Effects of Gas Flow Ratio on Optical Properties of PECVD Grown Single Layer Anti-reflecting Coating for Silicon Solar Cells

Zahidur R. Chowdhury, Hooman Nabovati, and Nazir P. Kherani

Abstract: Design of SiN_x/SiO_x single layer antireflection coating has been developed which tunes both the layer thickness and the deposition gas flow ratio. The method is built up for achieving maximum available carrier generation rate in single crystalline Silicon solar cells. The carrier generation rate estimation is based on internal and external quantum efficiency calculations. While the internal efficiency describes photons transport to the substrate and internal efficiency is related carrier generation mechanism. In this report the effect of optical reflection and absorption on external efficiency is widely studied. The model is based on wideband photonic parameters of silicon nitride/oxide which are deposited with PECVD machine under different deposition criteria. Effect of gas flow ratio on the dielectric refractive index and extinction factor are investigated by wideband optical measurements. For silicon nitride anti reflection coating, the optimized coating consists of 63 nm SiN_x layer with Silane to Ammonia gas ratio of 4. The estimated carrier generation rate is 1.88×10^{17} $cm^{-2}s^{-1}$. The best possible results for silicon oxide has been derived with 88.9 nm SiO_x with Silane to Nitrous Oxide gas ratio of 1. In this case the carrier generation rate will be 1.83×10^{17} $cm^{-2}s^{-1}$. The proposed anti reflection coatings are deposited on single crystal silicon substrate. The measured optical reflection coefficients are in very good agreement with the developed theory.

Keywords: Anti reflection coating, solar cells, PECVD, optical index.

1. Introduction

The high refractive index of the silicon substrate leads to high incident light reflection which significantly decreases power capability of the solar cells. The reflectivity of solar cells surface could be minimized using antireflection coating. A simple approach for thickness calculation of a single layer anti-reflection coating is the quarter wave coating. It means that, if the dielectric thickness is chosen so that the incident wave travels one quarter of the wavelength, the reflected waves from dielectric top and bottom surfaces will be out of phase, thus they would have destructive interferencewhich terminatesthe reflection [1].

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As the refractive index and wavelength in dielectric materials are functions of incident wavelength, this technique merely vanishes the reflection for a certain wavelength. For a broadband optimization of reflection, total reflection over solar spectrum should be considered for achieving minimum reflection [2] or maximizing the total carrier generation rate in the semiconductor substrate.

Using Plasma Enhanced Chemical Vapor Deposition (PECVD) technique provides accurate options for altering deposition parameters such as gas flow rates, temperature and RF power. The gas flow rates determine nitrogen per silicon content in SiN_x or oxygen per silicon in SiO_x films, which causes significant photonic effects. This phenomenon could be employed for designing high efficiency anti reflection coating layers. These coatings also improve cell passivation by adding large amount of atomic hydrogen [3-5].

2. Photonic Parameters

The schematic view if the structure is presented in Fig. 1. The efficiency of the solar cell is related to light transmission through ARC layers.

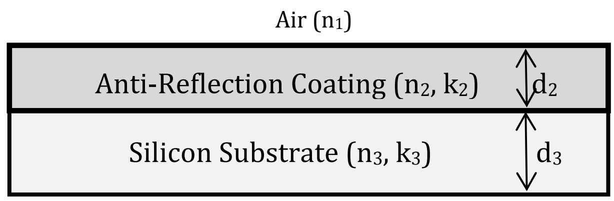


Fig. 1. Schematic view of the structure presenting opto-geometrical parameters.

The Transmission coefficient, *T(λ)*, defines the portion of the incident light power that is transmitted to the silicon substrate and can be calculated as follows [9];

$$T(\lambda) = [1 - R(\lambda)] \times A(\lambda) \tag{1}$$

where *R(λ)* and *A(λ)* are reflectivity and absorptivity coefficients for a single layer anti reflection coating respectively. Based on classic wave equations, the reflectivity can be calculated as follows [10];

$$R = \frac{r_1^2 + r_2^2 + 2r_1r_2\cos2\theta_1}{1 + r_1^2r_2^2 + 2r_1r_2\cos2\theta_1} \tag{2}$$

In this equation $r_i = (n_i - n_{i+1})/(n_i + n_{i+1})$ represent the reflection factors for orthogonal incident waves at the interfaces and $\theta_1 = 2\pi d_2 n_2/\lambda$ denotes the phase shift for the light traveling in dielectric layer. The subscripts 1, 2 and 3 are assigned for air, dielectric coating, and the substrate respectively.

