Finite element analysis of antireflective silicon nitride sub-wavelength structures for solar cell applications

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Abstract

We numerically calculate the spectral reflectivity of the silicon nitride (Si3N4) sub-wavelength structure (SWS) using a two-dimensional finite element simulation. The geometry-dependent effective reflectance of the Si3N4 SWS over the wavelength ranging from 400 nm to 1000 nm is examined and the structure of Si3N4 SWS is further optimized for the lowest effective reflectance. A p–n junction solar cell efficiency based on the optimized Si3N4 SWS is also calculated, resulting in an improvement of 0.98% in efficiency than that of single layer antireflection coatings.

1. Introduction

Antireflection coating (ARC) has been a vital part in designing high efficient solar cells. Double layer antireflection (DLAR) coatings have attracted much attention due to the advantages in covering a broad range of solar spectrum than single layer antireflection (SLAR) coatings. However, the DLAR coatings or multilayer ARCs usually require expensive facilities to precisely control the vacuum conditions, material compositions, and layer thickness. A relatively low cost alternative to the multilayer ARCs is the sub-wavelength structure (SWS) using a two-dimensional finite element simulation. The geometry-dependent effective reflectance data obtained is then used in PC1D to estimate the electrical characteristics of a p–n junction solar cell, i.e., the short-circuit current, JSC, the open-circuit voltage, VOC, and the cell efficiency, η. The solar efficiencies of Si3N4 SWS, SLAR, and DLAR coatings are further compared to each other.

The effective reflectance of the optimized pyramid-shaped silicon nitride (Si3N4) SWS has been examined and compared with SLAR and DLAR coatings using a rigorous coupled-wave approach (RCWA). The simulation results clearly show that the Si3N4 SWS can act as a second ARC layer which can facilitate the efficiency in solar cell. Herein, we continue to numerically calculate the effective reflectance of the Si3N4 SWSs, which comprise a Si3N4 layer superimposed an etched Si3N4 grating with the cross-section of the strip in triangular shape using a real space finite element analysis, where RF module in COMSOL is performed. Instead of using a constant refractive index for Si, a wavelength-dependent dispersion expression is implemented in this calculation for the Si3N4 SWS. We optimize the geometry of Si3N4 SWSs to get the best effective reflectance. The effective reflectance data obtained is then used in PC1D to estimate the electrical characteristics of a p–n junction solar cell, i.e., the short-circuit current, JSC, the open-circuit voltage, VOC, and the cell efficiency, η. The solar efficiencies of Si3N4 SWS, SLAR, and DLAR coatings are further compared to each other.

2. Numerical model

The proposed geometry of Si3N4 SWSs is displayed in the Fig. 1(a), which mainly includes a Si3N4 layer superimposed an etched Si3N4 grating with the cross-section of the strip in triangular shape. Assuming an infinite long grating, the three-dimensional (3D) structure can be further reduced to a 2D domain with a unit cell by taking the cross-section of the Si3N4 SWS. Fig. 1(b) shows the geometry parameters of the 2D case, in which we define the height and base width of the etched Si3N4 grating and the thickness of the Si3N4 layer to be h, b, and s, respectively. Furthermore, the spacing...
between two adjacent strips is defined as 2w. These parameters make it possible to study the density effect of the etched Si$_3$N$_4$ SWS that is infeasible in the previous analytical model by RCWA [15]. In the present 2D study, there is no variation in the z direction; the electromagnetic field propagates in the xy-plane only. The polarization of the incident electromagnetic wave can be then decoupled and separated as the transverse electric and transverse magnetic polarizations (TE and TM, respectively). In the TE polarization the magnetic field is a scalar and is normal to the 2D plane while the electric field is a vector and is in the transverse (in-plane) direction. On the contrary, for the TM case, the electric field and magnetic field switch orientation relative to TE one. Thus, Maxwell’s equations for these two cases are then expressed as the following formulas.

\[
\nabla \times (\varepsilon_r^{-1} \nabla \times H_z) = \left(\frac{\omega}{c}\right)^2 H_z (\text{TE polarization}),
\]

and

\[
\nabla \times (\nabla \times E_z) = \varepsilon_r \left(\frac{\omega}{c}\right)^2 E_z (\text{TM polarization}),
\]

where \(\varepsilon_r\) is the relative permittivity and is equal to \(n^2\), in which \(n\) is the refractive index. In the model, the port boundary condition (BC) [16] is applied on the top edge to excite a normal incident plane wave with TE polarization. While using port BC, the reflection coefficient at this port, \(S_{11}\), is automatically defined. The definition of \(S_{11}\) in terms of the power flow is expressed below.

\[
S_{11} = \frac{\sqrt{\text{Power reflected from port 1}}}{\text{Power incident on port 1}}
\]

Such a definition results in the absolute value and does not contain any phase information. The reflectance can then be computed by taking \(|S_{11}|^2\). At the left and right edges of the 2D model, we used the Floquet BC:

\[
H_{\text{dest}} = H_{\text{source}} \exp[-ik(r_{\text{dest}}-r_{\text{source}})].
\]

This periodic BC ensures that a wave, when reaching the left edge (source), is transposed to the right edge (destination) with the appropriate phase shift. Note that an additional perfect matched layer (PML) is applied just below the silicon substrate, which absorbs incoming waves without any reflection. At the bottom edge of the PML, a scattering BC is considered to further reduce the residual reflection.

