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# Simulation photoconverters of porous-Si/Si with different anti-reflective coatings

**Abstract.** This work is aimed at researching promising photosensitive solar energy structures based on the porous-Si/Si heterostructure with and without anti-reflective coatings. The PC1D program was used to model the photoconverted parameters. The reflection spectra of silicon solar cells without coating and with anti-reflective coatings $SiO_2$, $TiO_2$, ZnO, ZnS were studied. It was found that the reflection coefficient of the pure porous-Si/Si heterostructure at a wavelength about 500 nm reaches 37%, while the reflection coefficient from ARC is not more than 13% for the same wavelength in the case of light incidence at a 30º angle, and for the 45º angle incidence sunlight the value of the reflection coefficient becomes ~31% for porous-Si/Si and does not exceed 16% for solar cells with anti-reflective coatings at a wavelength about 500 nm. The light photoconverter characteristics were calculated on the basis of the studied structures, and the current-voltage characteristics were also constructed. Initial simulation results show that porous-Si/Si solar cells efficiency is about 17.5%. A significant increase in solar cells efficiency was achieved thanks to the use of anti-reflective coatings. Among the four materials, anti-reflective coatings $TiO_2$ has the highest efficiency value, which reached 26.4%. Frontal surface texturing effect on solar cell efficiency was studied. In texturing absence, the efficiency of the porous-Si/Si solar cell was 17.1%, and with texturing it reached the 18.1% value. For structures with anti-reflective coating, the efficiency is 17.3% ($SiO_2$), 25.4% ($TiO_2$), 19.8% (ZnO), 19.8% (ZnS) without surface texturing and 18.3% ($SiO_2$), 26.4% ($TiO_2$), 20.7% (ZnO), 20.9% (ZnS) with texturing. Operating temperature effect on the electrical solar cell characteristics is considered. It was established that an increase in temperature leads to a decrease in the efficiency of the studied structures by: 2.5% (without anti-reflective coatings), 2.3% ($SiO_2$), 1.8% ($TiO_2$), 2.4% (ZnO), 2.9% (ZnS).
**Key words:** solar cell, porous Si, PC1D, simulation, anti-reflective coating.

## Introduction

Today, the use of solar energy is a promising means of solving the global energy crisis [1]. Photoelectric solar energy conversion into electrical energy occurs with the help of photovoltaic cells. In recent years, semiconductor heterojunctions have been involved in one of the most active research and development photovoltaic areas – due to a wide range of technological applications and excellent flexibility [2].

Such heterostructural transitions as a-Si:H/c-Si, CdTe/CdS, n-ZnO/p-GaAs, ZnO/ZnSe and others are used in photoenergetics [3-6]. However, during the manufacture of multilayer structures, problems can arise that lead to a decrease in the electrical and optical material properties, which are associated with lattice mismatches and differences in the thermal deposited semiconductor coefficients. In order to solve such inconsistencies, it is suggested to use perforated buffer layers. The works [7-9] give experimental and theoretical calculation results of the photoelectric converter efficiency in the intermediate layer presence of a porous semiconductor. Previously, we showed in our work [10] that the energy conversion efficiency of a solar cell using a layer of porous silicon increases by ~10%, reaching 23.6%.value.

An important factor that greatly affects solar cells efficiency and allows to reduce reflection, increase absorption and sunlight transmission is the use of anti-reflective coating (ARC) [11].

Light absorption, transmission and reflection are the important parameters affecting the solar cell conversion system efficiency [12]. That is, coating a solar cell with anti-reflective coatings can greatly improve the amount of light absorbed by the cell surface. This is primarily due to such destructive interference and multiple reflection mechanisms. Currently, the most common ARCs used for both Si solar cells are $TiO_x$, $SiO_2$, ZnO, and $SiN_x$:H, etc.

However, research is still being conducted to optimize the silicon photocells parameters (stability, hysteresis, materials used as a charge transport layer and an absorber layer, etc.) in order to improve their performance.

