



Optimization of antireflection multilayer for industrial crystalline silicon solar cells

Nordine Sahouane*, Abdellatif Zerga

IIIrd Generation Solar Cells Team, Materials and Renewable Energies Research Unit, Faculty of Sciences, University of Abou Bekr Belkaid-Tlemcen, BP: 119 Tlemcen 13000 Algeria

Abstract

Reflection of the incident photons by the silicon surface is a major source of losses during photovoltaic conversion. However, these losses can be minimized by depositing an antireflection layer, usually silicon nitride SiN_x : H, combined with an appropriate texturing. This layer should also provide a good passivation where a real dilemma can be arising. In contrast the surface passivation gets better with increasing Si content (large optical index for $n > 2.3$) and the minimum reflectivity was found for small optical index. To achieve this, one first approach consists to use a double antireflective layer with two materials of different refractive index n . Among the materials that are appropriate from the standpoint of physics and technology are SiN_x :H-rich silicon, Oxynitride SiO_xN_y and silicon oxide SiO_x . To optimize the antireflection multilayer, we have developed a numerical simulation code with Matlab software package where we have used the method of transfer matrix to solve the optical equation. These solutions permit us to plot the optical reflectivity and the absorption versus wavelengths and layer thicknesses. The optical refractive index and thicknesses of considered materials, which allowed us to have the lowest reflection, were used to simulate the electrical properties of the cell with PC1D and Silvaco software. Thus, our results showed the cell efficiency increase by 0.3 % and effective reflectivity of 7.4 % is obtained with a first oxide layer ($n_1=1.5$ and $d_1=55$ nm), and a second layer of silicon nitride ($n_2=2.1$ and $d_2=53$ nm) non-encapsulated compared to a reference solar cell (with a SARC SiN). In the case of multilayer non-encapsulated, our optimization has shown that it is possible to increase the efficiency by 0.7 % with the refractive index (1.48, 2 and 2.4) and thicknesses (80, 5 and 50) nm.

© 2013 The Authors. Published by Elsevier Ltd. Open access under [CC BY-NC-ND license](https://creativecommons.org/licenses/by-nc-nd/4.0/).

Selection and peer-review under responsibility of The European Materials Research Society (E-MRS)

Keywords AR coating, Silicon-Nitride, Silicon-Oxynitride, solar cell

1. Introduction

During the last decade, diverse antireflection layers (ARC) deposited on non-encapsulated or encapsulated solar cells have been optimized theoretically and experimentally [1]. Many works are reported on the double antireflection layers where different types of materials were employed like $\text{SiO}_2/\text{Si}_3\text{N}_4$, $\text{SiO}_2/\text{TiO}_2$ and ZnS/MgF_2 [2, 3, 4]. However, few works are done on the optimization of multilayer antireflection (MARC, Fig. 1) using the SiN_x :H, SiO_xN_y and SiO_x as basic materials.

The reflection of the incidental photons by surfaces of the silicon substrates is an important source of losses for photovoltaic conversion.

* Corresponding author. Phone: +213 773 150 914 / +213 661 22 16 95.

E-mail adress: nordine_84@yahoo.fr / nordine.sahouane@yahoo.com.

The deposition of multilayer antireflection seems to be a good solution to reduce the optical losses (the silicon surface reflects more than 30%). From this perspective, the appropriate materials considered physically and technologically are SiN_x :H-rich silicon, Oxynitride SiO_xN_y and silicon oxide SiO_x . They can be used as antireflection coating due to their low absorption and adjustable optical properties and as a layer of passivation.

The refractive index n and the extinction coefficient k of SiN_x :H increase with the content of silicon in the layer [5]. Thus, it can vary from 1.9 to 3.0 at 628 nm. The optimal optical index of a transparent antireflection layer of non-encapsulated solar cell silicon is 2.05 and about 2.4 for an encapsulated solar cell (glass, acetate and EVA).

According to Soppe and al [6], the best efficiency of solar cells is obtained for optical low refractive indexes. However, surface passivation becomes better for indexes above 2.3 and the bulk passivation is good for a refractive index between $n = 2.1$ and 2.2.