The refractive index of Si$_3$N$_4$ is kept to be a constant value of 2.05 in our model since it is a weakly absorbing material [18]. Moreover, an empirically fitted formula for the wavelength-dependent refractive index, \(n_\text{Si}\), of Si is employed in this model [19].

\[
n_\text{Si} = \sqrt{\frac{C + A}{\lambda^2} + \frac{B \lambda^2}{(\lambda^2 - \lambda^2_0)^2}}
\]

where \(C = 11.6858\), \(A = 0.939816 \times 10^{-12} \text{ m}^2\), \(B = 8.10461 \times 10^{-3}\) and \(\lambda_0 = 1.1071 \times 10^{-6} \text{ m}\).

Instead of calculating the reflectance for a certain wavelength, an effective reflectance \(R_{\text{eff}}\) [20] is computed for the Si$_3$N$_4$ SWS over the wavelength \(\lambda\) ranging from 400 nm to 1000 nm.

\[
R_{\text{eff}} = \frac{\int R(\text{Si}) \text{d}\lambda}{\int E(\text{Si}) \text{d}\lambda},
\]

where \(E(\lambda)\) is spectral irradiance given by ATMG173 AM1.5G reference [21], \(E(\lambda)\) is photon energy and \(R(\lambda)\) is the calculated reflectance \(|S_{11}|^2\). To optimize the geometrical parameters, the 2D simulation results of COMSOL RF module are then exported and linked to the command line of MATLAB®. Such procedure enables us to parametrically study the geometry-dependent effective reflectance.

Notably, the incident angle \(\theta\) of sunlight is assumed to be normal to the plane (i.e., \(\theta = 0\)), for the calculation of the reflection properties. For a normal incidence, the degree of polarization is irrelevant [22]. Once light enters into a solar cell with a surface grating, it propagates through the solar cell at a particular diffraction angle based on the diffraction order. Higher order diffractions that are caused by surface gratings for a 2D case is given by:

\[
n_\text{Si} \sin \theta_{\text{mn}} \cos \phi_{\text{mn}} = m \frac{\lambda}{\lambda_0},
\]

and

\[
n_\text{Si} \sin \theta_{\text{mn}} \sin \phi_{\text{mn}} = n \frac{\lambda}{\lambda_0},
\]

where \(\theta_{\text{mn}}\) and \(\phi_{\text{mn}}\) are the diffraction polar angle and azimuthal angle at the diffraction order of \((m, n)\), respectively. These gratings increase optical path lengths and light absorption near the band gap wavelength and are dominant only for those with periods greater than the wavelength of incident light. However, for subwavelength structures whose period is much less than the wavelength of incident light, the incident light propagates through the medium in a straight direction [23]. Consequently, we merely focus on reflectivity in this work without considering the diffraction orders.

3. Results and discussion

We compare the simulated reflectance spectra of the Si$_3$N$_4$ SWS with \(h = 150 \text{ nm}\) and \(s = 70 \text{ nm}\) using the finite element method (FEM) and the transfer matrix method (TMM) [15]. The results from both methods are shown in the Fig. 2, in which they are closely matched in the higher wavelength regions and have similar trends in lower wavelength regions (i.e. \(\lambda = 400 \text{ nm}\) to \(600 \text{ nm}\)) within 3% absolute difference. Since, the results obtained from FEM and TMM
are matched well, the FEM is further advanced to explore the reflectance properties of Si$_3$N$_4$ SWS.

We then examine the effective reflectance of Si$_3$N$_4$ SWS by varying the $h$ and $s$, where $b = 50$ nm and $\lambda$ varying from 400 nm to 1000 nm. Fig. 3 shows the contour plot of the effective reflectance as a function of $h$ and $s$ for Si$_3$N$_4$ SWS. In this geometry setting of Si$_3$N$_4$ SWS, the minimum of $R_{\text{eff}} = 1.98\%$ occurs at $h = 180$ nm and $s = 70$ nm, which can be seen from the Fig. 3.

To examine the effect of height to base width ratio of the etched Si$_3$N$_4$ grating, we vary the $h$ and $b$ by keeping $s$ fixed at 70 nm for the same wavelength range (i.e. from 400 nm to 1000 nm). The result is shown in the Fig. 4; from which we obtain the lowest effective reflectance for $h = 180$ nm and $b = 60$ nm. The height to base width at this geometry of the etched Si$_3$N$_4$ grating is then calculated to be 3.6. This observation suggests that proper design of base width is crucial to get the lowest reflectance for Si$_3$N$_4$ SWS.

