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# Graded $SiO_xN_y$ layers as antireflection coatings for solar cells application

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The results of theoretical optical optimization of the graded index oxynitride antireflection coatings for silicon solar cells are presented. The calculation of reflectance and absorption of layers were carried out using the Bruggeman effective medium approximation with various concentration profiles of $SiN_x$:H in the $SiO_2$ matrices. The experimental optical data of $SiN_x$:H layers deposited by RF (13.56 MHz) plasma enhanced chemical vapour deposition system in various conditions were used for simulation. The highest improvement of the short-circuit current $J_{SC}$ (44.6%) was obtained with an $SiO_xN_y$ graded layer for $SiN_x$:H with a low refractive index (2.1 at 600 nm) and abrupt concentration profile which is characteristic of a double layer $SiO_2$–$SiN_x$:H. The graded index profile can be advantageous for $SiN_x$:H with higher indices ($n \geq 2.4$). Moreover, the enhancement of $J_{SC}$ obtained by application of the antireflection coating is smaller (42.3% for $n = 2.4$) in this case. The improvement should be higher if the effect of surface passivation is taken into account.

Key words: *graded refractive index; oxynitride; antireflection coating*

## 1. Introduction

Antireflection coatings are very important parts of solar cells. Presently, application of $SiN_x$:H layers obtained by plasma enhanced chemical vapour deposition (PECVD) is the crucial step to obtain high-efficiency silicon solar cells. The most important is the possibility to use them for surface and bulk passivation [1]. $SiN_x$:H layers can be used as excellent antireflection coatings due to a high flexibility of their optical parameters. Refractive indices of such layers can be changed in a wide range (from 1.8 to 2.9 at 600 nm) by adjustment of gas composition ($SiH_4$:$NH_3$) [2]. High values of $n$ are advantageous in respect of good surface passivating properties. Moreover, the layer with a high value of $n$ has a considerable absorption due to a high extinction coefficient. Therefore, a compromise has to be reached between reflectance,

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absorption and passivation properties. It is supposed that one of the ways to obtain good optical and passivation properties is application of graded index antireflection coatings based on the silicon oxynitride ($SiO_xN_y$:H) which changes its composition from $SiO_2$ to $SiN_x$:H. This kind of coating can be accomplished by PECVD by changing composition of the $SiH_4$:$NH_3$:$N_2O$ atmosphere.

In Ref. [3], a theoretical model of graded oxynitride films is presented based on the Bruggeman effective medium approximation. In this model, $SiO_xN_y$ is a $SiO_2$ matrix with $SiN_x$:H particles. Although this is not the case in reality, the approximation gives good results in the visible and near-infrared range. In the paper, the results of simulation using the same model are presented together with experimental optical parameters of $SiN_x$:H layers deposited by PECVD.

## 2. Simulation

For the simulation of optical parameters of the $SiO_xN_y$ layers the SCOUT software was used [4]. The Bruggeman effective medium approximation (EMA) [6] was chosen [3, 5]. In the EMA, an $SiO_xN_y$ film is considered as a composite of two phases: $SiO_2$ matrix and $SiN_x$:H particles. The effective dielectric function $\varepsilon_{ff}$ of the composite $SiO_xN_y$ layer can be expressed by the formula:

$$(1-f)\frac{\varepsilon_m - \varepsilon_{ff}}{\varepsilon_m + 2\varepsilon_{ff}} + f\frac{\varepsilon_p - \varepsilon_{ff}}{\varepsilon_p + 2\varepsilon_{ff}} = 0 \tag{1}$$

where $\varepsilon_m$ is the dielectric function of $SiO_2$ matrix, $\varepsilon_p$ – the dielectric function of the particle ($SiN_x$:H) material, $f$ – the volume fraction of the particle material in the matrix material, $f \le 1$ ($f = 0$ for $SiO_2$, $f = 1$ for $SiN_x$:H).

