Comprehensive Study on Reflectance of Si_3N_4 Subwavelength Structures for Silicon Solar Cell Applications Using 3D Finite Element Analysis

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ABSTRACT

In this work, a full 3D finite element analysis for the silicon nitride (Si_3N_4) subwavelength structure (SWS) deposited on the antireflection coating (ARC) of a-Si thin film solar cell is conducted. We investigate the reflectance property of cylinder-, right circular cone-, and square pyramid shape of Si_3N_4 SWS with various heights and incident angles. The results show that the pyramid shape of SWS possesses the best reflectance property in the optical region from 400 nm to 1000 nm. Comparison with the RCWA work is also reported.

KEYWORDS: Finite Element Analysis, Silicon Nitride, Sub-Wavelength Structure, Shape Effect, Morphological Effect, Antireflection Coating, Reflectance, Solar Cell, Rigorous Coupled-Wave Approach.

1 INTRODUCTION

Solar cell is one of the most promising renewable energy technologies in order to relieve the impact of the climate change. In semiconductor based solar cells, electron-hole pairs are generated via absorption of impinging photons. Due to high refraction index of semiconductor materials, especially silicon, the incident sunlight power is largely reflected back, resulting in the reduction of light absorption and poor energy conversion efficiency. Antireflection coating (ARC) is mounted over absorption layers, resulting in three effects: (a) reduction in surface reflection, (b) increase in light absorption due to an increase in optical path length by diffraction, and (c) enhancement of internal reflection that reduces the amount of escaping light. Bases on the theory of impedance matching, single layer and multilayer of antireflection coating are proposed for reduced reflectance property; however, the resulting reflectance spectra meet the demand only within a narrow spectral domain. Subwavelength structure, whose dimensions are much smaller than the wavelengths of light, with ARC on the surface of solar cells can substantially reduce the reflectivity and improve the capability of light trapping, then achieve the enhanced efficiency, which was studied both numerically and experimentally recently [1-3]. Figure 1(a) to 1(c) exhibit the solar cell panel with Si_3N_4 SWS fabricated by our group [4]. Compared to Si solar cell with SLAR, the efficiency of solar cell with Si_3N_4 SWS is better shown in Table 1 [4]. Yet, the morphological effect on reflectance property is obscure. A rigorous coupled-wave analysis (RCWA) [5] has been reported to estimate the reflectance of Si_3N_4 SWS by approximating structural shapes with partitioned uniform homogeneous layers. However, RCWA has limited capability to investigate 3D problems, especially with non-azimuthally symmetric structural shapes. Therefore, a full 3D finite-element (FE) analysis of Si_3N_4 SWS will be an interesting examination for quantitative understanding of the reflectance property.

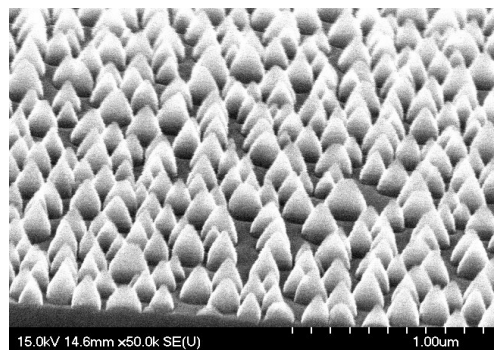

Figure 1: Photo-graphic images of the fabricated silicon solar cells with Si_3N_4 SWS. [4].

