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Numerical Simulations of Optical Transmission for Pyramidally Textured Silicon Surface with Antireflection Dielectric Coating

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Abstract

Numerical modeling of a pyramidally textured crystalline silicon solar cells with single (SiO_2) and double (SiO_2 + Si_3N_4) layer antireflection coating (ARC) are presented in this work. The simulation was used to analyze conversion efficiency of solar energy taking into account the optical transmittance of solar cell surface structure. The simulation was performed using Synopsys TCAD software package. Optimization possibilities of texture dimensions and geometrical parameters of antireflection coating were considered.

Keywords: solar cell, antireflection coating, texture, transmittance, efficiency, optimization.

Introduction

In recent years many companies focus their efforts on the development of highly efficient solar cells based on crystalline silicon. To achieve high solar energy conversion efficiency design and technological parameters of the solar cells must satisfy many requirements. One of the main requirements is a high transmittance of sunlight by the surface of the cell. Due to the fact that the silicon surface reflects large part of electromagnetic radiation across most of the solar spectrum from about 350 to 1100 nm [1] a thin dielectric antireflection coatings (ARC) are used [2-4].

Further improvement of light absorption can be achieved by structuring the silicon surface in the form of inverted pyramids by anisotropic etching [5]. This kind of texturing combined with an optimized antireflection coating of the solar cell surface provides a significant increase in optical absorption. In order to predict the best parameters of such combined structure for increasing efficiency a detailed simulation study is required. Synopsys TCAD software package allows to define the optimized parameters of the texturing and antireflection coatings taking into account the technological capabilities of solar cells manufacturing.

This paper presents the simulation results of the spectral dependence of solar radiation transmittance through the textured surface of silicon with single and double layer dielectric antireflection coating. The efficiency of solar energy conversion depending on geometrical parameters of the structure and the antireflection film thickness is determined.

The Modeling Technique

Synopsys TCAD software package was used to calculate the absorption coefficient of electromagnetic radiation for structures with different geometric parameters.

Modeling method was as follows:

1) Creating patterns using graphical interface Sentaurus Structure Editor;
2) Setting boundary conditions and optical parameters of materials;
3) Selection of light propagation models;
4) Calculation of the absorption coefficient depending on the wavelength of the radiation;
5) Calculation of the integral utilization of solar energy by integrating the spectrum of light.

The structure model

Fig. 1 shows a two-dimensional structure of one cell of the inverted pyramid which was used for the simulation.

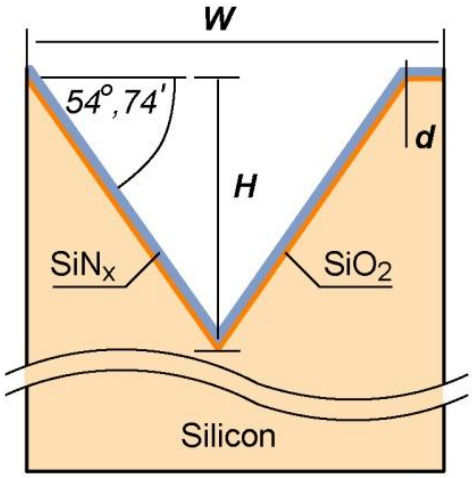

Fig. 1. Two-dimensional structure of the inverted pyramid

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The main geometrical parameters of the structure are step pyramids W, the width of the masking grid d, the height of the pyramid H and the angle between the base and the face of the pyramid α=54°,74'.

Boundary conditions and optical parameters of materials

Taking into account that main part of solar radiation is absorbed at a depth of 250-300 μm it was assumed for the model that the radiation intensity at the cell borders is equal to zero.

Single and double layer antireflection coating was simulated. For double layer antireflection coating the bottom SiO_2 layer with a thickness of 30 nm was considered in the model due to the fact that the interface of Si-SiO_2 has a low density of surface recombination centers. The dependence of solar radiation transmittance on the step of the inverted pyramids and the thickness of the top layer Si_3N_4 was investigated.