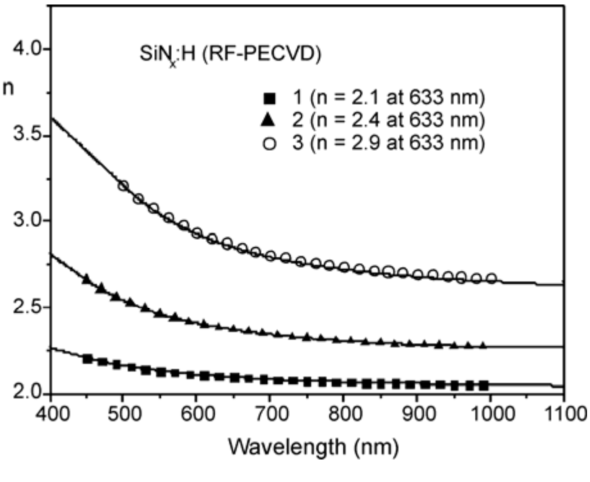

Fig.1. The measured dispersion of the refractive index $n$ for various RFPECVD $SiN_x$:H films [2]

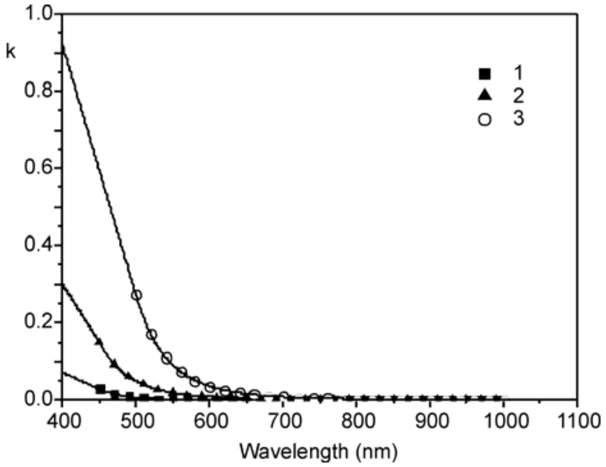

Fig. 2. The measured dispersion of the extinction coefficient *k* for the RFPECVD $SiN_x$:H films from Fig. 1

The wavelength-dependent refractive index $n(\lambda)$ and the extinction coefficient $k(\lambda)$ of $SiN_x$ layers deposited by the RF PECVD for various $NH_3/SiH_4$ ratios [2] were used to calculate optical parameters of the graded $SiO_xN_y$ layers. Figures 1, 2 show the dispersion of the optical constants of these layers. The dielectric function for the $SiO_2$ layer and Si (polycrystalline) base material was taken from the database of the SCOUT program.

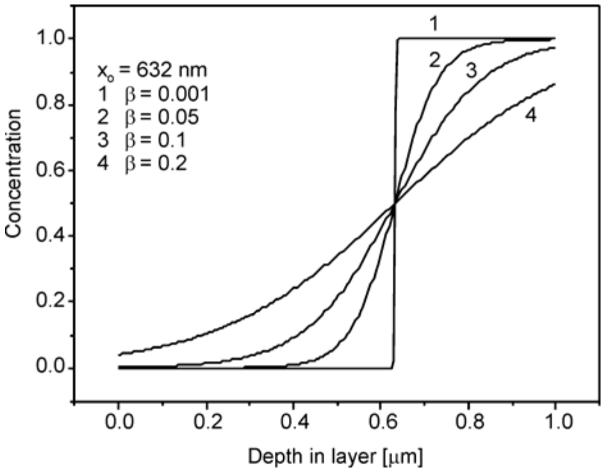

Fig. 3. The profiles of $SiN_x$:H concentration in the $SiN_xO_y$ material [3]

The optical parameters of graded $SiO_xN_y$ layers were determined for various concentration gradients. The latter was exposed by the volume fraction of silica in the

$SiN_x$:H material $f(x)$ as a function of the parameter $x$ being the ratio of the layer depth to its thickness. According to Ref. [3], $f(x)$ was taken in the form:

$$f(x) = 1 - \left[1 + \exp\left(\frac{x - x_0}{\beta}\right)\right]^{-1} \tag{2}$$

The examples of concentration profiles for various $\beta$ values are shown in Fig. 3. The parameter $x_0$ was fixed to obtain the minimum reflectance $R_{\min} = 0$. The thickness of the antireflection coating (ARC) layer $d$ was chosen to obtain $R_{\min}$ for $\lambda = 700$ nm.