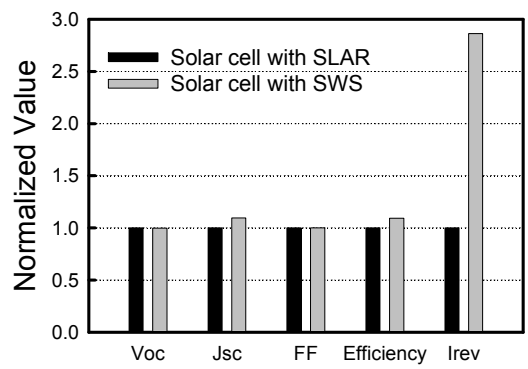

Figure 2: Measured solar cell I-V data for silicon nitride SLAR and silicon nitride SWS [4]. The difference of electrical characteristics is presented, where the I_{rev} is the leakage current. The p-type multi-crystalline Si wafer with resistivity of 1 Ω-cm and thickness of 200 μm is cleaned with H_2SO_4/H_2O_2 and followed by chemical polishing to remove surface damage. When a PSG is deposited on Si substrate, phosphorous starts to diffuse into the bulk and emitter is formed with junction depth of 0.6 μm. The area is 1 cm^2.

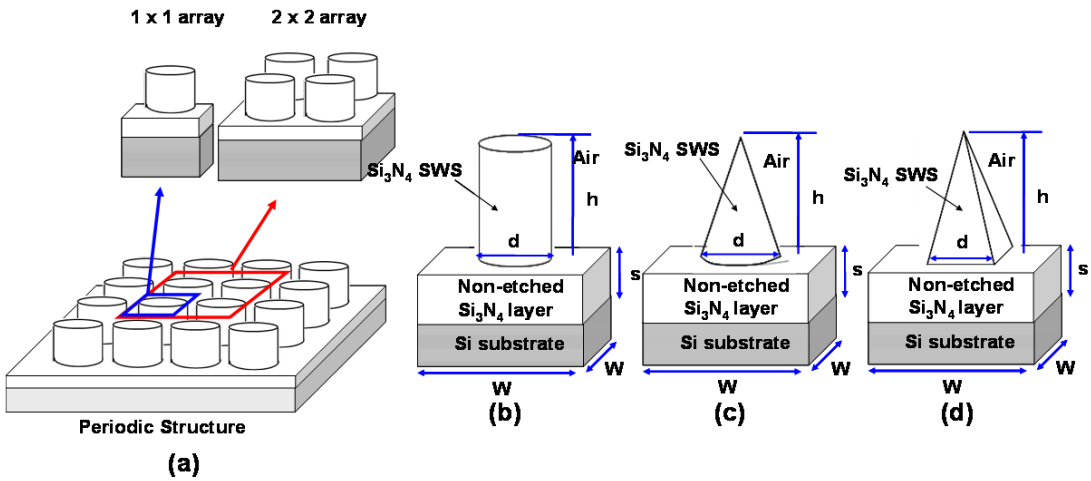

Figure 3: (a) Illustration of periodic structure of Si_3N_4 SWS with 1x1 and 2x2 array as unit cell. Schematic of (b) cylinder-, (c) right circular cone-, (d) square pyramid-shaped structure.

In this work, 3D FE analysis for the reflectance of Si_3N_4 SWS with three types of structural shapes was conducted for quantitative understanding of reflectance property. Proper selection on the boundary conditions can alleviate the computational load from simulating a holistic ARC. The reflectance of Si_3N_4 SWS with shapes of cylinder, right circular cone, and square pyramid on the Si substrate is thus calculated. The analysis of reflectance spectrum with wide-angle incidences of electromagnetic wave and the average reflectance with various heights are presented. Besides, according to the previous work our group studied earlier, which presented the optimal design parameters of Si_3N_4 SWS based on RCWA [4], a numerical verification is accomplished following the discussion.

2 Subwavelength Structure and Optical Model

2.1 Subwavelength Structure

Figure 2(a) illustrates the periodic structure of Si_3N_4 SWS which is used in FE simulation for simplicity. We study Si_3N_4 SWS with cylinder, right circular cone, and square pyramid, as shown in Figure 2(b), 2(c) and 2(d), respectively. With a constant volume, the diameter of cylinder- and right circular cone- shaped Si_3N_4 SWS and the edge length of square pyramid are 130 nm, the heights (h) of the etched part of Si_3N_4 SWS are 200 nm, 600 nm and 471.3 nm, the height (s) of the non-etched part is 70 nm, and the base (W) of a unit cell is 200 nm [4]. Note that the thickness of Si substrate is given 600 nm.

