Comprehensive Study on Reflectance of Si₃N₄ Subwavelength Structures for Silicon Solar Cell Applications Using 3D Finite Element Analysis

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1. INTRODUCTION

Semiconductor solar cell is one of promising renewable energy technologies 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. 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's dimensions are much smaller than the wavelengths of light; therefore, using SWS on the surface of silicon solar cells (Fig. 1) can substantially reduce the reflectivity and improve the capability of light trapping [1-4].

In this study, 3D FE simulation for the reflectance of Si_3N_4 SWS with three types of structural shapes: the cylinder, the right circular cone, and the square pyramid shapes is conducted with respect to different geometry parameters and lighting angles for quantitative understanding of reflectance property.

2. SWS AND OPTICAL MODEL

Fig. 2(a) illustrates a periodical structure of Si₃N₄ SWS which is used in our 3D FE simulation without loss of generality, based upon our recent experimental characterization [4]. We study Si₃N₄ SWS with the cylinder, the right circular cone, and the square pyramid shapes, as shown in Figs. 1(b)-(d), respectively. Throughout the paper, we consider time-harmonic fields assuming a time-dependence in $e^{-j\omega t}$. The diffraction problem is governed by the well-known Maxwell equations. A repeated pattern is applicable to use periodic boundary conditions, thus the Floquet theorem is adopted to simulate the boundary condition of periodic structure:

$$\overline{E}_{2}(\overline{r}) = \overline{E}_{1}(\overline{r} + \overline{L}) = \overline{E}_{1}(\overline{r})e^{-j\theta}, \qquad (1)$$

where r is position vector, L is the distance between the periodic boundaries, and θ is a phase factor.

3. RESULTS AND DISCUSSION

To verify the effect of Floquet boundary condition in 3D FE analysis, as shown in Fig. 3, we compare the difference between the simulated unit cells of 1×1 and

2x2 array of Si_3N_4 SWS. We find at the wavelengths above 600 nm, the reflectance of 1x1 array of Si_3N_4 SWS as unit cell is almost consistent with unit cell of 2x2 array, meanwhile insignificant discrepancy occurs at wavelengths shorter than 600 nm.

Fig. 4 shows the reflectance spectra with incident angles of 0°, 30° and 60° for the cylinder-, right circular cone-, and square pyramid-shaped Si₃N₄ SWS, respectively. For the normal incidence case, the lowest average reflectance among three structural shapes is 3.47% of square pyramid-shaped structure. Fig. 5 shows the reflectance dependence on the structural height and wavelength. The pyramid-shaped Si₃N₄ SWS has lower reflectance and less sensitivity on structure height in comparison with the cylinder-shaped Si₃N₄ SWS. Hence, the impact of process variation of structure height on solar cell performance is relatively smaller for the pyramid-shaped Si₃N₄ SWS.

Based on solar spectrum at the sea level revealed in ASTM Standard Tables for Reference Solar Spectral Irradiances [5], we further estimate the reflected power density defined by reflectance times incident power density, as shown in Fig. 6(a). The higher reflected power density of cylinder-shaped Si₃N₄ SWS (red line) indicates the less efficiency in the solar cell application. Fig. 6(b) shows the normalized reflectance for three structure shapes of Si₃N₄ SWS. The square pyramid-shaped Si₃N₄ SWS again shows the lowest normalized reflectance 3.13% while the cylinder- and the right circular coneshaped Si₃N₄ SWSs have 6.66% and 4.12%, respectively.

4. CONCLUSIONS

The reflective property of unit cell with a validated Floquet boundary condition has been calculated using a full 3D FE simulation. Considering various incidence angles and height effect on three experimentally observed structural shapes of Si_3N_4 SWS, we have concluded that the pyramid-shaped Si_3N_4 SWS has best reflective property in the analysis of morphological effect for silicon solar cell applications.

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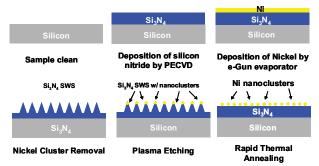


Fig. 1. Schematic illustration of the fabricated silicon solar cells with Si_3N_4 SWS. [4].

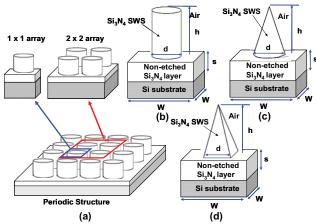


Fig. 2. (a) Illustration of periodic structure of Si_3N_4 SWS with 1x1 and 2x2 array as unit cell. Schematic of (b) cylinder-, (c) right circular cone-, (d) square pyramid-shaped structure.

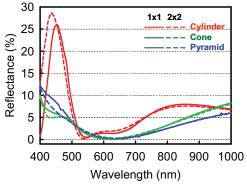


Fig. 3. Plot of the reflectance spectrum of Si3N4 SWS with three structural shapes as well as two different periodical configurations: 1x1 and 2x2 arrays in the 3D FEM simulation

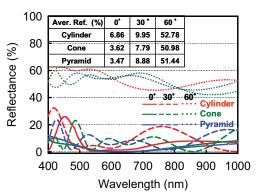
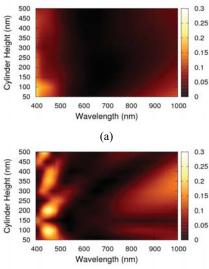


Fig. 4. Plot of reflectance spectrum of three structural shapes of Si_3N_4 SWS with incident angles of 0°, 30°, and 60°.



(b)

Fig. 5. 3D view for the height effect on the reflectance with respect to different wavelength. (a) The pyramid-shaped Si_3N_4 SWS has lower reflectance and less sensitivity on structure height in comparison with (b) the cylinder-shaped Si_3N_4 SWS.

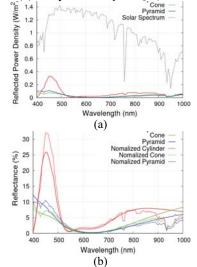


Fig. 6. (a) Plot of the reflected power density among three different shapes. (b) Plot of reflectance with and without considering incident solar spectrum at sea level.