To combine between the minimization of the reflectivity and the adequate surface passivation, one first approach consists to use a double antireflective layer DARC with two materials of different refractive index n : a lower layer relatively rich in silicon to allow good surface passivation and a top layer with low refractive index to minimize reflection at the surface of the solar cell [7]. Optimization calculations of such a DARC were already carried out by Wright et al [8]. These results indicate a failure of the double layer concept. To resolve this problem, we have studied antireflective multilayer composed of three layers with a variable index $1.45 \leq n \leq 3$. The indexes of three materials used are: SiO_x ($1.45 \leq n_1 \leq 1.5$), SiO_xN_y ($1.5 \leq n_2 \leq 1.8$) [9] and SiN_x :H ($1.8 \leq n_3 \leq 3$) [10].

In this work, a lower thickness limit of $d_{(\text{SiN})} > 30$ nm was assumed for the inner layer because referring to Lauinger et al [11] a minimum thickness is needed to achieve an effective surface passivation. It is important to note that the optical properties of materials used vary considerably with the method and the deposition conditions that generate the inhomogeneity of the refractive index along the depth of materials.

The theory of antireflection coating is examined by many authors [2, 7, 11, 12]. The transfer matrix method [13] is usually employed for calculation of reflection coefficient.

In this paper, we present the result of calculation obtained by our computer program of single, double and multilayer ARC on silicon substrate.

2. Simulation of multilayer antireflective coating

2.1. Modeling

Let us consider an external environment “0” with refractive index n_0 and N thin layers C_n . The refractive indexes of these layers are: $n_i, n_{i+1}, n_{i+2}, \dots, n_{i+n}$, and their thicknesses are: $d_i, d_{i+1}, d_{i+2}, \dots, d_{i+n}$. The refractive index of a substrate S is n_s (Fig.1).

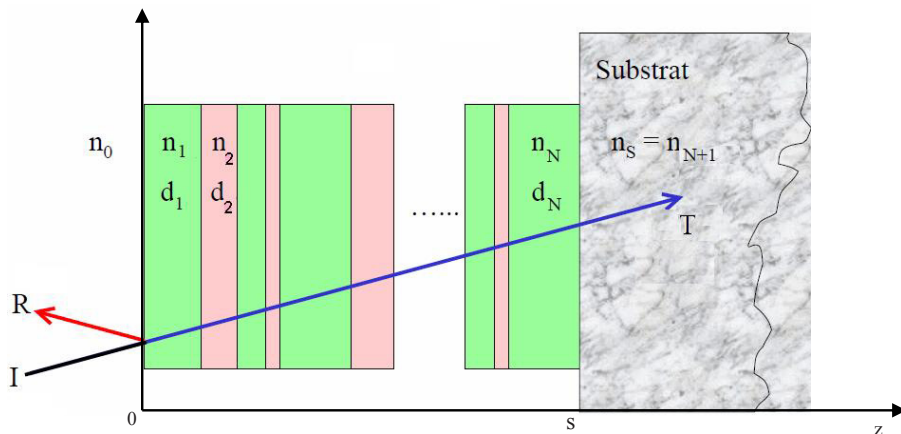


Fig. 1. Model of multilayer reflection coating (MARC), $n_N > \dots > n_2 > n_1$.

First, we describe the characteristic matrix of a single layer. As mentioned earlier, the matrix relates tangential components of the electric $E(z)$ and magnetic $H(z)$ fields at the layer boundaries $z=0$ and $z=s$.

$$\begin{pmatrix} E(0) \\ H(0) \end{pmatrix} = M \begin{pmatrix} E(s) \\ H(s) \end{pmatrix} \quad (1)$$

The matrix itself is

$$M = \begin{pmatrix} \cos \varphi & j \sin \varphi / n_c \\ j n_c \sin \varphi & \cos \varphi \end{pmatrix} \quad (2)$$

The characteristic matrix of a multilayer is a product of corresponding single layer matrices. If i is the number of layers, then the field at the first ($z=z_0$) and the last ($z=z_i$) boundaries are related as follows:

$$\begin{pmatrix} E(z_0) \\ H(z_0) \end{pmatrix} = M_1, M_2 \dots M_i \begin{pmatrix} E(z_i) \\ H(z_i) \end{pmatrix} \quad (3)$$