The purpose of this work is to model the silicon solar cell parameters using ARC in the PC1D software package in order to further optimize the photovoltaic converter designs.

**Work methodology**

The solar cell model (Fig. 1) was simulated in PC1D taking into account two cases: one porous-Si/Si solar cell model without anti-reflective coating materials (Fig. 1, a) and the other with four ARC materials (Fig. 1, b). The influence of a single-layer anti-reflective coating based on semiconductor materials on solar cells efficiency is analyzed.

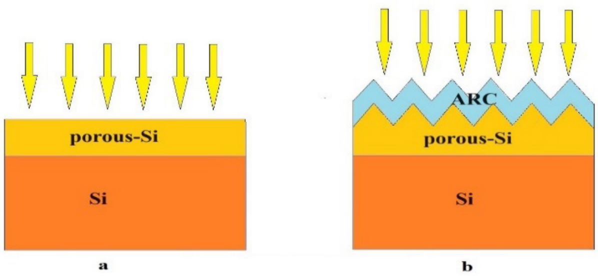



**Figure 1** – Schematic representation of a solar cell based on the porous-Si/Si structure without ARC (a) and with ARC (b).

The parameters of each layer at the proposed model are given in Table 1. The simulation was carried out under AM 1.5 solar radiation.

Anti-reflective coating choice (Table 2) was based on the statement that in order to minimize the reflection coefficient in a wide spectrum, the layers should be laid in order of decreasing refractive index with the material with the highest index. The thickness of the ARC layer should be one quarter of the wavelength within the material [13]. The refractive index of porous silicon is between the refractive indices of monocrystalline silicon and air, depending on the degree of porosity and other properties of specific porous silicon. In this work, the refractive index of porous silicon was taken as 2.04 [14].

**Table 1** – List of parameters used in the simulation

| Parameter | Value |
|---|---|
| Area | 1 $cm^2$ |
| Front surface texture depth | 0-5% (varied) |
| *Layer porous-Si* | |
| Thickness | 0.2 mkm |
| Band gap | 2.05 eV |
| Dielectric constant | 1.6 |
| N-type background doping | $1 \cdot 10^{16}$ $cm^{-3}$ |
| Bulk recombination | 800 mks |
| *Layer Si* | |
| Thickness | 5 mkm |
| Band gap | 1.124 eV |
| Dielectric constant | 11.9 |
| P-type background doping | $1 \cdot 10^{16}$ $cm^{-3}$ |
| Bulk recombination | 1000 mks |

From Fig. 2 clearly shows that the thickness of the layer will be greater for materials with a lower refractive index.

The peak energy in the solar spectrum is about 500 nm, while the peak of the relative spectral response in silicon cell is in the wavelength range about 800-900 nm, so the wavelength range of the best anti-reflection is in the range of 500-700 nm [12]. Accordingly, the ARC-material thickness was chosen precisely for this range (Fig. 2).

**Table 2** – ARC-material with their refractive index

| Material | Refractive index |
|---|---|
| $SiO_2$ | 1.458 |
| $TiO_2$ | 2.468 |
| ZnO | 2.105 |
| ZnS | 2.470 |

