short wavelength range).

3) As mentioned in the previous section, a 100 Å thin oxide must always be present between the AR coating and the Si substrate (unless the coating’s first layer is oxide).

The initial theoretical calculations used ‘ideal’ materials, i.e. without losses and with no dispersion (i.e. constant refractive index in the entire wavelength range: $n_{\text{SiO}_2} = 1.46$, $n_{\text{Si}_3\text{N}_4} = 2$, $n_{\text{low-stress nitride}} = 2.2$, and $n_\text{Si} = 4.218$). However, the computer optimizations were carried out replacing these ideal materials with the real ones. The optical properties of the real silicon oxide, silicon nitride, low-stress silicon nitride and for the Si substrate itself used in the simulations are based on values tabulated in literature (EMIS Data reviews, 1988). These materials are denoted by LIT-SIO2, LIT-SIN, LS-SIN and LIT-Si in the Tables presented in the following sections that will detail the final structures of the designed filters.

![Figure 1](image_url)  
**Figure 1.** The influence of a $\text{SiO}_2$ layer on the reflectance of monocrystalline Si.
The first attempted design was a coating with a one order stopband suppression at $\lambda_0/\lambda = 2$. A three symmetrical layer, $aAbBaA$, with oxide ($n=1.46$) as the A component and nitride ($n=2$) as the B component, was employed. From the formulae derived by Nenkov and Pancheva (1997), the thickness of these layers can be calculated. By setting the wavelength design at $\lambda_0 = 1100$ nm, the periodic multilayer which is constructed by this symmetrical structure can provide a wide passband between $\lambda_1 = 380$ nm and $\lambda_2 = 780$ nm.

A matching layer with the substrate at $\lambda = 550$ nm is needed for this design since its equivalent index ($N_{aAbBaA} = 1.239$) is very different from the optical admittance of silicon. The necessary layer should have an equivalent index $N_{ms} = \sqrt{N_{aAbBaA} \cdot n_{\text{substrate}}} = 2.294$, which means that low-stress silicon nitride can be employed for this matching layer. The resultant theoretical design structure is presented in Table 1, and its reflectance curve can be seen in Figure 2.

Taking dispersion into account, the reflection within the passband decreases but the passband becomes narrower as it can be seen in Figure 3.

The optimization was done by varying both the thicknesses and refractive indices of the coating’s layers. It can be seen that the optimized coating provides a good performance due to the good performance of the initial theoretical design. The final structure after optimization and its performance are presented in Table 3 and in Figure 3, respectively.

### Table 1. The structures designed by using one order stopband suppression ($\lambda_0 = 1100$ nm).

<table>
<thead>
<tr>
<th>Matching Structure</th>
<th>Basic Structure (aAbBaA)$^3$</th>
<th>Matching Structure With Substrate</th>
</tr>
</thead>
<tbody>
<tr>
<td>With Air</td>
<td>OXIDE \ n=1.46; d=94.18 nm</td>
<td>LOW-STRESS NITRIDE \ n=2.2; d=125 nm</td>
</tr>
<tr>
<td></td>
<td>NITRIDE \ n=2; d=137.5 nm</td>
<td></td>
</tr>
<tr>
<td></td>
<td>OXIDE \ n=1.4; d=94.18 nm</td>
<td></td>
</tr>
</tbody>
</table>

**Figure 2.** The reflectance curves of the design resulted in Table 1, without matching layer (dashed line), and with matching layer (solid line), respectively.
However, there is one difficulty with the one-order stopband suppression. The width of the design passband resulted theoretically is determined by choosing which order is suppressed and by the design wavelength selection. If inappropriate values are taken for these parameters, a poorly performing coating may result. An example is given in the following design. A passband within 380 to 780 nm can also be achieved by suppressing the third order ($\lambda / \lambda_0 = 3$) and selecting the design wavelength at 1650 nm. Compared to the design shown in Figure 2, this design will result having a narrower passband, as it can be seen in Figure 4. Obviously, this limitation will then affect the result of the subsequent optimizations.