The transfer matrix method is used to evaluate the optical properties of a multilayer system deposited on a substrate. A system of N layers is characterized by the equivalent matrix M_i

$$M_i = \prod_{i=1}^N \begin{pmatrix} \cos \varphi_i & j \sin \varphi_i / n_i \\ j n_i \sin \varphi_i & \cos \varphi_i \end{pmatrix} \quad (4)$$

With $j^2 = -1$, n_i the refractive index of the i^{th} layer, φ_i is dephasing between the reflected waves of layers i and $i+1$

$$\varphi_i = \frac{2\pi}{\lambda} n_i d_i \cos \phi \quad (5)$$

ϕ is the angle of wave propagation in the layer. The detailed derivation of amplitude reflection (r) and transmission (t) coefficients is given in [16]. The resulting expressions are shown in Equations 6 and 7.

$$r = \frac{n_0 M_{11} + n_0 n_s M_{12} + M_{21} - n_s M_{22}}{n_0 M_{11} + n_0 n_s M_{12} + M_{21} + n_s M_{22}} \quad (6)$$

$$t = \frac{2n_0}{n_0 M_{11} + n_0 n_s M_{12} + M_{21} + n_s M_{22}} \quad (7)$$

M_{ij} are the elements of the characteristic matrix of the multilayer. The energy coefficients (reflectivity, transmissivity, and absorptance) are given by

$$R = |r|^2 \quad (8)$$

$$T = \frac{n_s}{n_0} |t|^2 \quad (9)$$

$$A = (1 - R) \left[1 - \frac{R_e(n_s)}{R_e[(M_{11} + n_s M_{12})(M_{21} + n_s M_{22})^*]} \right] \quad (10)$$

With R_e the real part, n_s and n_0 is refractive index of the silicon and vacuum respectively.

$$R + T + A = 1 \quad (11)$$

The absorption coefficient α is defined by the following equation.

$$\alpha = \frac{4\pi k}{\lambda} \quad (12)$$

2.2. Optimization of the MARC

A good antireflective coating (ARC) is vital for solar cell performance as it ensures a high photocurrent by minimising reflectance. Unlike many other optoelectronic devices, solar cells operate at a range of wavelengths, from 300 – 1200 nm, which means they need a broadband ARC.

The dispersion n and k were used to determine the optimum parameters of antireflection coatings on silicon non encapsulated solar cells and encapsulated ones using glass and EVA copolymer encapsulate, we have developed a numerical simulation code with a Matlab software package where we have used the method of transfer matrix to solve the optical equation and that to have different reflectivity for each index and layer thickness. These simulations were done with a flat front surface.

The IQE was calculated using PC1D and Silvaco software. For the simulation of the cell « Al BSF cell », the parameters used are grouped in Table 1.

Table.1. Parameters used to calculate the electrical parameters of silicon solar cells « Al BSF cell » using simulation software (PC1D and Silvaco).

Parameters	Value
Cell thickness [μm]	200
Diffusion length within the base [μm]	140
Specific resistivity of the base [$\Omega\cdot\text{cm}$]	1, p-type
First emitter peak doping [cm^{-3}]	1.10^{21} , 0.1 μm , Erfc
Second emitter peak doping [cm^{-3}]	1.10^{20} , 0.4 μm , Gauss
BSF	5.10^{19} , p ⁺ -type
Emitter sheet resistance [Ω/sq]	40
Front surface recombination velocity[cm/s]	10^5
Back surface recombination velocity [cm/s]	10^7
J_{SCmax} (R = 0, A = 0) [mA/cm^2]	35.0
J_{SCmin} (without ARC) [mA/cm^2]	22.3

2. Result and discussion

3.1. Reflection of MARC

The table.2 includes the best results of effective reflectivity (R_{eff} average across a wavelength range 300-1100 nm) of SARC, DARC and MARC. The best results of R_{eff} are for a stacking of three layers SiO_x ($n_1 = 1.48$, $d_1=80$ nm), SiO_xN_y ($n_2 = 2$, $d_2=5$ nm) and SiN_x : H ($n_3= 2.4$, $d_3=50$ nm).