## 3. Optimization of ARC

The following expressions were applied for the optimization of antireflection coating: the density of the short-circuit current $J_{SC}$ losses due to the reflection $J_{\mathrm{ref}}$, and absorption $J_{\mathrm{abs}}$ :

$$J_{SC} = J_{SC\,\max} - J_{\mathrm{ref}} - J_{\mathrm{abs}} \tag{3}$$

$$J_{SC\,\max} = q \int_{\lambda_{\min}}^{\lambda_{\max}} F_{ph}(\lambda) IQE(\lambda) d\lambda \tag{4}$$

$$J_{\mathrm{ref}} = q \int_{\lambda_{\min}}^{\lambda_{\max}} R(\lambda) F_{ph}(\lambda) IQE(\lambda) d\lambda \tag{5}$$

$$J_{abs} = q \int_{\lambda_{\min}}^{\lambda_{\max}} A(\lambda)\, F_{ph}(\lambda) IQE(\lambda) d\lambda \tag{6}$$

where $\lambda_{\min} = 300$ nm, $\lambda_{\max} = 1200$ nm, $q$ is the charge of electron, $F_{ph}(\lambda)$ – the incident photon flux calculated from the AM1.5G solar spectrum (normalized to the power density of 100 mW·cm$^{-2}$), $R(\lambda)$ – the reflectance, $A(\lambda)$– the absorption of the ARC layer, $IQE(\lambda)$ – the internal quantum efficiency of the solar cell. $J_{SC\max}$ is the maximal $J_{SC}$ value for the reflectance $R(\lambda) = 0$ and absorption of antireflection coating $A(\lambda) = 0$ for the whole $\lambda$ range.

The $IQE(\lambda)$ was calculated using the PC-1D program [7] for the two sets of parameters given in Table 1. For the simulation of cell 1, the parameters used were typical of the polycrystalline silicon solar cell (efficiency 16%) and for the simulation of cell 2 – the parameters for the single crystalline solar cells characterized by the efficiency of about 20% as in Ref. [8]. The *IQE*s for these two solar cells are presented in Fig. 4.

Table 1. Parameters used for the calculation of the IQE of two n$^+$-p silicon solar cells using the simulation programme PC-1D and calculated values of the maximal and minimal (without ARC) values of $J_{SC}$

| Parameter | Cell | |
|---|---|---|
| | 1 | 2 |
| Cell thickness [μm] | 300 | 350 |
| Diffusion length within the base [μm] | 150 | 810 |
| Specific resistance of the base [Ω·cm] | 1 | 1.5 |
| Emitter peak doping [cm$^{-3}$] | $2\times10^{20}$ | $7\times10^{19}$ |
| Junction depth [μm] | 0.5 | 0.4 |
| Emitter sheet resistance [Ω/sq.] | 40 | 100 |
| Front surface recombination velocity [cm/s] | $10^5$ | $1.5\times10^4$ |
| Back surface recombination velocity [cm/s] | $10^7$ | 60 |
| $J_{SC\max}$ ($R$ = 0, $A$ = 0) [mA/cm$^2$] | 35.4 | 40.8 |
| $J_{SC\min}$ (without ARC) [mA/cm$^2$] | 23.0 | 26.5 |