According to Beer's law, the absorptivity, $A(\lambda) = e^{-4\pi k_2 d_2/\lambda}$ defines the light attenuation in the dielectric coating. In all equations n_i and k_i denote real and imaginary parts of the dielectric refractive index and d is the thickness. Assuming a specular front surface substrate the total path of the travelling photon is assumed $2d_3$ where d_3 is the substrate thickness, beside, the back surface is simply considered as a perfect reflector. Consequently the absorption probability could be calculated as follows [6];

$$AP(\lambda) = \frac{4\pi k_3}{4\pi k_3 + \frac{\lambda}{2d_3}} \tag{3}$$

In conclusion, the external optical efficiency which is the ratio of the absorbed light power to the incident light can be calculated as follows;

$$\eta_{ext} = [1 - R(\lambda)] \times A(\lambda) \times AP(\lambda) \tag{4}$$

Up to photon energies of $3eV$, the internal quantum efficiency is unity, hence each incident photon with energy greater than the band gap, can produce an *electron hole* pair. The number of generated *electron hole pairs* increases by factor of $1 + 33.5(0.45\mu m - \lambda)^2$. The additional pairs are created by impact ionization [10]. Considering this phenomenon, the *electron hole pair* generation rate per area of the solar cell can be presented by

$$\mathrm{EHPGR} = \int_0^{0.45\mu m} \frac{\eta_{ext}(\lambda) I(\lambda)}{hc} \lambda \left[1 + 33.5(0.45\mu m - \lambda)^2\right] d\lambda + \int_{0.45\mu m}^{\lambda_{eff}} \frac{\eta_{ext}(\lambda) I(\lambda)}{hc} \lambda d\lambda \tag{5}$$

where $\lambda_{eff}(\mu m) \approx 1.24/E_g(eV)$ is the effective wavelength for the semiconductor material with the band gap of E_g and $I(\lambda)$ represents solar intensity according to the Air Mass 1.5 standard. The parameters h and c represent Plank's constant and the speed of light.

The equation (5) has been examined for several dielectric thicknesses and different deposition parameters to find optimum values which maximize overall EHP generation rate.

3. SiN_x/SiO_x Deposition and Measurements

The SiO_x/SiN_x films were deposited using PlasmaPro System100 PECVD machine from Oxford Instruments. This technique uses appropriate gaseous mixtures of Siliane *(5% $SiH4/N_2$)* and Nitrous oxide (N_2O) or Ammonia *(NH_3)*. The gas ratio have been altered while other deposition parameters were kept constant. The gas ratio factor is defined as Silane flow which is divided by Ammonia or Nitrous Oxide. Hence the deposition gas ratio alters the portion of silicon in SiO_x/SiN_x films. It provides an interesting option for tuning the factor *'x'* and accordingly photonic specifications of the materials. Figure 2 shows broad band measured refractive index and extinction factor for SiO_x and SiN_x while the gas ratio is varying from *4* to *7* for SiN_x and *1* to *4* for SiO_x

Dielectric function has been measured using optical ellipsometer from Sopra in energy band of *1-5 eV*. The ellipsometry measures the change in polarization state of the incident wave which is affected by the sample refractive index. This measuring method provides the parameter ρ, which is ratio of the reflectivity for p-polarized light divided by the reflectivity for s-polarized light.