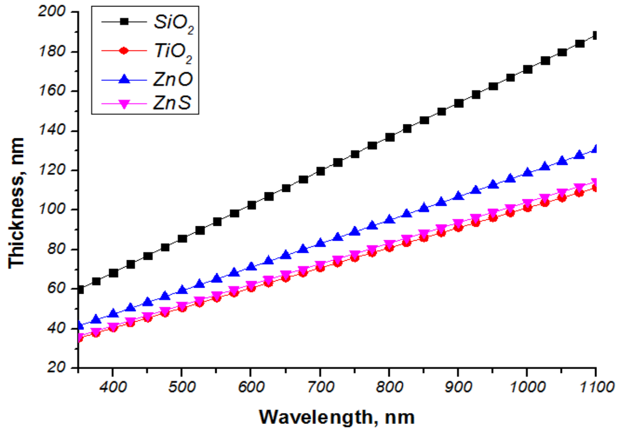


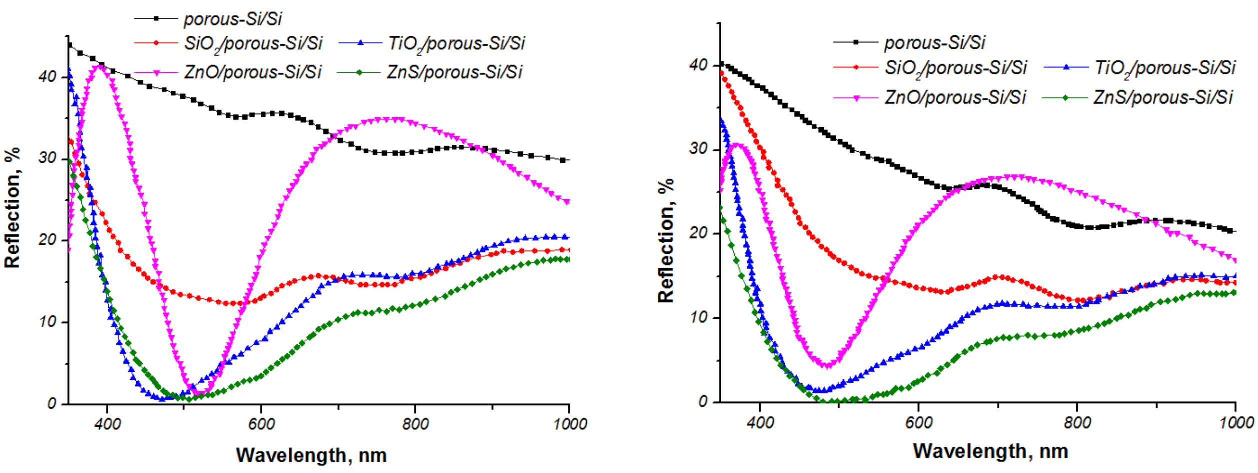

**Figure 2 –** Optimal thickness ARC.

**Simulation results and it's discussion**

***The reflectance spectra of uncoated and coated silicon solar cell with ARC using different materials***

In Fig. 3 shows the change in reflectance as a function of wavelength for a pure porous-Si/Si heterostructure covered with different ARC layers at a light incidence angle of 30º (Fig. 3, a) and 45º (Fig. 3, b). The reflection coefficient for all cases for the thickness of a quarter of the wavelength is calculated using the equations given in [15-16].

From Fig. 3 shows that the reflection coefficient of the pure porous-Si/Si heterostructure at a wavelength about 500 nm reaches 37%, while the reflection coefficient from ARC is no more than 13% for the same wavelength in the case of light incident at an angle of 30º, and for the angle of incidence sunlight of 45º, the value of the reflection coefficient becomes 31% for porous-Si/Si and does not exceed 16% for solar cells with ARC at a wavelength about 500 nm. The graphs show that the reflectivity is minimum at mostly one wavelength and high at other wavelengths.




a b

**Figure 3** – Reflectance variation as a wavelength function for bare porous-Si/Si and with ARC. (a) incident angle 30º and (b) 45º.

In the case of the porous-Si/Si structure, there is no such change the minimum value of reflectivity is observed falls on the red region of the spectrum.

***Modeling of electrical silicon solar cell properties with ARC using different materials***

According to Fig. 4, the ARC layer helps to significantly reduce the reflection coefficient, which, in turn, changes the electrical solar cells properties made on the studied heterostructures.

ARC increases the short-circuit current due to increased absorption of incident light photons. As can be seen from Table 3, the efficiency of the porous-Si/Si solar cell without ARC is 17.5%, and with the use of ARC it increases by more than 0.6%, reaching a value of 26.4% for the TiO2/porous-Si/Si structure.

