Simulation of Multilayer Layer Antireflection Coating for Visible and Near IR Region on Silicon Substrate Using Matlab Program

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ABSTRACT
In this work, double layer and three antireflection coating were designed and simulated, optical reflection values were deduced with a matrix formulation via a personal computer using matlab program, six materials has been selected to investigated of the reflection as function of wavelength in visible region and near IR between (400-1200nm) on silicon substrate and central wavelength at 900nm the result show double layer quarter-quarter wave optical thickness has good preference antireflection has been reduced reflection from 32% for silicon surface to 3% and for three layer coatings, the results obtained broadband antireflection spectra and several form antireflection that have zero reflection in double and three layer antireflection coating. The refractive index and the optical thickness of each layer are adjusting to optimum antireflection coatings on silicon solar cells.

Keywords: antireflection, thin film, matlab, simulation, reflection.

محاكاة متعدد الطبقات لطلاء مضاد للانعكاس بالنسبة للمنطقة المرئية وتحت الحمراء القريبة على قاعدة من السليكون باستخدام برمجة الماتلاب

الخلاصة
في هذا البحث تم دراسة طلاء مضاد للانعكاس مكون من طبقتين وثلاثة طبقات باستخدام تصميم نظام محاكاة حساب القيم البصرية للانعكاس باستخدام نظم المصفوفات باستخدام الحاسب
Simulation of Multilayer Layer Antireflection Coating for Visible and Near IR Region on Silicon Substrate Using Matlab Program

INTRODUCTION

In an attempt to reduce the surface reflectance, silicon (Si) surfaces were textured, which could reduce the surface reflectance to about 11% [1]. Since a mirror-polished Si surface reflects about 36% of the incident light beams, a surface texturing improves surface reflectance by 30.6%. However, the reflectance of a textured surface is still high for solar-cell application, so single crystal Si substrates were investigated antireflection (AR) coatings [2,3].

Conventional single layer AR (Antireflection) coatings with minimum reflectance are not enough to cover the broad rage of the solar spectrum, many research groups have investigated double and more layer AR coatings [4].

Antireflection (AR) coatings for the visible and the infrared regions have long been the subject of much research and development because they are very important and useful in the solar cell [2].

Silicon is a semiconductor optical material with relatively high refractive index [3]. It is used in infrared devices as windows, lenses and transmission filters AR coatings have been widely used in many applications including glass lenses, eyeglasses, lasers, mirrors, solar cells, IR diodes, multipurpose broad and narrow band-pass filters, architectural and automotive glass and displays such as cathode ray tubes, as well as plasma, liquid crystal and flat panel displays [2,4]. In addition, highly reflecting dielectric mirrors have been developed to be used in gas lasers and in Fabry-Perot interferometers [5]. The most important application of silicon in the visible near IR region is photovoltaic solar cells [6].

Conversion of solar energy into other energy forms is more effective if the reflectance of light-receiving surface of solar device is minimal in the solar spectrum range [4]. Efficiency of a solar cell and its lifetime can be raised by coating the light sensitive surface of the cell with an antireflection coating [7-8].

This coating reduces the reflectance of the light incident on the cell surface and also protects it from radiations and atmospheric effects [7].

و باستخدام برنامج الماتلاب ، تم استخدام ستة مواد بصرية لدراسة انعكاساتها في المنطقة المرئية و تحت الحمراء القريبة بين (1200-400nm) على قاعدة من السليكون عند طول موجة تessions الملاحظات التي تم الحصول عليها في طلاء طبقتين لسمك بصري ربع طول موجة تـ900nm الحصول على أفضل مضادة للانعكاس حيث قلت الانعكاسية من 32% بالنسبة لسطح السليكون إلى 3% أما في الطلاء ثلاث طبقات فقد تم تقليل الانعكاسية بدء طيفي أومع وتم الحصول على عدد انعكاس لكلا الطبقتين وثلاث طبقات في عدة أشكال . معالع الاكسار والسمك البصري لكل طبقة ينظم لأفضل طبقة طلاء مضادة للانعكاس على الخلايا الشمسية السليكونية.
The high reflection index of silicon causes important reflection loss from its surface, even in thin film form. Therefore, its surface should be coated with an antireflection coating to reduce the reflectance or to increase the transmittance. The principle of the single and multilayer antireflection coatings is based on the destructive interference of light reflected from the interfaces of the coating layers [9].