Table. 2. Results of simulation of reflectivity (Matlab)

Cells non-encapsulated	n_1 (d_1) (SiO_x)	n_2 (d_2) (SiO_xN_y)	n_3 (d_3) (SiN_x :H)	R_{eff} (%)
no ARC				35,4
SARC			2,03 (73)	11,7
DARC		1,5 (55)	2,1 (53)	7,4
MARC	1,48 (80)	2 (5)	2,4 (50)	4,4

Fig 2 shows the losses due to reflection and absorption in MARC. On the one hand one can see that the reflectivity of the surface non-textured of the cell with MARC is reduced to less than 30 % compared to a standard cell and has two minima at about 380 nm and 700 nm. On the other hand the absorption loss especially in the UV range of the spectrum is considerably high and thus dominates the total losses of the MARC, this is due to the layer of SiN that a large refractive index $n=2.4$ and the extinction coefficient $k = 0.18$.

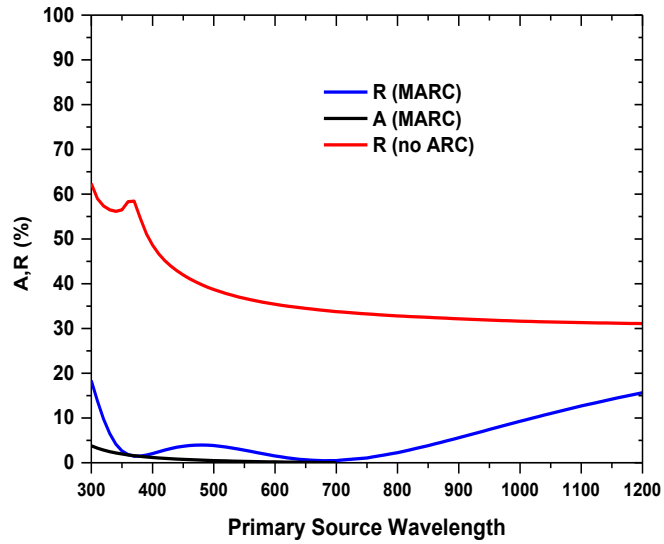


Fig.2. Reflection and absorption losses as a function of wavelengths of non-encapsulated MARC

The effects of the optical index n_2 (SiO_xN_y) and the optical index n_3 ($\text{SiN}_x\text{:H}$) on the reflectivity are represented in the Fig. 3.

The results confirm that the minimum reflectivity is assigned to MARC with a layer of $\text{SiN}_x\text{:H}$ refractive index $n_3 = 2.5$, $d_3 = 50$ nm, but it does not lead to the optimal result photovoltaic. This is due to the strong absorption of the layer. The best compromise between the minimization of the reflectivity and absorption is obtained for a $\text{SiN}_x\text{:H}$ layer with refractive index about $n_3=2.4$ and $d_3=50$ nm thickness.

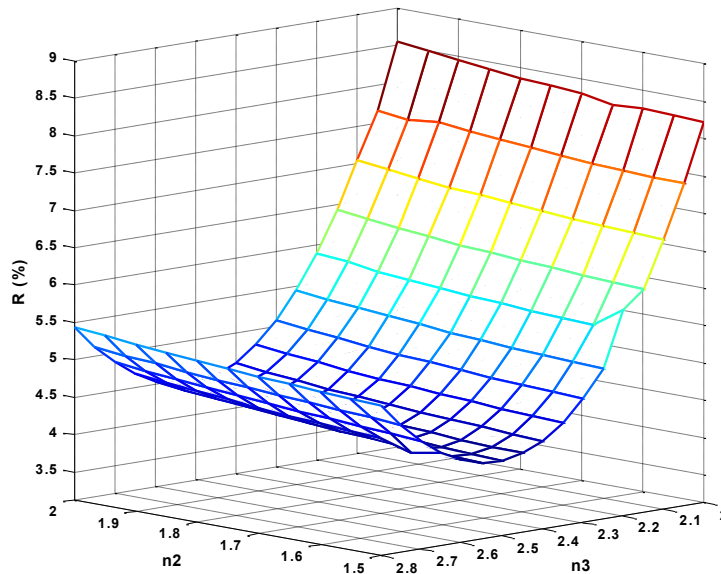


Fig.3. The influence of the optical indexes n_2 , n_3 on the effective reflectivity of the cell.