$$\rho = \tan\psi \times e^{j\Delta} \tag{6}$$

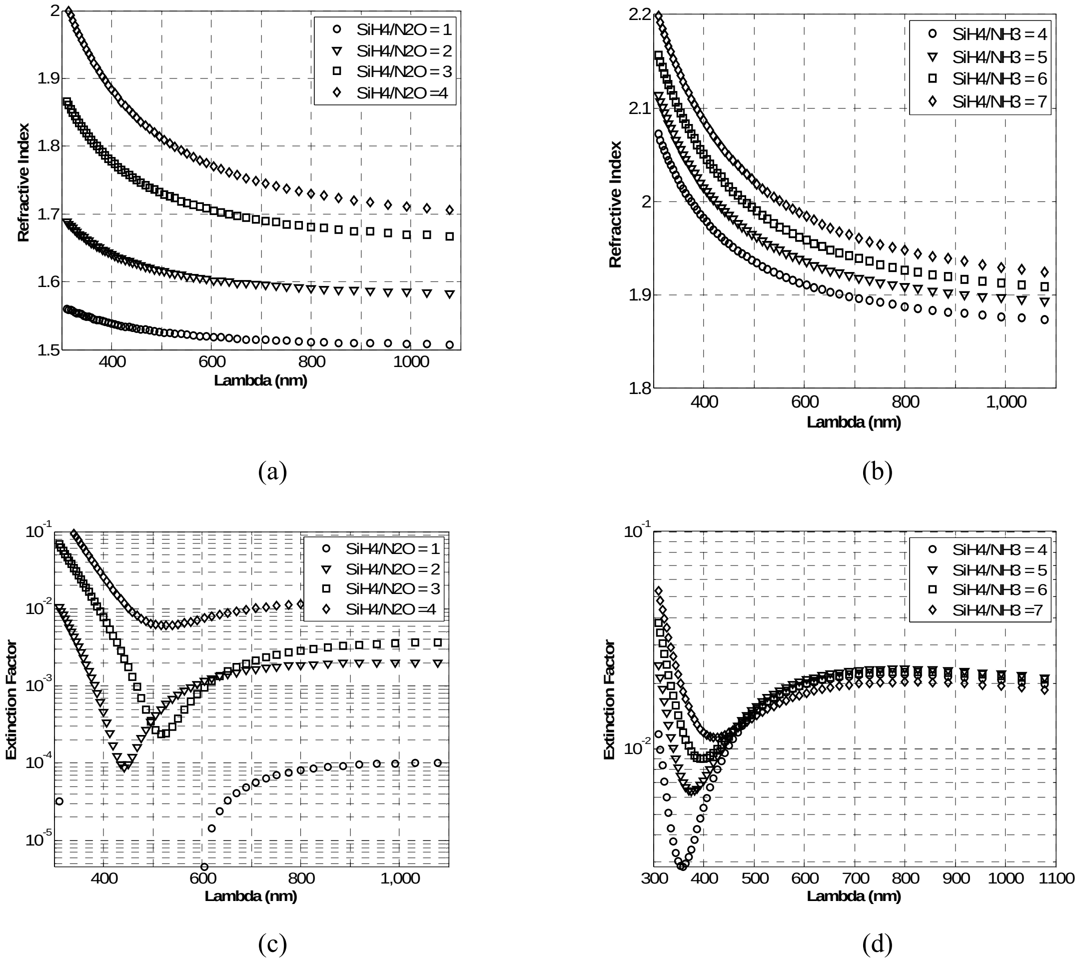
The measured data, $tan\,\psi$ and $cos\,\Delta$, were analyzed by WinElli software acquiring the refractive index, extinction factor and the film thickness.

4. Optimization Results

The optimization techniqueis applied for a single layer silicon oxide/nitride anti reflection coatings with examining wide range of important parameters. The optimum thickness is varying whileSiH_4/NH_3 and SiH_4/N_2O gas flow ratio changes. Table 1 represents the optimization results when the method has been applied for oxide and nitride layers respectively.

It can be seen that nitride layers show better overall optical efficiency. Table 2 presents detailed deposition parameters for the best possible antireflection coatings. Fig. 3 presents the external optical efficiency versus wavelength for different gas combinations. The spectrum is summarized from 300 nm to 900 nm.

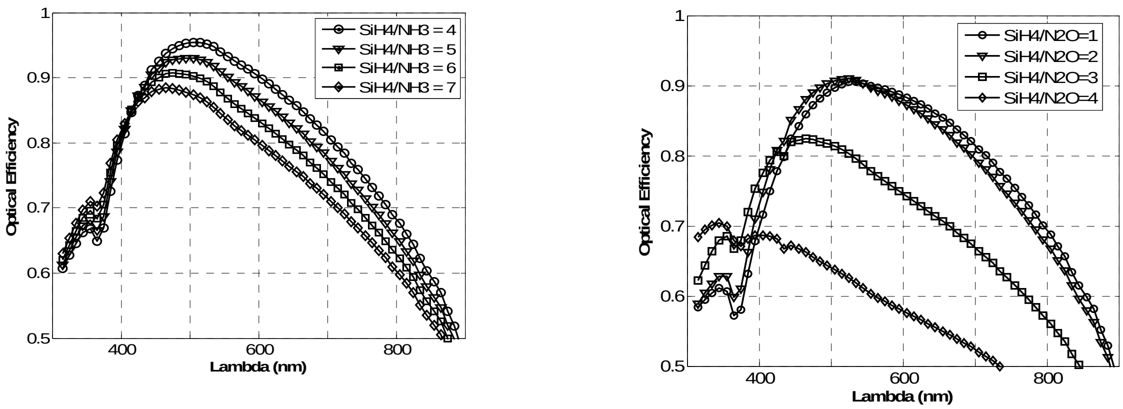
The reflectivity coefficients are presented in Fig. 4. The dielectric thickness is selected *63 nm* for SiN_x and *88 nm* for SiO_x which are optimized values for achieving maximum available carrier generation rate. The spectrometric measured data are plotted as well which show good matching between simulated and measured values. The reflectivity of the coated samples has been measured using Perkin-Elmer *UV/VIS* spectrometer in wavelength range of *300-900 nm*.