Alternatively, one can design a coating with a two-order stopband suppression in order to achieve a wide enough passband. The basic structure is a five symmetrical layer, $a_1AbBaAbB_1A$, composed of two materials, oxide ($n=1.46$) and nitride ($n=2$). From the formulae derived by Nenkov and Pancheva (1997), the thicknesses of these layers can be calculated. By setting the design wavelength at $\lambda_0 = 1800$ nm, the periodic multilayer which is constructed by this symmetrical structure, can provide a wide passband between 380 to 780 nm.

Again, a substrate matching layer is needed at $\lambda = 550$ nm for this design since its equivalent index ($N_{a_1AbBaAbB_1A} = 1.124$) is very different from the optical admittance of silicon. Low-stress silicon nitride with $n=2.2$ can be employed for this matching layer. The resulting theoretically designed structure is presented in Table 2, and its reflectance curve can be seen in Figure 5.

<table>
<thead>
<tr>
<th>Matching Structure With Air</th>
<th>Matching Structure With Substrate</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Basic Structure</strong> $(a_1AbBaAbB_1A)^5$</td>
<td><strong>LOW-STRESS NITRIDE</strong> $n=2.2; d = 62.5$ nm</td>
</tr>
<tr>
<td>OXIDE $n = 1.46; d = 90$ nm</td>
<td><strong>OXIDE</strong> $n = 1.46; d = 90$ nm</td>
</tr>
<tr>
<td>NITRIDE $n = 2; d = 150.3$ nm</td>
<td>NITRIDE $n = 2; d = 136.6$ nm</td>
</tr>
<tr>
<td>OXIDE $n = 1.46; d = 24.7$ nm</td>
<td>OXIDE $n = 1.46; d = 90$ nm</td>
</tr>
</tbody>
</table>

Taking dispersion into account, the performance of this design improves considerably due to a significant decrease in reflectance within the passband, as it can be seen in Figure 6.
Figure 4. The reflectance curves of one order stopband suppressed structure resulted by setting $\lambda/\lambda_0 = 2, \lambda_0 = 1100$ nm (solid line) and $\lambda/\lambda_0 = 3, \lambda_0 = 1650$ nm (dashed line).

Figure 5. The reflectance curves of the two order stopband suppressed coatings: As designed, without matching structure (solid line), and with matching structure (dashed line), respectively.
The optimization of this design was quite easy since the initial design provided a good performance. The optimization was done by varying both the thicknesses and refractive indices of the coating's layers and setting the optimization bandwidth target from 390 nm to 780 nm. The final structure after optimization and its performance are presented in Table 3 and in Figure 6, respectively.

Conclusions

1. A broadband anti-reflecting coatings using Silicon-compatible materials was designed. The AR provides a low reflectance (<10% within the passband) for a Si substrate (not glass, as is the target in the majority of literature sources) in the wavelength range 380 to 780 nm.

2. The method based on the main properties of symmetrical multilayer periods could be used in the design of broadband anti-reflecting thin film filters using Silicon-compatible material, but needs optimization process by varying both thicknesses and refractive indices of the coating’s layers.

3. The final design performance provides a larger reflectance ripple in the passband. However, as long as a low reflectance can be achieved within passband, this feature is not a problem.

4. The real limitation in the optical thin-film filters is the capability of the fabrication process to produce layers of precisely the correct optical constants and thickness. This aspect could not be examined here because, on one hand, of the limited available time, and on the other hand, due to the limited scope of the project which had to focus only on the finding the best optimized designs most suitable for subsequent practical realization. Therefore, an important recommendation for future work is related to performing the actual implementation of the filters and then measuring their performance and compare the measured characteristics with the theoretically predicted ones.