3.2. Electrical parameters of solar cells

Simulations using Silvaco and PC1D software, allowed us to optimize the antireflection layer to reach the maximum photogenerated current. Table. 3 combine the electrical results of different designs of the antireflection layer. The obtained results for MARC show that the J_{SC} is increased by 11, 6 $\text{mA} \cdot \text{cm}^{-2}$ compared to a reference solar cell (no ARC).

Table.3. Results of simulation of J_{SC} and η (PC1D and Silvaco)

	n_1 (d_1) (SiO_x)	n_2 (d_2) (SiO_xN_y)	n_3 (d_3) ($\text{SiN}_x\text{:H}$)	J_{SC} ($\text{mA} \cdot \text{cm}^{-2}$) (PC1D) (Silvaco)	η (%) (PC1D) (Silvaco)
no ARC				22,9	11,2
				22,3	10,9
SARC			2,03 (73)	32,9	16,4
				32,2	16,0
DARC		1,5 (55)	2,1 (53)	33,4	16,7
				32,9	16,3
MARC	1,48 (80)	2 (5)	2,4 (50)	34,5	17,1
				34,1	16,7

Fig 4 shows a good improvement in external quantum efficiency (EQE) for a solar cell with the MARC compared to the DARC and SARC designs. This improvement at $\lambda < 450 \text{ nm}$ (emitter region) and $\lambda > 700 \text{ nm}$ (base region) is important and it's due mainly to the role of the different layers of the MARC. Thus, the SiO_x and SiO_xN_y layers can reduce the reflection of high energy photons. The losses caused by the absorption of layer $\text{SiN}_x\text{:H}$ ($n > 2.3$) is compensated with the passivation of the surface of the cell was achieved by Soppe et al [6].

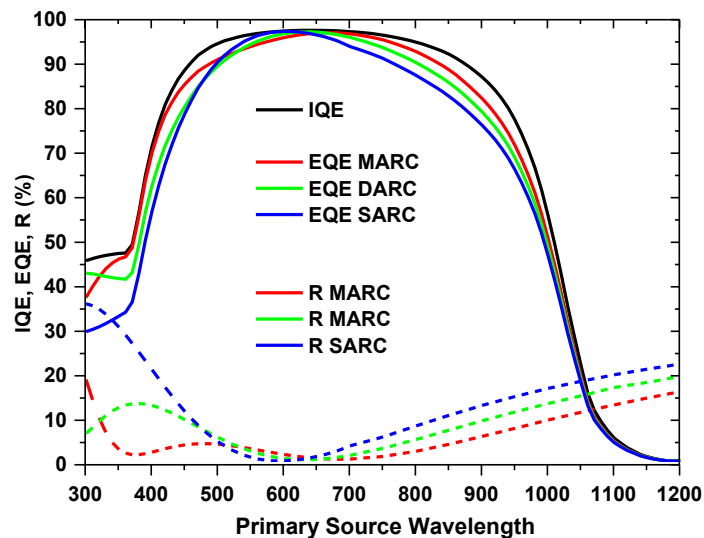


Fig.4. Reflectivity, EQE and IQE of the solar cells with a SARC, DARC and MARC versus the wavelength λ

The thicknesses influences of the second layer d_2 (SiO_xN_y) and the third layer d_3 ($\text{SiN}_x\text{:H}$) and the index refractive n_3 on the current of short circuit J_{SC} is shown in fig. 5 and fig. 6. The influence of the layer of $\text{SiN}_x\text{:H}$ is considerable compared to the influence of the SiO_xN_y layer. The best results of J_{SC} are for small thicknesses of d_2 and for the average thicknesses d_3 ($40 \text{ nm} < d_3 < 55 \text{ nm}$).