The optical parameters of materials used in the model are given in Fig. 2.

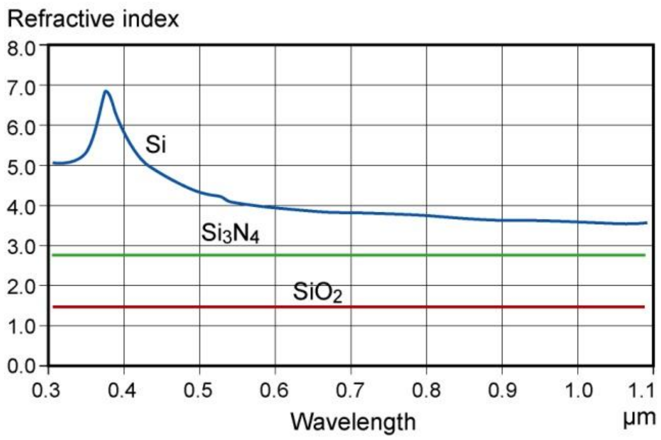

Fig. 2. Optical parameters of materials

Models used in the calculations

Model of the complex refractive index

$$\tilde{n} = n + ik$$

n is the real refractive index and k is the attenuation coefficient (complex part of the refractive index). The absorption coefficient depends on k and λ:

$$\alpha = 4\pi k/\lambda$$

The beam passing through the interface of two transparent mediums with different refractive indexes is split into reflected and refracted rays. In the absence of absorption in this mediums the condition $I=R+T$ is satisfied, where I, R and T the intensity of the incident, reflected and refracted ray respectively. To calculate the values of R and T the Raytracer method was used.

Raytracer

If you know the angle of the incident light and the refractive indices of two mediums it is possible to calculate the angle of refraction by the Snellius formula. Then amplitude coefficients of reflection and transmission can be calculated:

$$r_{TE} = \frac{k_1 - k_2}{k_1 + k_2}\ ;\ t_{TE} = \frac{2k_1}{k_1 + k_2}$$

for s-polarized waves, and

$$r_{TM} = \frac{\varepsilon_2 k_1 - \varepsilon_1 k_2}{\varepsilon_2 k_1 + \varepsilon_1 k_2}\ ;\ t_{TM} = \frac{2\varepsilon_2 k_1}{\varepsilon_2 k_1 + \varepsilon_1 k_2}$$

for p-polarized waves.

The energy coefficients are expressed in terms of amplitude ones as follow:

$$R_{TE} = |r_{TE}|^2, T_{TE} = \frac{k_2}{k_1}|r_{TE}|^2,$$

$$R_{TM} = |r_{TM}|^2, T_{TM} = \frac{\varepsilon_1 k_2}{\varepsilon_2 k_1}|r_{TM}|^2,$$

where

$$k_2 = \frac{2\pi n_2}{\lambda_0}cos\theta_t,\ k_1 = \frac{2\pi n_1}{\lambda_0}cos\theta_i$$
$$\varepsilon_1 = n_1^2,\ \varepsilon_2 = n_2^2$$

To determine the efficiency of solar cells the radiation that passes through the interface between two media, is of interest. In this work we used a light transmittance of antireflection coating, which was calculated by the formula

$$\text{Transmittance} = 1 - R/I$$

The transfer matrix method was used for the simulation of antireflection coating.

Transfer Matrix Method

The transfer matrix for two adjacent layers j and j+1:

$$T_{j,j+1} = \frac{1}{2Z_j}\begin{bmatrix} Z_j + Z_{j+1} & Z_j - Z_{j+1} \\ Z_j - Z_{j+1} & Z_j + Z_{j+1} \end{bmatrix}$$

where $Z_j = n_j cos\theta_j$ is the complex impedance in the case of s-polarization, and $Z_j = n_j/cos\theta_j$ for p-polarization, $cos\theta_j$ is the cosine of the angle of refraction. When modeling the polarization vector was set randomly.