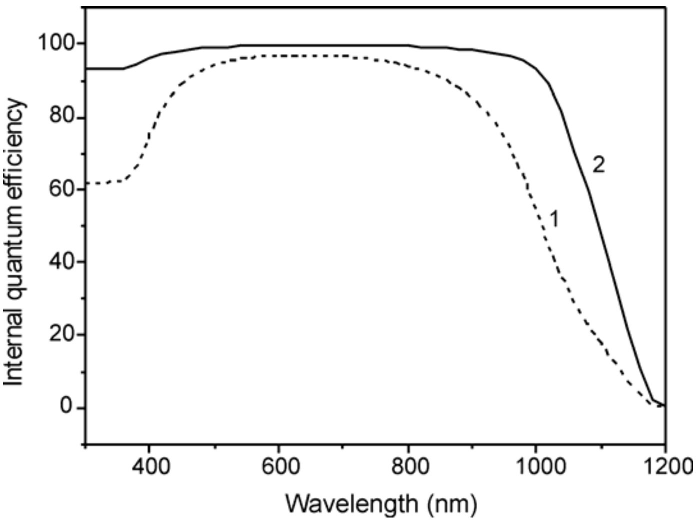

Fig. 4. Internal quantum efficiencies for two solar cells (1 and 2) simulated by the PC-1D program

In order to describe the improvement in $J_{SC}$ due to ARC, the ratio $\Delta J_{SC}/J_{SC}$ was calculated according to the equation:

$$\frac{\Delta J_{SC}}{J_{SC}} = \frac{J_{SC}(\text{with ARC}) - J_{SC}(\text{without ARC})}{J_{SC}(\text{without ARC})} \tag{7}$$

One can see that the maximum values of $\Delta J_{SC}/J_{SC}$ for the cell 1 and cell 2 are close to 54%.

## 4. Results

Figure 5 presents reflectances for various profiles *f*(*x*) of graded $SiN_xO_y$ and single homogenous $SiN_x$:H layers for comparison (1 and 2). Table 2 shows the results of calculation of the parameters from Eqs. (3)–(6) used for the optimization of antireflection coatings. The results of optical optimization of the $SiO_xN_y$ antireflection coatings for the various gradient profiles depending on $\beta$ and $x_0$ parameters are presented in Table 3.

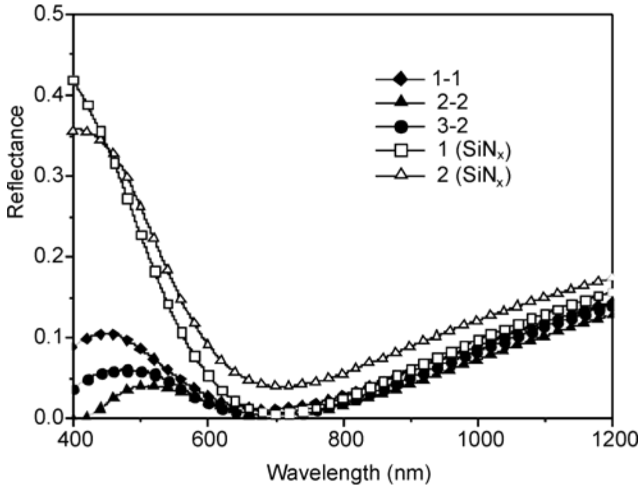

Fig. 5. Reflectances of some graded ARCs and $SiN_x$:H layers for the comparison

Table 2. Calculated short circuit current densities and losses factors due to the reflectivity and absorption for single homogeneous $SiN_x$ antireflection coatings

| Cell | $n$ | $D$ [nm] | $J_{\mathrm{ref}}$ | $J_{\mathrm{abs}}$ | $J_{sc}$ | $\Delta J_{sc}/J_{sc}$ [%] |
|---|---|---|---|---|---|---|
| | | | [mA/cm$^2$] | | | |
| 1 | 2.1 | 85.0 | 3.42 | 0.71 | 31.42 | 36.6 |
| 2 | 2.4 | 75.5 | 4.35 | 2.79 | 28.78 | 25.1 |

It is seen from Table 3 that the highest $J_{SC}$ value is obtained for the layer 1–1 which can be considered as a double $SiO_2$–$SiN_x$:H layer where $SiN_x$:H has a low index $n$ (2.1). In the case of $SiN_xO_y$ layer composed of $SiO_2$ and $SiN_x$:H with a higher index $n$, the optimal layer is obtained for the graded concentration with the $\beta$ factor equal to 0.05 and 0.2 for the $SiN_x$:H with $n = 2.4$ and 2.9, respectively. The reflectance losses $J_{\mathrm{refl}}$ are lower (for $SiN_x$:H with $n = 2.4$ and 2.9) than in the case of double $SiO_2$ –$SiN_x$:H layer (for $n = 2.1$) but the values of $J_{SC}$ are lower, too, due to high absorption losses.