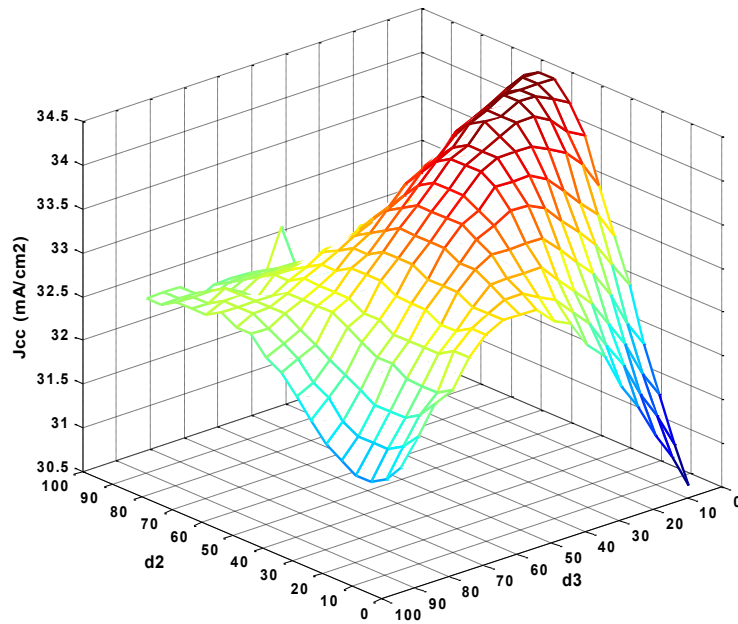


Fig.5. Current density as a function of d_2 and d_3 of solar cells with MARC.

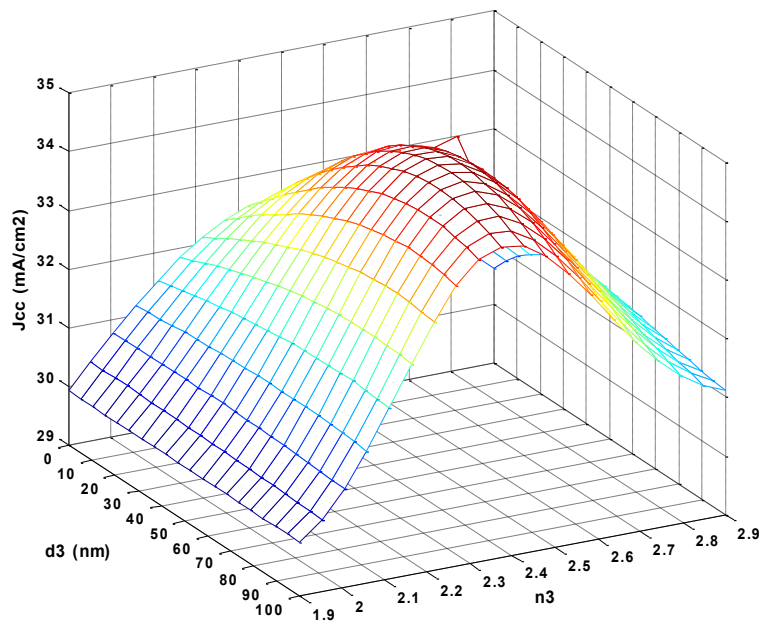


Fig. 6. Current density as a function of n_3 and d_3 of solar cells with MARC

4. Conclusions

The SiN_x , H , SiO_xN_y and SiO_x are remarkable materials for the photovoltaic applications with silicon. From their optical and electric properties, the combination of these three materials can be exploited to reduce both the optical losses and the losses related to the recombination of the minority carriers.

Finally, we have shown that antireflection multilayer composed of silicon nitride, silicon oxynitride and silicon oxide could induce a significant improvement in the photogenerated current ($+1.6 \text{ mA}\cdot\text{cm}^{-2}$) compared to cells with a SARC, in

the case of a non-encapsulated cell. Nevertheless, we did not get a satisfactory combination of layers in the case of encapsulation. The use of a SiN_x : H layer with an index $n_3=2.4$ and $d_3>30$ nm is supposed to lead a good bulk and surface passivation.