The aim of this study is to present an computational process for the numerical design and simulated of antireflection coatings.

THEORY AND NUMERICAL DESIGN OF ANTIREFLECTION COATINGS

The optical matrix approach was employed for $N$-layer design of antireflection coatings. The main idea of this method is matching the $E$ and $H$ fields of the incident light on the interfaces of multilayer optical coatings. The matrix relation defining the $N$-layer antireflection coating problem is given by [7]

$$
\begin{bmatrix}
B \\
C
\end{bmatrix} = \prod_{j=1}^{N} \begin{bmatrix}
\cos \delta_j & i \sin \delta_j/n_j \\
- i n_j \sin \delta_j & \cos \delta_j
\end{bmatrix} \begin{bmatrix}
1 \\
n_e
\end{bmatrix} 
$$

where $B$ and $C$ are total electric and magnetic field amplitudes of the light propagating in the medium. Thus optical admittance is given by the ratio

$$
Y = C/B 
$$

Characteristics matrices are usually used to calculate the reflectance of an assembly of thin films layers. The characteristic matrix at a wavelength $\lambda$ for the assembly of $N$ layers is given by

$$
M = M_1 M_2 \cdots \cdots \cdots M_N 
$$

Thus, each layer is represented by a $2 \times 2$ matrix $M$, of the form

$$
M_j = \begin{bmatrix}
\cos \delta_j & i \sin \delta_j/n_j \\
n_j \sin \delta_j & \cos \delta_j
\end{bmatrix} 
$$

where $n_j$ is the refractive index of the layer and $\delta_j$ is its phase thickness given by:

$$
\delta_j = 2\pi n j/\lambda 
$$
with the physical thickness of the layer being \( d_j \), then the reflection coefficient \( r \) and the reflectance \( R \) are, respectively, given by

\[
r = \frac{n_0 - Y}{n_0 + Y}
\]

\[
R = \frac{r}{r^*}
\]

\[
\begin{align*}
R &= \left( \begin{array}{c}
\frac{n_0 - Y}{n_0 + Y} \\
\frac{n_0 + Y}{n_0 - Y}
\end{array} \right) \left( \begin{array}{c}
\frac{n_0 - Y}{n_0 + Y} \\
\frac{n_0 + Y}{n_0 - Y}
\end{array} \right)^* \\
&= \frac{r}{r^*}
\end{align*}
\]  

\[ \text{(7)} \]

where \( R = \frac{r}{r^*} \)

**DOUBLE-LAYER ANTIREFLECTION COATINGS**

According to the double layer AR coating theory for nonabsorbing films and for normal incidence of light, the matrix equation becomes [7].

\[
\begin{pmatrix}
B \\
C
\end{pmatrix} = \begin{pmatrix}
\cos \delta_1 & i \sin \delta_1/n_1 & \\
i \sin \delta_1 \cos \delta_1
\end{pmatrix} \begin{pmatrix}
\cos \delta_2 & i \sin \delta_2/n_2 & \\
i \sin \delta_2 \cos \delta_2
\end{pmatrix}
\]  

\[ \text{\begin{align*}
\begin{pmatrix}
B \\
C
\end{pmatrix} = \begin{pmatrix}
\cos \delta_1 & i \sin \delta_1 \\
i \sin \delta_1 \cos \delta_1
\end{pmatrix} \begin{pmatrix}
\cos \delta_2 & i \sin \delta_2 \\
i \sin \delta_2 \cos \delta_2
\end{pmatrix} \begin{pmatrix}
\cos \delta_3 & i \sin \delta_3 \\
i \sin \delta_3 \cos \delta_3
\end{pmatrix}
\end{align*}\]  