2.2 Optical Model

Throughout the paper, we consider only time-harmonic fields assuming a time-dependence in $e^{-j\omega t}$. The diffraction problem is governed by the well-known Maxwell equations given by:

$$\nabla \times \overline{E} = -j\omega\mu\overline{H}\,, \tag{1}$$

$$\nabla \times \overline{H} = \overline{J} + j\omega\varepsilon\overline{E}\,, \tag{2}$$

$$\nabla \cdot \overline{E} = \rho/\varepsilon\,, \tag{3}$$

and

$$\nabla \cdot \overline{B} = 0\,, \tag{4}$$

where E and D are eletric field intensity and flux density, H and B are magnetic field intensity and flux density, ω is the corresponding frequency to the wavelength λ, J and ρ are current density and charge density, ε is electric permittivity, μ is magnetic permeability.

A repeated pattern is applicable to use periodic boundary conditions, thus the Floquet theorem is adopted to simulate the boundary condition of periodic structure. Floquet theorem asserts that the analysis region can be reduced significantly in one periodicity cell to characterize the propagation property. The electric fields in periodic structure are related in the following:

$$\overline{E}_2(\overline{r}) = \overline{E}_1(\overline{r} + \overline{L}) = \overline{E}_1(\overline{r})e^{-j\theta}\,, \tag{5}$$

where r is position vector, L is the distance between the periodic boundaries, and θ is a phase factor determined by wave vector k and L:

$$\theta = \overline{k} \cdot \overline{L}\,. \tag{6}$$

The polarization of transverse electric (TE) mode, which the electric field is normal to the direction of wave propagation, is excited as the normal incident light source with wavelengths sweeping from 400 nm to 1000 nm. The

bottom region of Si substrate is assigned as perfect matched layer (PML) in avoidance of reflected wave. The refraction index of Si_3N_4 is 2.05, and the refraction index of Si is frequency dependent with this empirical relation [1]:

$$n_{Si} = \sqrt{\varepsilon + \frac{A}{\lambda^2} + \frac{B\lambda_1^2}{\left(\lambda^2 - \lambda_1^2\right)}}, \quad (7)$$

where λ is the incident wavelength, A = 0.939816, B = 8.10461x10^{-3}, λ_1 = 1.1071 μm and ε = 11.6858 .

In order to examine the effect of Floquet boundary condition in 3D FE analysis, Figure 3 shows the difference between the simulated unit cells of 1x1 and 2x2 array of Si_3N_4 SWS. Obviously, at the wavelengths above 600 nm, the reflectance of 1x1 array of Si_3N_4 SWS as unit cell is agreed with unit cell of 2x2 array, meanwhile insignificant discrepancy occurs at wavelengths shorter than 600 nm. Based on this consequence, it is more efficient using 1x1 array of Si_3N_4 SWS as simulated unit cell with acceptable accuracy.

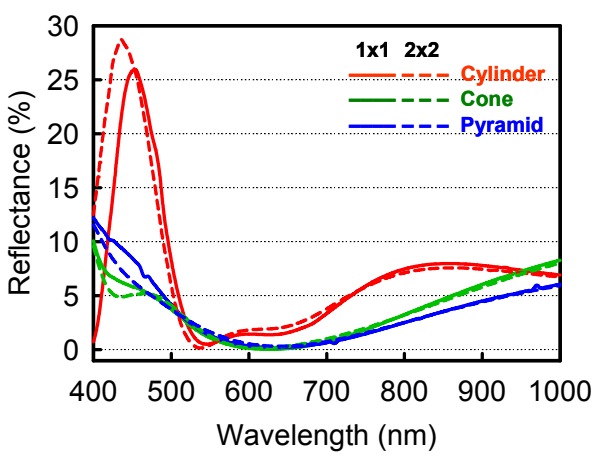

Figure 4: Reflectance spectrum of Si_3N_4 SWS with 1x1 (solid line) and 2x2 array (dashed line) as simulated unit cell in 3D FE analysis.