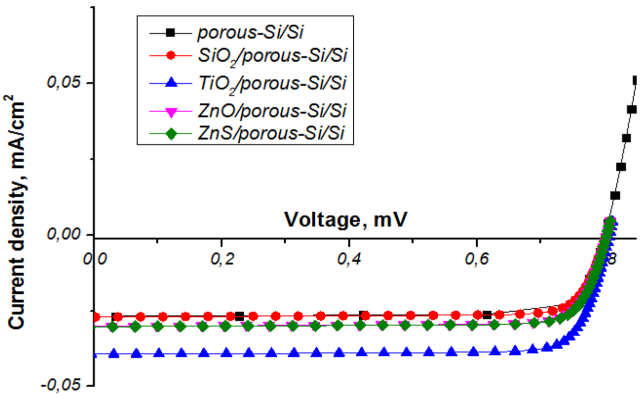



**Figure 4** – Volt-ampere curves of the studied solar cells.

**Table 3** – Electrical properties of different ARC materials based on silicon solar cells

| Structure | $J_{SC}$ (mA/cm²) | $V_{OC}$ (mV) | FF (%) | Efficiency (%) |
|---|---|---|---|---|
| porous-Si/Si | 26.9 | 800.0 | 81.3 | 17.5 |
| $SiO_2$/porous-Si/Si | 27.1 | 801.7 | 83.3 | 18.1 |
| $TiO_2$/porous-Si/Si | 39.4 | 807.5 | 83.0 | 26.4 |
| ZnO/porous-Si/Si | 30.2 | 803.7 | 83.2 | 20.2 |
| ZnS/porous-Si/Si | 30.3 | 803.3 | 83.4 | 20.3 |

***Texturing of the solar cell front surface***

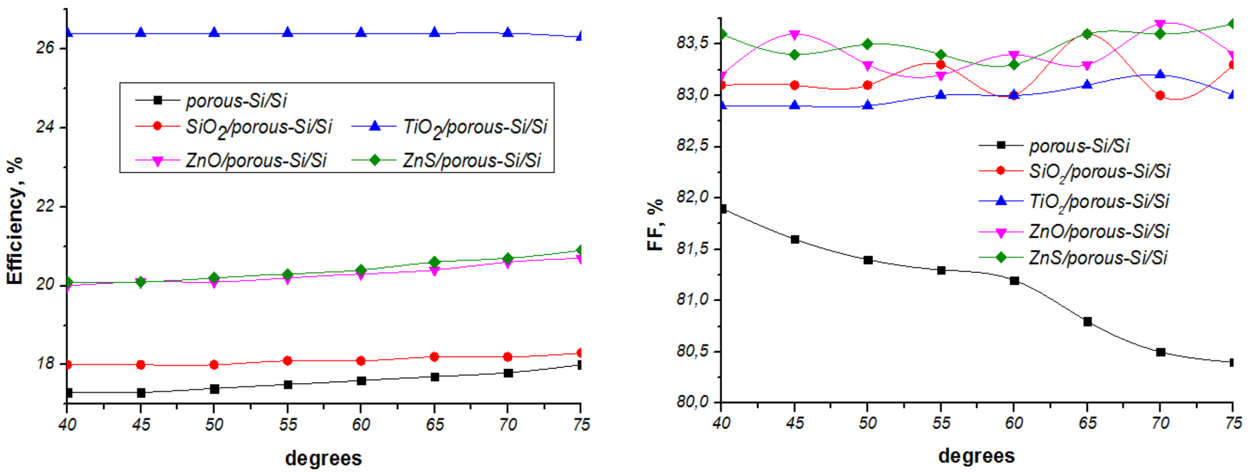
One of the important parameters for reducing reflected light and reducing optical losses is the texturing of solar cell surface.

The modeling used a pyramidal texture (Fig. 1, b), containing pyramids 3 μm deep with an angle that varies between 40-75°. Fig. 5, a shows the dependence of solar cells efficiency on the pyramid texture angle.