\[ \text{\begin{align*}
\begin{pmatrix}
B \\
C
\end{pmatrix} = \begin{pmatrix}
\cos \delta_1 & i \sin \delta_1 \\
i \sin \delta_1 \cos \delta_1
\end{pmatrix} \begin{pmatrix}
\cos \delta_2 & i \sin \delta_2 \\
i \sin \delta_2 \cos \delta_2
\end{pmatrix} \begin{pmatrix}
\cos \delta_3 & i \sin \delta_3 \\
i \sin \delta_3 \cos \delta_3
\end{pmatrix}
\end{align*}\]  

\[ \text{(8)} \]

**Three-layer antireflection coatings**

According to the double layer AR coating theory for nonabsorbing films and for normal incidence of light, the matrix equation becomes [7].

\[
\begin{pmatrix}
B \\
C
\end{pmatrix} = \begin{pmatrix}
\cos \delta_1 & i \sin \delta_1 \\
i \sin \delta_1 \cos \delta_1
\end{pmatrix} \begin{pmatrix}
\cos \delta_2 & i \sin \delta_2 \\
i \sin \delta_2 \cos \delta_2
\end{pmatrix} \begin{pmatrix}
\cos \delta_3 & i \sin \delta_3 \\
i \sin \delta_3 \cos \delta_3
\end{pmatrix} \begin{pmatrix}
\cos \delta_4 & i \sin \delta_4 \\
i \sin \delta_4 \cos \delta_4
\end{pmatrix} \begin{pmatrix}
\cos \delta_5 & i \sin \delta_5 \\
i \sin \delta_5 \cos \delta_5
\end{pmatrix} \begin{pmatrix}
\cos \delta_6 & i \sin \delta_6 \\
i \sin \delta_6 \cos \delta_6
\end{pmatrix} \begin{pmatrix}
\cos \delta_7 & i \sin \delta_7 \\
i \sin \delta_7 \cos \delta_7
\end{pmatrix}
\]

\[ \text{(9)} \]

**Quarter-wave optical thickness antireflection coating**

The reflectance for a quarter wave thickness at normal incidence the matrix equation becomes
HALF- WAVE OPTICAL THICKNESS ANTIREFLECTION COATING

The reflectance for a half wave thickness at normal incidence the matrix equation becomes

\[
\begin{pmatrix}
0 & \frac{1}{n_j}
\end{pmatrix}
\begin{pmatrix}
\frac{1}{n_j}
& 0
\end{pmatrix}
\]

……………(10)

From (8), (7), (10) and (11) The reflectance reduced to zero (\( R=0 \)) then

\[
n_2/n_1=(n_0n_s)^{1/2}
\]

………………(12)

or

\[
n_{13}=n_02n_s
\]

………………..(13)

\[
n_{23}=n_0n_s2
\]

………………..(14)

where \( n_0=1 \) for air and \( n_s=3.5 \) for Si
can be written in \( n_1=(n_s)^{1/3} \) and \( n_2=(n_s)^{2/3} \)

\[
n_1=1.51
\]

so must be select materials have refractive index about 1.5 , the materials (SiO\(_2\)=1.44, MgF\(_2\)=1.38) have been selected for top layer antireflection antireflection coating in our program [7,5]

\[
n_2=2.3
\]

so must be select materials have refractive index about 2.3 , the materials (CeO\(_2\)=2.2, ZnS=2.3) have been selected for bottom layer coating in our program [7]

2.6 Solution of three- layer antireflection coatings

From (9), (7), (10) and (11) The reflectance reduced to zero (\( R=0 \)) then

\[
n_{14}=n_03n_s
\]