Integral factor of solar energy utilization

Taking into account the transmittance of the antireflection coating the integral factor of solar energy utilization was calculated by the formula

$$\eta_k = \frac{\int_0^\infty F(\lambda_0)\varkappa(\lambda_0)\kappa(\lambda_0)d\lambda_0}{\int_0^\infty F(\lambda_0)\varkappa(\lambda_0)d\lambda_0}$$

$F(\lambda_0)$ is the spectral distribution of solar energy AM1.5G, $\varkappa(\lambda_0)$ is the silicon spectral sensitivity, $\kappa(\lambda_0)$ is the calculated absorption coefficient.

Results

The SiO_2+S_3N_4 double layer antireflection coating of the silicon solar cell surface is of primary interest because of silicon oxide provides surface passivation and silicon nitride allows to optimize the surface optical transmission.

Fig. 3 (a, b) shows the simulation results of spectral dependence of solar radiation transmission by the solar cell surface for different surface modifications.

The calculations were made for piramidally textured surface with double-layer antireflection coating (30 nm SiO_2 + 40 nm Si_3N_4) with different step-distance of inverted pyramid in comparison with a plane coated and uncoated surfaces (see Fig. 3a). It was assumed that the width of the masking grid d is equal to 2 μm because of the contact photolithography limitations. By increasing the accuracy of photolithography, which allows to reduce the width of the masking grid, the values of the step pyramid ***W***, whereby is achieved the maximum optical transmittance, changes in the direction of smaller values. This is illustrated by the simulation results in which ***d*** relied equal to zero (see Fig. 3b).

Fig. 4 shows the simulation results of spectral dependence of solar radiation transmission by the piramidally textured surface (W=20 μm, d=2 μm) with double-layer antireflection coating (30 nm SiO_2) for different thicknesses of silicon nitride.

It was also considered transmission properties of SiO_2 single layer antireflection coating. The simulation results of such a coating for piramidally textured surface (step-distance 20 μm, masking grid width 2 μm) are presented in Fig. 5.

It is seen that the transmittance maximum is shifted to longer wavelengths with increasing SiO_2 thickness. Curves fracture in the short-wave region of the spectrum is due to the dependence of silicon refractive index (see Fig. 2).

To determine the optimum parameters of antireflection coatings the dependence of the integral factor of solar energy utilization on the thickness of silicon nitride was calculated. The results of the calculation are presented in Fig. 6, 7.

As can be seen from the graphs in Fig. 6, the efficiency loss due to reflection losses of the sunlight in piramidally textured substrates with double-layer antireflective dielectric coatings can be reduced to 2-3%. The maximum transmission for such a structure is reached when total coating thickness is equal 50 μm.

The use of a single-layer coating gives slightly worse results (Fig. 7), but because of simplification of technology is also worthy of attention.