Table 3. Results of the optical optimization of graded $SiO_xN_y$ ARCs considered as a the mixture of $SiO_2$ with $SiN_x$:H

| No. | $n$ | $x_o$ | $\beta$ | $d$ [nm] | $J_{ref}$ | $J_{abs}$ | $J_{ref}+J_{abs}$ | $J_{sc}$ | $J_{sc}^*$ | $\Delta J_{sc}/J_{sc}$ [%] |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | [mA/cm$^2$] | | | | | |
| 1–1 | 2.1 | 0.63 | 0.001 | 128 | 1.68 | 0.47 | 2.15 | 33.28 | 38.05 | 44.6 |
| 1–2 | 2.1 | 0.63 | 0.050 | 126 | 2.06 | 0.35 | 2.41 | 33.03 | 37.78 | 43.5 |
| 1–3 | 2.1 | 0.46 | 0.100 | 119 | 2.05 | 0.50 | 2.55 | 32.88 | 37.63 | 42.9 |
| 2–1 | 2.4 | 0.63 | 0.001 | 136 | 0.82 | 1.95 | 2.77 | 32.66 | 37.30 | 41.9 |
| 2–2 | 2.4 | 0.63 | 0.05 | 136 | 0.94 | 1.75 | 2.69 | 32.74 | 37.40 | 42.3 |
| 2–3 | 2.4 | 0.63 | 0.100 | 132 | 1.23 | 1.64 | 2.87 | 32.55 | 37.21 | 41.5 |
| 3–1 | 2.9 | 0.64 | 0.1 | 142 | 0.54 | 4.46 | 5.00 | 30.43 | 34.88 | 32.2 |
| 3–2 | 2.9 | 0.72 | 0.2 | 121 | 1.16 | 3.41 | 4.57 | 30.86 | 35.28 | 34.1 |
| 3–3 | 2.9 | 0.72 | 0.3 | 109 | 1.47 | 3.33 | 4.80 | 30.63 | 35.01 | 33.1 |

For $n$ = 2.1, 2.4 and 2.9 (at 633 nm) for the IQE cell 1. Additionally, the results of $J_{SC}^*$ simulated for the IQE cell 2 (see Fig. 4) are given.

For the $SiN_x$:H layer with $n = 2.9$, the reflectance losses are the lowest, however, the absorption losses are very high. For the optimal profile with $\beta = 0.2$, the $J_{sc}$ is considerably lower in comparison with others layers (1–1 and 2–2).

Comparing the values of the $\Delta J_{SC}/J_{SC}$ parameter and $J_{SC}$ values from Tables 2 and 3 one can conclude that all the graded $SiO_xN_y$ films composed of $SiO_2$ and $SiN_x$:H with $n = 2.1$ or 2.4 are better than simple homogeneous $SiN_x$:H layers.

## 5. Conclusion

Optical improvement of graded layers can be obtained due to the reduction of total optical losses in comparison with single layers. The mixture of $SiO_2$ and $SiN_x$:H with the large index $n$ ($n = 2.4$ or $n = 2.9$) has high absorption losses which can be reduced by the optimal profile concentration. The graded index profile can be profitable for $SiN_x$:H with the high refractive index $n$ ($n \geq 2.4$). Moreover, the enhancement of $J_{SC}$ obtained by the antireflection coating is smaller (42.3% for $n = 2.4$) in comparison with the $SiO_2$–$SiN_x$:H double layer for $n = 2.1$. In the presented simulation, the surface passivation effect was not considered. It is supposed that the influence of refractive index on the surface recombination makes the graded profile to be more profitable with higher refractive index.

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