To study the density effect on the reflection of Si$_3$N$_4$ SWS, we have changed the unit cell width, $W$, which is given by $(2w + b)$, in the Fig. 1, from 60 nm to 360 nm and kept the $h$, $s$, and $b$ constant at 180 nm, 70 nm, and 60 nm, respectively. The effective reflectance obtained from this variation of $W$ is shown in the Fig. 5. It is observed that when the unit cell width increases, i.e. the spacing between two adjacent strips increases, the effective reflectance decreases from around 9% to 2%, meaning that the effective reflectance decreases with decreasing the density. However, over a certain $W$, the effective reflectance increases gradually. The minimum of $R_{\text{eff}}$ is obtained for $W = 210$ nm.

Finally, the optimized Si$_3$N$_4$ SWS with $h = 180$ nm, $s = 70$ nm, $b = 60$ nm and $W = 210$ nm is obtained with effective reflectance of 1.97%. The reflectance spectra for this optimized structure for wavelength from 400 nm to 1000 nm is compared with those of SLAR coating with Si$_3$N$_4$ and DLAR coating with Si$_3$N$_4$/MgF$_2$ [15]. The reflectance spectra in comparison to each other are shown in the Fig. 6 and the effective reflectance for these three structures are tabulated in Table 1. From Table 1, it can be seen that the lowest effective reflectance is obtained for Si$_3$N$_4$ SWS as compared to SLAR and DLAR coatings.

To calculate the solar cell electrical characteristics including $J_{\text{SC}}$, $V_{\text{OC}}$, and $\eta$, we have used the simulated reflectance spectra of the optimized Si$_3$N$_4$ SWS as the input of the PC1D program, which solves...
the fully coupled nonlinear equations for the quasi-1D transport of electrons and holes in photovoltaic solar cells [17]. In the simulation, the solar cell settings used are the same as the previous study [15]. The $J_{SC}$ and $V_{OC}$ of the solar cell are calculated under the standard AM1.5 global spectrum [21] from its $I–V$ characteristics. Then, the $\eta$ of a solar cell is deduced out of the three photovoltaic parameters: $V_{OC}$, $J_{SC}$ and fill factor (FF) and is given by:

$$\eta = \frac{FF \cdot J_{SC} \cdot V_{OC}}{P_I};$$

where $P_I$ is defined as the incident power ($P_I = 0.1 \text{ W/cm}^2$ under illumination AM1.5 G), and

$$FF = \frac{P_{max}}{J_{SC} \cdot V_{OC}}.$$

In addition, the external quantum efficiency (EQE) is calculated using

$$\text{EQE} = 1 - \frac{\text{SR}}{q \left( \frac{hc}{\lambda} \right) / (1 - R)};$$

where SR is spectral response, $R$ is reflectance and $q$ is the elementary unit of charge. Electrical characteristics obtained from the PC1D simulation for the tested silicon solar cell using the reflectance spectra for the three different kinds of antireflection structures (i.e. $\text{Si}_3\text{N}_4$ SWS, DLAR and SLAR) are shown in the Fig. 7(a). The reflectance spectra for SLAR and DLAR structures are taken from our recent study [15]. It is clear that $J_{SC}$ and $V_{OC}$ of $\text{Si}_3\text{N}_4$ SWS are higher than those of $\text{Si}_3\text{N}_4$ SLAR and $\text{Si}_3\text{N}_4$/MgF$_2$ DLAR structures. A clear increase in $\eta$ of 0.98% has been observed for the silicon solar cell with $\text{Si}_3\text{N}_4$ SWS over a cell with single layer $\text{Si}_3\text{N}_4$ ARC calculated under the standard AM1.5 global spectrum. As shown in the Fig. 7(b), the calculated EQE over wavelength from 400 nm to 1000 nm also confirmed the higher efficiency of the simulated $\text{Si}_3\text{N}_4$ SWS, compared with $\text{Si}_3\text{N}_4$ SLAR and $\text{Si}_3\text{N}_4$/MgF$_2$ DLAR coatings.

4. Conclusions

In this paper, we have simulated $\text{Si}_3\text{N}_4$ SWS and optimized the reflectance properties for the $\text{Si}_3\text{N}_4$ SWS in terms of the effective reflectance. A lowest effective reflectance of 1.97% has been obtained for $\text{Si}_3\text{N}_4$ SWS with $h = 180 \text{ nm}$, $s = 70 \text{ nm}$, $b = 60 \text{ nm}$ and $W = 210 \text{ nm}$, respectively, which is much less than those obtained from 80 nm $\text{Si}_3\text{N}_4$ SLAR and $\text{Si}_3\text{N}_4$/MgF$_2$ DLAR coatings. The estimation of this study has shown that the increase of solar cell efficiency is 0.98% from the explored SWS, compared with the results of SLAR coating. This model provides an alternative to numerically investigate reflectance properties of the SWS for solar cell applications.

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