3 Results and Discussion

3.1 Reflectance Spectra with Incident Angles

Figures 4-6 show the reflectance spectra with incident angles of 0°, 15°, 30°, 45° and 60° for cylinder-, right circular cone-, and square pyramid-shaped Si_3N_4 SWS. For normal incidence case, the lowest average reflectance among three structural shapes is 3.47% of square pyramid-shaped structure. The others are 6.86%, 4.42% for cylinder-, right circular cone-shaped Si_3N_4 SWS respectively. Meanwhile, in Figures 4-6, one can observe that the reflectance increases significantly with larger incident angles, resulting in average reflectance beyond 50%. Table 2 summarizes the average reflectance for various incident angles.

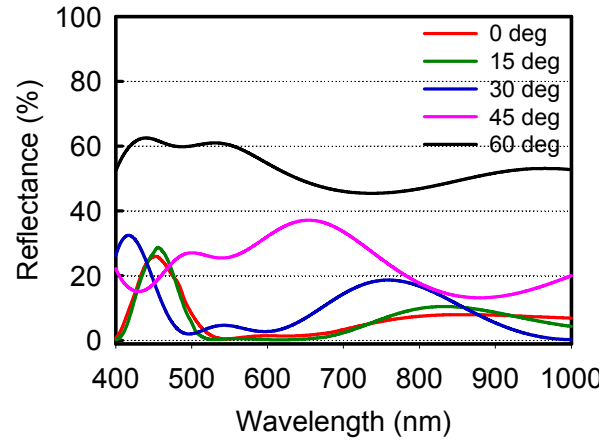

Figure 5: Plot of reflectance spectrum for cylinder-shaped Si_3N_4 SWS with incident angles of 0°, 15°, 30°, 45° and 60°.

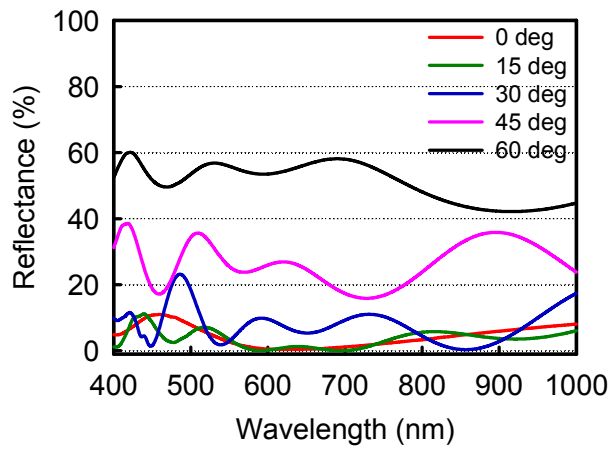

Figure 6: Plot of reflectance spectrum for circular-cone-shaped Si_3N_4 SWS with incident angles of 0°, 15°, 30°, 45° and 60°.

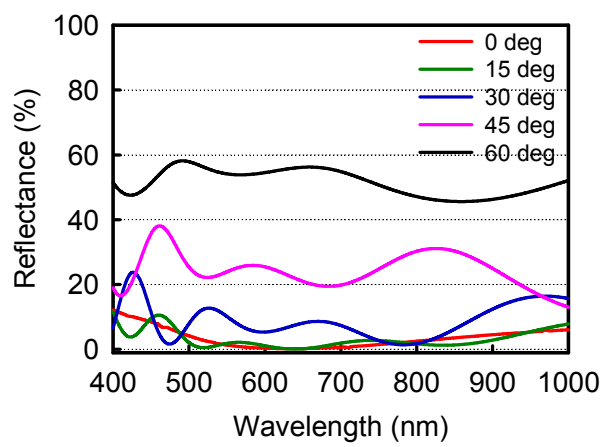

Figure 7: Plot of reflectance spectrum for square-pyramid-shaped Si_3N_4 SWS with incident angles of 0°, 15°, 30°, 45° and 60°.

Table 1: Average reflectance of Si_3N_4 SWS with various incident angles.