So \( n_1=1.36 \)

………………..(15)

\[
n_{24}=n_02n_s2
\]

So \( n_2=1.87 \)

………………..(16)

\[
n_{34}=n_0n_s3
\]

So \( n_3=2.5 \)

………………..(17)
for

\[ n_1 \text{ was selected materials (SiO}_2=1.44, \text{MgF}_3=1.38) \]
\[ n_2 \text{ was selected materials (SiO}=1.95, \text{CeF}_3=1.7) \]
\[ n_3 \text{ was selected materials (ZnS}=2.3, \text{CeO}_2=2.2) \] [8].

3. Simulation in Matlab

The simulation of the reflection in matlab have been the main assignment of this work. The reflectivity of the silicon has been simulated with two, three layers of antireflection coatings the program optimize at \( \lambda_0=900\text{nm} \) central wavelength for visible and near infrared spectral region. the parameters of antireflection optical thickness for each layers.

Reflection index for each layer coating and substrate [10].

The materials must be select that low wave absorption, homogeneity, high packing density, good adhesion, low stress, hardness and ability to survive in deferent environmental, low cost and easy preparation [11].

RESULTS AND DISCUSSION

Double-layer antireflection coating

The refractive index \( n_s \) of silicon in the region between (400-1200nm) is 3.5 [9], therefore when the surrounding medium is air \( n_0=1 \) the reflective index of the first layer should have coating materials value about 2.3 according to the condition in equation (13) and (14) so the first layer (SiO2,MgF2) and second layer (CeO2,ZnS) materials was selected, the Figs. (1-4) show reflectance spectra of double-layer coating for four dielectric materials with variety optical thickness.

The figure (1) show the reflectance spectra as a function of wavelength for quarter-quarter antireflection coating on silicon and uncoated silicon surface, all curves in the figure have nearly the same behavior, the silicon reflectance surface reduced from 32\% to less than 5\% in range between (700-1200nm) and zero reflection at 700nm and the best curve antireflection is (d) illuminated in the figure.

The higher reflection values at the shorter wavelengths particularly in the region between (400-700nm) are attributed to small variation in thickness and refractive index of the materials leading to higher reflection value. This is form its suitable for antireflection coating on silicon and can be used in silicon solar cells [6].

The multilayer antireflection coatings are based on the destructive interference of beams reflected from the interfaces of the layers [4].

figures (2) and (3) show the reflectance spectra of quarter-half for figure (2) and half-quarter for fig.(3) wave optical thickness of bauble layer coating. These figures have nearly the same behavior and have broadband antireflection spectral region in range between (580-1200nm) but there is no zero reflection because the different thickness compared with figure (1), they good application in silicon solar cells, they would be increase quantum efficiency of optoelectronic device [12].
Fig. 4 shows reflectance spectra of half-half wave optical thickness of double-layer coating the figure, showing failure to reduce reflection particularly between 700-1200 nm but only range between 550-700 nm was reduced reflection. This form couldn’t be used in antireflection on silicon solar cells but they may be capable of using antireflection coating in green and red light detectors or as filter applications [3].

**Three-layer antireflection coating**

Figure (5) shows reflectance spectra of three-layer coating for six dielectric materials. The form antireflection coating was shown below the figure, in this figure, two dielectric materials have been changed in each layer according to paragraph (2-6). Figure 5 shows the reflectance spectra of quarter-quarter-quarter layer coating on silicon all curves exhibit the same behavior, the figure shows that antireflection coating reduces the reflection from 32% to less than 10%. In this figure there are two zero reflections, the first at 600 nm and the second at 900 nm due to high transmittance in these regions [8].

Figure 6 shows reflectance spectra of three-layer coating with the form antireflection coating was shown below the figure, this figure has broadband antireflection if compared with figure (5), it has reduced reflectance in the range between 540-1200 nm. The two figures above are just suitable for use in silicon solar cells [3].