In the texturing absence (or almost no texturing), efficiency of the porous-Si/Si solar cell was 17.1% ($I_{SC}$=26.0 mA, $V_{OC}$=801.1 mV), and with texturing it reached a value within the given range of angle values about 18.1%. For structures with ARC, the efficiencies are 17.3% ($SiO_2$), 25.4% ($TiO_2$), 19.8% (ZnO), 19.8% (ZnS) without surface texturing and 18.3% ($SiO_2$), 26.4% ($TiO_2$), 20.7% (ZnO), 20.9% (ZnS) with texturing. Thus, the presence of texturing leads to a reduction in light reflection losses and an increase in photocurrent (a light beam can be reflected from one inverted pyramid to a neighboring pyramid, thereby increasing absorption) and solar cells efficiency is ~1%.

***An operating temperature influence on the electrical solar cell characteristics***

Solar cell heating in the operating mode significantly affects the solar cells parameters and can significantly worsen their operating characteristics [18]. Modeling the parameters of the investigated photoconverters when the temperature changes in the interval T=290-320 K with a step of ΔT=5 K. The dependence of the efficiency of the investigated photoconverters is shown in Fig. 6.




a b

**Figure 5 –** a) Solar cell efficiency at different texturing values for bare porous-Si/Si and with ARC; b) dependence of FF on the texturing angle.

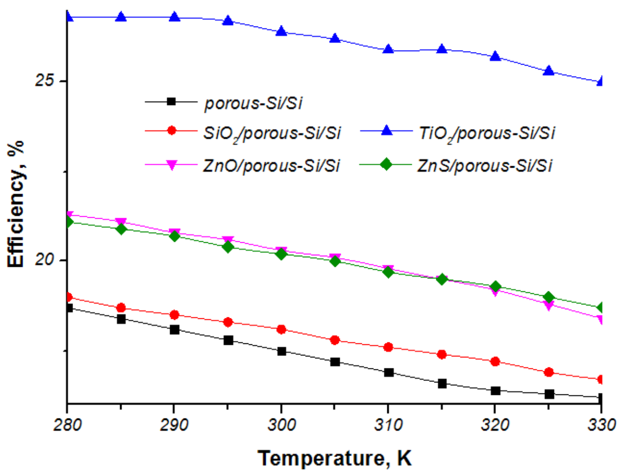



**Figure 6 –** Efficiency elements for bare porous-Si/Si and with ARC at different temperature values.

From the simulation results, it can be seen that with an increase in the operating solar cell temperature, there is a slight increase in the value of the $J_{SC}$ short-circuit current [19]. This phenomenon is associated with the excitation of a large numbers electron-hole pairs. The voltage value of the $V_{OC}$ open circuit in the specified temperature range decreases by 70-90 mV. As the temperature increases, the number of charge carriers generated due to thermal processes increases. This can promote their recombination, which reduces the open-circuit voltage. In addition, an increase in temperature in solar photoconverters can be a consequence of a decrease in the band gap of a semiconductor material, which leads to an increase in radiation from non-electronic charge carriers.

An increase in temperature also lead to a decrease in the efficiency of the studied structures by: 2.5% (without ARC), 2.3% ($SiO_2$-ARC), 1.8% ($TiO_2$-ARC), 2.4% (ZnO-ARC), 2.9% (ZnS-ARC). Although the change in the solar cells efficiency value without ARC is comparable to the photoconverter efficiency with ARC, the change in FF value in a given temperature range for structures with ARC does not exceed 2%, while the change in FF reaches 4.4%.

## Conclusion

Photosensitive structures based on a pure porous-Si/Si heterostructure and with anti-reflective coatings were investigated in the paper. The PC1D program was used to model the photoconverter parameters. The reflection spectra of silicon solar cells without coating and with anti-reflective coatings $SiO_2$, $TiO_2$, ZnO, ZnS were studied. The light photoconverter characteristics were calculated based on the studied structures. Initial simulation results show that the porous-Si/Si solar cells efficiency is about 17.5%. A significant increase in solar cell efficiency of up to 26.4% was achieved through the ARC material use. Texturing impact of the front surface and operating temperature on solar cell efficiency was studied.

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