References

- [1] J. Zhao and M. A. Green, IEEE Trans. Electr. Dev. 38, pp. 1925, (1991).
- [2] Daniel N. Wright, Erik S. Marstein and Arve Holt, double layer anti-reflective coatings for silicon solar cells, IEEE, pp. 7803-8707, (2005).
- [3] A. Lennie, H. Abdullah, Z.M. Shila and M. A. Hannan, Modeling and simulation of $\text{SiO}_2/\text{Si}_3\text{N}_4$ as Anti-reflecting coating for silicon solar cell by using Silvaco Software, World Applied Sciences Journal 11(7), pp.786-790,(2010).
- [4] S-M Jung, Y-H Kim, S-I Kim, S-I Yoo, Design and fabrication of multi-layer antireflection coating for III-V solar cell, Current Applied Physics 11, 538-541,(2011).
- [5] L. Remache, A. Mahdjoub, E. Fourmond, J. Dupuis, and M. Lemiti, "Influence of PECVD SiO_x and SiN_x :H films on optical and passivation properties of antireflective porous silicon coatings for silicon solar cells" Phys. Status Solidi C8, No. 6, 1893–1897 (2011).
- [6] W.J. Soppe, H. Hong, W.M.M. Kessels, M.C.M. van de Sanden, W.M. Arnoldbik, H. Schlemm, C. Devilee, H. Rieffe, S.E.A. Schiermeyer, J.H. Bultman, and A.W. Weeber, On combining surface and bulk passivation of SiN :H layers for mc-Si solar cells, in Proc. 29th IEEE Photovoltaic Specialists Conference, New Orleans, (2002), pp. 158-161.
- [7] J. Hofstetter, C. del Cafiizo, S. Ponce-Alcantara, A. Luque, Optimization of SiN_x : H anti-reflection coatings for silicon solar cells, IEEE, (2007), pp. 4244-0869
- [8] D.N. Wright, E.S. Marstein, and A. Holt, Double layer anti-reflective coatings for silicon solar cells, in Proc. 31th IEEE Photovoltaic Specialists Conference, Orlando, (2005), pp. 1237-1240
- [9] M. Lipinski, A. Kaminski, J. F. Llzievre, Investigation of graded index SiO_xNy antireflection coating for silicon solar cell manufacturing, phys. stat. sol, C4(4)(2007)1566–1569.
- [10] M. Carrada, A. Zerga, M. Amann, J.J. Grob, J.P. Stoquert, A. Slaoui, C. Bonafos, S. Schamm, Structural and optical properties of high density Si_n synthesized in SiN_x :H by remote PECVD and annealing, Materials Science and Engineering B 147 (2008) 218–221.
- [11] T. Lauinger, J. Schmidt, A.G. Aberle, R. Hezel, Comparison of direct and remote PECVD silicon nitride films for low temperature surface passivation of p-type crystalline silicon, in Proc. 14th Europ. Photovoltaic Solar Energy Conference, Stephens, Bedford, (1997), p. 863.
- [12] H. Nagel, A.G. Aberle, and R. Hezel, Determination of optical constants of semitransparent films and substrates for silicon solar cell application, Proc. 2nd World Conf. and Exhibition on Photovoltaic Solar Energy Conversion, 1422–1425(1998).
- [13] Abeles F, Recherches sur la propagation des ondes électromagnétique sinusoïdales dans les milieux stratifiés, Application aux couches minces, Annal de Physique 1950(5): 596–640; 706–782.
- [14] H. Nagel, A.G. Aberle, and R. Hezel, Optimized antireflection coatings for planar silicon solar cells using remote PECVD silicon nitride and porous silicon dioxide, Prog. Photovolt.: Res. Appl., Vol. 7, vol. 7 pp. 245-260,(1999).
- [15] M. Rubin, Optical properties of soda lime silica glasses, Solar Energy Materials 12, 275–288 (1985).
- [16] Kacic, A.D., and M.L. Majewski. Cavity and Mirror Design for Vertical-Cavity Surface-Emitting Lasers", Vertical-Cavity Surface-Emitting Laser Devices. Springer Series in Photonics, 2003