Fug. 2. Refractive index over wavelength for different gas ratios for SiO_x (a) and SiN_x (b); Extinction factors for SiO_x (c) and SiN_x (d).

Table 1. Effect of SiO_x/ SiN_x deposition gas ratio on optimum anti reflection coating thickness and available carrier generation rate.

Material	**Gas Ratio**	**Optimum Thickness(nm)**	**Available EHP Generation Rate ($\times 10^{17}$/cm^{-2}.s^{-1})**
SiO_x	1	88.9	1.8343
	2	78.9	1.8190
	3	61.5	1.6063
	4	45.3	1.3012
SiN_x	4	63.2	1.8818
	5	60.1	1.8269
	6	57.1	1.7711
	7	54.2	1.7163



(a) (b)

Fig. 3. Total optical efficiency for different gas ratios. The coating thickness is optimized for the maximum available carrier generation rate; (a) SiN_x and (b) SiO_x dielectric layers.

Table 2. SiO_x and SiN_x Deposition Conditions

Deposition Parameter	**SiNx**	**SiOx**
Temperature	400^{o}C	400^{o}C
RF Power	40W	34W
Pressure	1000 mTorr	1000 mTorr
SiH_4 Flow	200 sccm	200 sccm
N_2O Flow	0	200 sccm
NH_3 Flow	50 sccm	0
Deposition Rate	1.49 nm/s	0.27 nm/s
Deposition Time	42 seconds	326 seconds
Thickness (estimated)	63nm	88nm
Thickness (measured)	65nm	90nm

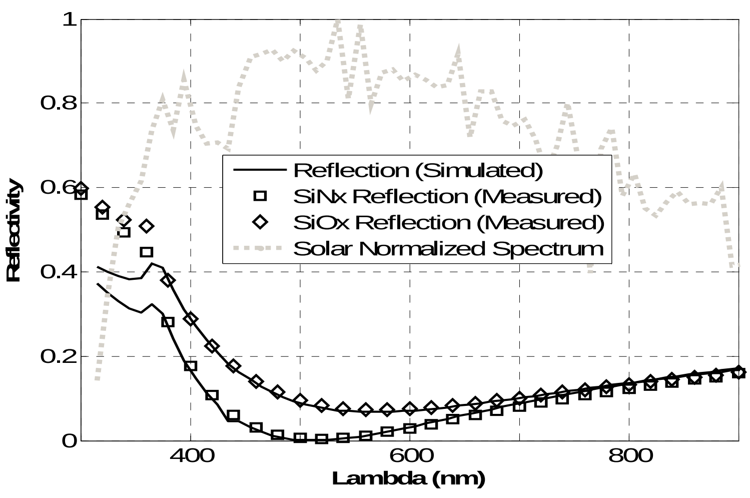


Fig. 4. Measured and simulated reflectivity coefficient forSiN$_x$ ARC with gas ratio of 4 and thickness of 63nm, SiO_x ARC with gas ratio of 1 and thickness of 88nm.

5. Conclusion

Design of PECVD SiN_x/SiO_x single layer antireflection coating has been developed which tunes both the layer thicknesses and the deposition gas flow ratio. The optimized coating consists of *63nm* SiN_x layer with Silane to Ammonia gas ratio of *4* or *88nm* SiO_x with Silane to Nitrous Oxide gas ratio of *1*. The estimated carrier generation rate would be 1.88×10^{17} $cm^{-2}s^{-1}$ and 1.83×10^{17} $cm^{-2}s^{-1}$ respectively under *AM1.5* solar spectrum. The proposed antireflection coatings are deposited using PECVD technique, the exact layers thickness was measured *67nm* and *90nm*. The measured reflectivity coefficients are in very good agreement with simulated values especially in visible and infra red spectrum. It can be vividly seen that silicon nitride single layer antireflection coatings shows better optical performance with proper passivation characteristics.

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