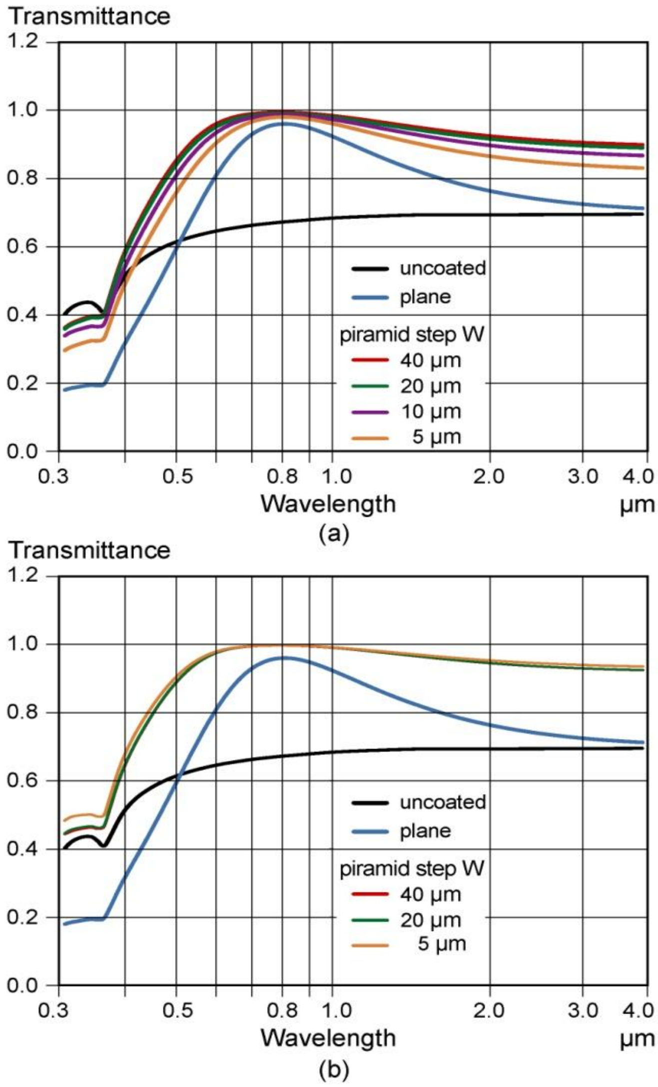

Fig. 3. Spectral dependence of solar radiation transmission by the solar cell surface for different surface modifications (a) for piramidally textured surface with double-layer antireflection coating (30 nm SiO_2 + 40 nm Si_3N_4) when W=20 μm, d=2 μm (b) for the same texture but d=0 μm

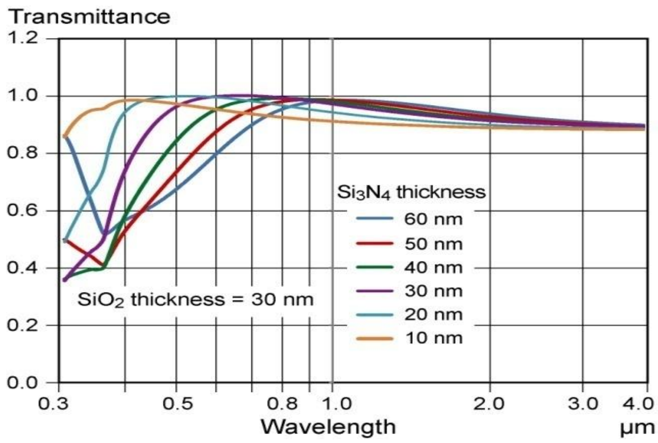

Fig. 4. Spectral dependence of optical transmission for different thicknesses of silicon nitride

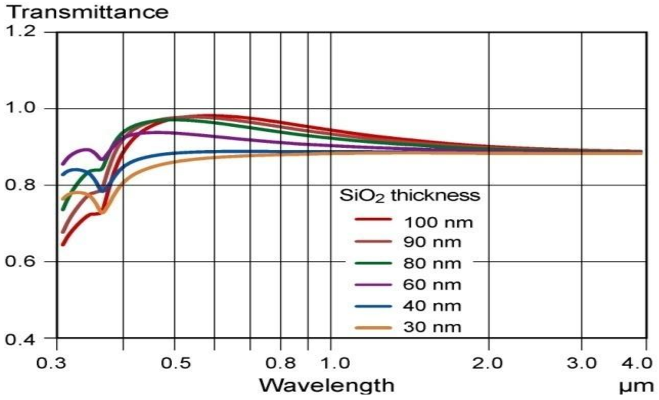

Fig. 5. Spectral dependence of solar radiation transmission by the solar cell piramidally textured surface for different thicknesses of SiO_2 antireflection coating