The figures 7 and 8 show reflectance spectra, the form of the antireflection coating was shown below the figures. The figures aren't different in form; they exhibit the same behavior; the two figures have a maximum reflectance of 17% for broadband spectra; this form may be unsuitable or ineffective in silicon solar cells [9].

The figures (9) and (11) show reflectance spectra, the form of the antireflection coating was shown below the figure, the figures exhibit the same behavior, the antireflection coating reduces the reflection from 32% to less than 15% this figures, have broadband spectra; antireflection coating this form may be suitable for use in silicon solar cells.

The figure (10) exhibits the same behavior of the figure (4), this form couldn’t be used in antireflection on silicon solar cells.

**CONCLUSIONS**

In this work, we have presented the optical matrix approach method to design and simulated multilayer antireflection coatings in visible and near IR region using MATLAB program starting from double-layer up to three-layer at central wavelength $\lambda = 900$ nm. The refractive index and the optical thickness of each layer are adjusting to optimum antireflection coatings on silicon solar cells.

Since the refractive index of silicon is relatively high, its surface reflects a high portion of the incident radiation throughout the spectral range between 400 and 1200 nm. The way to reduce this reflectance is to coat the surface of silicon with at least a single layer, in this work, design and simulated antireflection coating of silicon with double and three layer. In the Double-layer antireflection coating, the form (d) in figure (1) is illuminated the best antireflection its reduce reflection less than 3%
between 700-1200nm A more effective reflectance reduction in a broad spectral region can be obtained with quarter-half-quarter wave optical thickness coatings, in narrow band antireflection spectra can be use (such as figure (4)) as filter application.

REFERENCE
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Figure (1) Reflectance spectra of (a) an uncoated Silicon surface and double-layer coating for four dielectric materials with optical thickness arranged below 
(b) SiO₂(1/4)+ZnS(1/4)/Si, (c)SiO₂(1/4)+CeO₂ (1/4)/Si, (d)MgF₂(1/4)+ CeO₂(1/4)/Si, 
(e) MgF₂(1/4)+CeO₂(1/4)/Si.

Figure (2) Reflectance spectra of (a) an uncoated Silicon surface and double-layer coating for four dielectric materials with optical thickness arranged below 
(b) SiO₂(1/4)+ZnS(1/2)/Si, (c)SiO₂(1/4)+CeO₂ (1/2)/Si, (d)MgF₂(1/4)+ ZnS(1/2)/Si, 
(e) MgF₂(1/4)+CeO₂(1/2)/Si.
Simulation of Multilayer Layer Antireflection Coating for Visible and Near IR Region on Silicon Substrate Using Matlab Program

Figure (3) Reflectance spectra of (a) an uncoated Silicon surface and double-layer coating for four dielectric materials with optical thickness arranged below (b) SiO$_2$(1/2)+ZnS(1/4)/Si, (c)SiO$_2$(1/2)+CeO$_2$ (1/4)/Si, (d)MgF$_2$(1/2)+ ZnS(1/4)/Si, (e) MgF$_2$(1/2)+CeO$_2$(1/4)/Si.

Figure (4) Reflectance spectra of (a) an uncoated Silicon surface and double-layer coating for five dielectric materials with optical thickness arranged below (b) SiO$_2$(1/2)+ZnS(1/2)/Si, (c)SiO$_2$(1/2)+CeO$_2$ (1/2)/Si, (d)MgF$_2$(1/2)+ ZnS(1/2)/Si, (e) MgF$_2$(1/2)+CeO$_2$(1/2)/Si.
Figure (5) Reflectance spectra of (a) an uncoated Silicon surface and three-layer coating for six dielectric materials with optical thickness arranged below (b) SiO$_2$(1/4)+SiO(1/4)+ZnS(1/4)/Si, (c) MgF$_3$(1/4)+SiO(1/4)+ZnS(1/4)/Si, (d) SiO$_2$(1/4)+CeF$_2$(1/4)+CeO$_2$(1/4)/Si, (e) MgF$_3$(1/4)+CeF$_2$(1/4)+CeO$_2$(1/4)/Si.