Figure 6. The reflectance curves of the two order stopband suppressed structures, calculated after taking into account the dispersion of the real materials and after optimization, respectively.
Table 3. The design structures after computer optimization

<table>
<thead>
<tr>
<th>λ₀</th>
<th>One order stopband suppression</th>
<th>Two order stopband suppression</th>
</tr>
</thead>
<tbody>
<tr>
<td>1100 nm</td>
<td></td>
<td>1800 nm</td>
</tr>
<tr>
<td>Band-width</td>
<td>380.3 nm - 780 nm</td>
<td>380.3 nm - 780 nm</td>
</tr>
<tr>
<td>Average R in bandwidth</td>
<td>2.1224 %</td>
<td>3.5609 %</td>
</tr>
<tr>
<td>Ripple Variation</td>
<td>3.8447</td>
<td>6.6718</td>
</tr>
<tr>
<td>R_max</td>
<td>5.3311 %</td>
<td>5.8513 %</td>
</tr>
</tbody>
</table>

Basic Structure

<table>
<thead>
<tr>
<th></th>
<th>LIT-SIO2 n=1.46 d= 89.38 nm</th>
<th>LIT-SIO2 n=1.46 d= 88.30 nm</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>LS-SIN n=2.253 d= 115.39 nm</td>
<td>LS-SIN n=2.253 d= 129.56 nm</td>
</tr>
<tr>
<td></td>
<td>LIT-SIO2 n=1.46 d= 177.03 nm</td>
<td>LIT-SIO2 n=1.46 d= 21.06 nm</td>
</tr>
<tr>
<td></td>
<td>LS-SIN n=2.253 d= 115.60 nm</td>
<td>LS-SIN n=2.253 d= 130.85 nm</td>
</tr>
<tr>
<td></td>
<td>LIT-SIO2 n=1.46 d= 171.07 nm</td>
<td>LIT-SIO2 n=1.46 d= 168.38 nm</td>
</tr>
<tr>
<td></td>
<td>LS-SIN n=2.253 d= 108.42 nm</td>
<td>LS-SIN n=2.253 d= 106.88 nm</td>
</tr>
<tr>
<td></td>
<td>LIT-SIO2 n=1.46 d= 165.59 nm</td>
<td>LIT-SIO2 n=1.46 d= 155.75 nm</td>
</tr>
<tr>
<td></td>
<td>LS-SIN n=2.253 d= 110.25 nm</td>
<td>LS-SIN n=2.253 d= 102.81 nm</td>
</tr>
<tr>
<td></td>
<td>LIT-SIO2 n=1.46 d= 173.75 nm</td>
<td>LIT-SIO2 n=1.46 d= 160.31 nm</td>
</tr>
<tr>
<td></td>
<td>LS-SIN n=2.253 d= 126.27 nm</td>
<td>LS-SIN n=2.253 d= 101.20 nm</td>
</tr>
<tr>
<td></td>
<td>LIT-SIO2 n=1.46 d= 39.22 nm</td>
<td>LIT-SIO2 n=1.46 d= 154.99 nm</td>
</tr>
<tr>
<td></td>
<td>LS-SIN n=2.253 d= 104.30 nm</td>
<td>LS-SIN n=2.253 d= 155.78 nm</td>
</tr>
<tr>
<td></td>
<td>LIT-SIO2 n=1.46 d= 159.95 nm</td>
<td>LS-SIN n=2.253 d= 100.13 nm</td>
</tr>
<tr>
<td></td>
<td>LS-SIN n=2.253 d= 103.95 nm</td>
<td>LIT-SIO2 n=1.46 d= 152.67 nm</td>
</tr>
<tr>
<td></td>
<td>LIT-SIO2 n=1.46 d= 152.67 nm</td>
<td>LS-SIN n=2.253 d= 107.16 nm</td>
</tr>
<tr>
<td></td>
<td>LS-SIN n=2.253 d= 152.67 nm</td>
<td>LIT-SIO2 n=1.46 d= 170.02 nm</td>
</tr>
<tr>
<td></td>
<td>LS-SIN n=2.253 d= 126.77 nm</td>
<td>LS-SIN n=2.253 d= 103.13 nm</td>
</tr>
<tr>
<td></td>
<td>LIT-SIO2 n=1.46 d= 39.22 nm</td>
<td>LIT-SIO2 n=1.46 d= 139.13 nm</td>
</tr>
</tbody>
</table>

Matching Structure With Substrate

<table>
<thead>
<tr>
<th></th>
<th>LS-SIN n=2.2 d= 65.23 nm</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>LS-SIN n=2.2 d= 64.81 nm</td>
</tr>
</tbody>
</table>

References