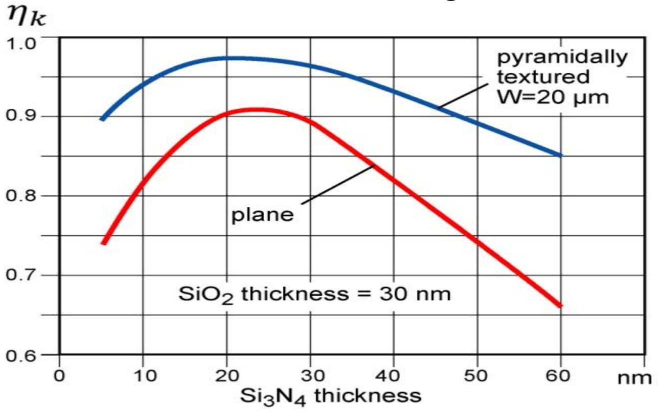

Fig. 6. The dependence of the integral factor of solar energy utilization for pyramidally textured surface on the thickness of the nitride for a double layer anti-reflection coating

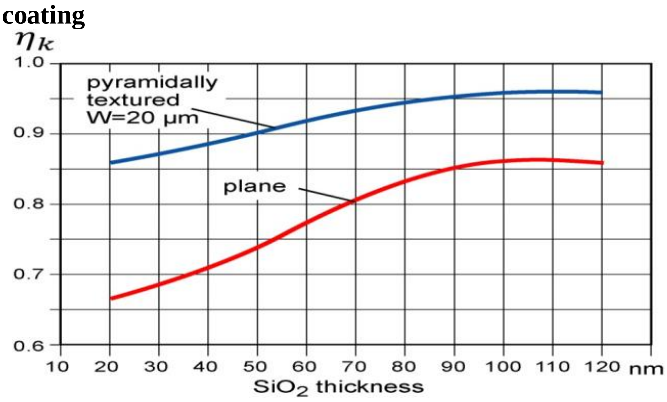

Fig. 7. The dependence of the integral factor of solar energy utilization for pyramidally textured surface on the single silicon oxide layer thickness

Discussion

The simulation of optical transmittance for a pyramidal textured silicon substrates with double layer anti-reflection coating illustrate opportunities to increase in energy conversion efficiency of solar cells. Transmittance of solar radiation increases with increasing step distance of the pyramids up to values of 40 microns (see Fig. 3). It is essential that the use of pyramidal structure increases optical transmittance in the shortwave part of the spectrum up to 30 %.

The maximum of optical transmittance is shifted toward shorter wavelengths with decreasing nitride thickness (Fig. 4).

As follows from modeling results textured silicon substrates with a single layer oxide coating also provide enhanced optical transmission (Fig. 5) however, double layers are some more effective. Double-layer dielectric coating of silicon is also preferred because of the high nitride resistance to the ion drift. In this case, the SiO_2 layer provides a low surface recombination of carriers.

Modeling has shown that it is possible to achieve the optimum parameters of antireflection layers to ensure maximum efficiency in the use of solar energy (Fig. 6, 7).

It should be noted that achieving high absorption of sunlight is only one part of creating high-efficiency solar cells. This problem must be solved taking into account other factors influencing the quality of solar cells, such as losses due to the recombination of photogenerated carriers in the bulk and on the surface and resistivity losses in contact grids.

In particular, an important point that should pay attention is that the pyramidal textured surface is characterized by increased rate of surface recombination due to the change in surface orientation from (100) to (111) and increasing the area by about 70%.

Conclusion

In this paper we have presented simulated results of single (SiO_2) and double (SiO_2 + Si_3N_4) layer anti-reflective coatings (ARC) on crystalline piramidally textured silicon. It was shown that the solar energy utilization can be significantly increased in silicon solar cells based on the pyramidal textured substrate in combination with a two-layer antireflection coating.

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