Aver. Ref. (%)	0°	15°	30°	45°	60°
Cylinder Shape	6.86	6.70	9.95	23.13	52.78
Circular Cone Shape	4.42	3.64	7.79	26.68	50.98
Square Pyramid Shape	3.47	3.15	8.88	24.40	51.44

Height effect on average reflectance of Si_3N_4 SWS at normal incident angle with d = 130 nm and s = 70 nm is also calculated, shown in Figure 7. The resulting average reflectance of pyramid-shaped Si_3N_4 SWS nearly keeps lowest in comparison with cylinder- and right circular cone-shaped Si_3N_4 SWS as height is ranged from 50 nm to 500 nm.

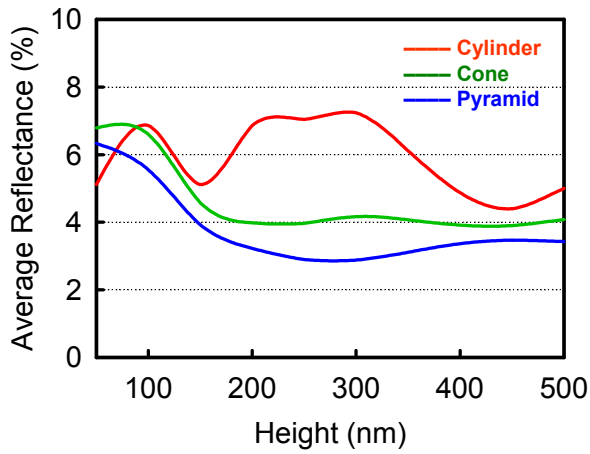

Figure 8: Plot of average reflectance for three structural shapes of Si_3N_4 SWS with heights from 50 nm to 500 nm.

3.2 Comparsion to RCWA

In the previous work reported earlier, which is based on RCWA [4], the reflectance spectra are plotted in Figure 8 using the optimal design parameters. Also, the spectra calculated by a full 3D FE analysis with the same design parameters are indicated by dashed lines. For cylinder-shaped Si_3N_4 SWS, the reflectance spectra for RCWA and FE analysis are similar, but not agreed for cone-shaped Si_3N_4 SWS.

4 Conclusions

In this study, the reflective property of unit cell with Floquet boundary condition, for the first time, has been calculated in a full 3D FE analysis. Considering various incidence angles and height effect on three structural shapes of Si_3N_4 SWS, we conclude that the pyramid-shaped Si_3N_4 SWS has best reflective property in the analysis of morphological effect. Compared to RCWA, the reflective property calculated by a full 3D FE analysis is significantly deviated from the results from RCWA, giving the hint that a detailed and comprehensive methodology is dispensable for the design of Si_3N_4 SWS. In the future, the optimal design of pyramid-shaped Si_3N_4 SWS for solar cell applications will be implemented to demonstrate this work presented here, which can be contributed to higher energy conversion efficiency.

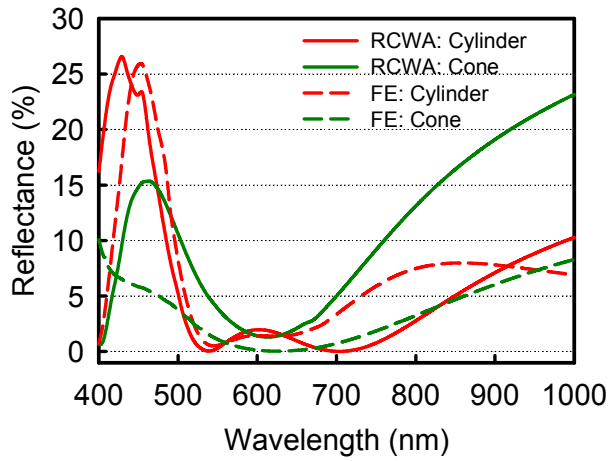

Figure 9: Comparsion of reflectance spectra for the cone- and cylinder-shaped Si_3N_4 SWS calculated by RCWA and FE analysis with the same design parameters.

Acknowledgement

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