Figure (6) Reflectance spectra of (a) an uncoated Silicon surface and three-layer coating for six dielectric materials with optical thickness arranged below (b) SiO$_2$(1/4)+SiO(1/2)+ZnS(1/4)/Si(c) MgF$_3$(1/4)+SiO(1/2)+ZnS(1/4)/Si, (d) SiO$_2$(1/4)+CeF$_2$(1/2)+CeO$_2$(1/4)/Si(e) MgF$_3$(1/4)+CeF$_2$(1/2)+CeO$_2$(1/4)/Si.
Simulation of Multilayer Layer Antireflection Coating for Visible and Near IR Region on Silicon Substrate Using Matlab Program

Figure (7) Reflectance spectra of (a) an uncoated Silicon surface and three-layer coating for six dielectric materials with optical thickness arranged below (b) SiO$_2$(1/2)+SiO(1/4)+ZnS(1/4)/Si, (c) MgF$_3$(1/2)+SiO(1/4)+ZnS(1/4)/Si, (d) SiO$_2$(1/2)+CeF$_2$(1/4)+CeO$_2$(1/4)/Si, (e) MgF$_3$(1/2)+CeF$_2$(1/4)+CeO$_2$(1/4)/Si.

Figure (8) Reflectance spectra of (a) an uncoated Silicon surface and three-layer coating for six dielectric materials with optical thickness arranged below (b) SiO$_2$(1/4)+SiO(1/4)+ZnS(1/2)/Si, (c) MgF$_3$(1/4)+SiO(1/4)+ZnS(1/2)/Si, (d) SiO$_2$(1/4)+CeF$_2$(1/4)+CeO$_2$(1/2)/Si, (e) MgF$_3$(1/4)+CeF$_2$(1/4)+CeO$_2$(1/2)/Si.
Figure (9) Reflectance spectra of (a) an uncoated Silicon surface and three-layer coating for six dielectric materials with optical thickness arranged below (b) SiO\(_2\)(1/4)+SiO(1/2)+ZnS(1/2)/Si, (c)MgF\(_3\)(1/4)+SiO(1/2)+ZnS (1/2)/Si, (d) SiO\(_2\)(1/4)+CeF\(_2\)(1/2)+CeO\(_2\)(1/2)/Si (e)MgF\(_3\)(1/4)+CeF\(_2\)(1/2)+CeO\(_2\)(1/2)/Si

Figure (10) Reflectance spectra of (a) an uncoated Silicon surface and three-layer coating for six dielectric materials with optical thickness arranged below (b) SiO\(_2\)(1/4)+SiO(1/2)+ZnS(1/2)/Si, (c)MgF\(_3\)(1/4)+SiO(1/2)+ZnS (1/2)/Si, (d) SiO\(_2\)(1/4)+CeF\(_2\)(1/2)+CeO\(_2\)(1/2)/Si (e)MgF\(_3\)(1/4)+CeF\(_2\)(1/2)+CeO\(_2\)(1/2)/Si
Figure (11) Reflectance spectra of (a) an uncoated Silicon surface and three-layer coating for six dielectric materials with optical thickness arranged below
(b) $\text{SiO}_2(1/2)+\text{SiO}(1/2)+\text{ZnS}(1/4)/\text{Si}$
(c) $\text{MgF}_3(1/2)+\text{SiO}(1/2)+\text{ZnS}(1/4)/\text{Si}$
(d) $\text{SiO}_2(1/2)+\text{CeF}_2(1/2)+\text{CeO}_2(1/4)/\text{Si}$
(e) $\text{MgF}_3(1/2)+\text{CeF}_2(1/2)+\text{CeO}_2(1/4)/\text{Si}$.