INFLUENCE OF SURFACE ROUGHNESS ON OPTICAL CHARACTERISTICS OF MULTILAYER SOLAR CELLS

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Abstract. *Increasing efficiency of solar cells is still a discussed problem. Even if it is well-known that specially formed substrates as Asahi U-type for solar cells are produced, there is still a continuing attention given to the applications of surface roughness to achieve better light trapping and absorptance in solar cells. It was found out the even an exact interface morphology can play an important role in light trapping. In this paper we focused on the issue how final absorptance of a solar cell structure could be affected and possibly increased. The goal of this article is to show which of interfaces has the greatest influence on specular absorptance of the whole structure.*

Keywords

Absorptance, a-Si, c-Si, efficiency, pc-Si, reflectance, roughness, solar cell, thin films.

1. Introduction

Thin film structures can reduce the cost of solar power produced by solar cells by using inexpensive substrates and a lower quantity and amount of semiconductor material. Silicon is still most widely used material for solar cells production. Its efficiency in solar cells has a restrictions set by the Shockley – Queisser limit [1].

Short optical path lengths and minority carrier diffusion lengths requiring either a high absorption coefficient or excellent light trapping are also important issues. The aim of light trapping is to maximize the absorption of light in the thin absorber layer of the solar cell [2], [3], [4], [5]. Randomly textured transparent conductive oxides (TCO) are commonly used in silicon thin-film solar cells as front contacts. Besides this technique other innovative light trapping methods including plasmonic nanoparticles or photonic structures have been reported recently [6], [7], [8], [9].

The surface textures of the transparent conductive oxides assist in reducing reflection losses and increasing scattering/diffraction of the incident light [2]. Randomly textured TCO can be realized by wet etching of sputtered zinc oxide (ZnO) films, direct deposition of textured ZnO by low pressure chemical vapor deposition (LPCVD) or tin oxide films by atmospheric pressure chemical vapor deposition (APCVD) [2], [10]. Aluminum induced texturing (AIT) is a method to texture glass surfaces. Previous studies have shown that AIT glass increased the quantum efficiency of micromorph thin-film solar cells in the long-wavelength range [11].

As previous studies indicated the enhanced light trapping can be achieved when both front and back contacts are textured [2], [11]. The texturing of the back contact is achieved by relief repetition of front contact surface textures during the solar cell deposition. Then it is usually supposedly that the back contact surface textures are an exact replica of the front contact textures, but experimental measurements have shown that between the front and back contact morphology of silicon thin-film solar cells are significant differences [2].

As the back and front contact textures differ the changes in the interface structures between two layers during the layer deposition are expected. This fact is significant and the simulations of different interface properties between various layers of a multilayer solar cell structure are expected as a tool for predicting the final solar cell performance.

Light trapping in silicon thin-film solar cells is determined by the front and back contact morphology. For the implementation of light trapping in hydrogenated amorphous silicon (a-Si:H) solar cells it is advantageous to suppose a rough interface just on interfaces of these contacts. If interface roughness is applied light is scattered into different directions at each rough interface in the solar cell. Scattered light beams fall on the interfaces non-perpendicularly which results in higher angular-dependent reflectance at the interfaces than in case of the normal incidence. Due to the increase of reflections at internal interfaces light trapping is more efficient, the light path and hence absorption of light in the solar cell additionally increases [12], [13].

In this article we focus on examining the impact of roughness of the interface between two layers of the multijunction solar cell structure. The aim is to determine the impact of interface roughness on the total specular transmittance, reflectance and absorptance in the investigated structure. The objective is also to investigate the impact of the change in roughness between individual layers in a multijunction system. We explore the impact of these changes on the total transmittance, reflectance and absorptance.

2. Simulation Theory

It is known that the performance of a multilayer structure (reflectance, transmittance, and absorptance) depends on optical properties of individual layers and their thicknesses. An ideal case predicates a homogeneous layer with ideally smooth and parallel interfaces. It is obvious to expect that any changes in surface and interface roughness of individual layers influence the performance of the whole structure.

In this section we give a brief theoretical background necessary for simulations of multilayer structures comprised of amorphous silicon (a-Si), crystalline silicon (c-Si) or polycrystalline silicon (pc-Si) that are broadly used in thin film solar cell technologies. Let us suppose that the multilayer structures are deposited on ZnO used as a TCO electrode and deposited on Corning Eagle glass substrates (CE) [14].

Electric fields representing the electromagnetic wave at the interface of the k-th and $(k-1)th$ layer of the structure can be described by the transfer-matrix method in the form:

$$\begin{pmatrix} E^{+}_{(k-1)} \\ E^{-}_{(k-1)} \end{pmatrix} = \frac{1}{t_k} \begin{pmatrix} e^{i\delta_{(k-1)}} & r_k e^{i\delta_{(k-1)}} \\ r_k e^{-i\delta_{(k-1)}} & e^{-i\delta_{(k-1)}} \end{pmatrix} \begin{pmatrix} E^{+}_{(k)} \\ E^{-}_{(k)} \end{pmatrix}, \quad (1)$$

where $\delta_{(k-1)}$ is the phase change of light in the $(k-1)th$ layer, and expressed by the equation:

$$\delta_{(k-1)} = \frac{2\pi}{\lambda} N_{(k-1)} d_{(k-1)} \cos\varphi_{(k-1)}. \quad (2)$$

In the phase change the wavelength (λ) dependent optical properties of layers are taken into account. The complex refractive index N is given by the expression:

$$N(\lambda) = n(\lambda) + ik(\lambda), \quad (3)$$

where k is extinction coefficient expressing absorption of light in optical medium. In Eq. (2) $d_{(k-1)}$ is the thickness of $(k-1)th$ layer and $\varphi_{(k-1)}$ is the angle of the wave propagation in the $(k-1)th$ layer [15]. In Eq. (1) r_k and t_k are the Fresnel coefficients representing the amplitude reflectance and transmittance of the $k-th$ layer, respectively, E^{+}_{k},E^{-}_{k} are amplitudes of forward (+) and backward (-) electric field of the $k-th$ interface, respectively [8]. The final reflectance R and transmittance T can be then calculated using the expressions:

$$R = \frac{E^{-}_{(0)} E^{-*}_{(0)}}{E^{+}_{(0)} E^{+*}_{(0)}}, \quad (4)$$

$$T = \frac{N_{(m+1)}}{N_{(0)}} \frac{E^{+}_{(m+1)} E^{+*}_{(m+1)}}{E^{+}_{(0)} E^{+*}_{(0)}}, \quad (5)$$

where m is the total layer number, N_0 is the refractive index of the CE substrate, $N_{(m+1)}$ is the refractive index of the ambient medium, usually air [15]. Via the conservation law the absorptance can be calculated as:

$$A = 1 - T - R. \quad (6)$$

If an interface which is not perfectly smooth occurs in the multilayer structure the final characteristics are obviously modified. Due to the scattering the wave propagations through rough and smooth interfaces differ. Figure 1 illustrates the wave propagation through the structure with the rough interface between layers with the refractive indices n_2, n_3. The appearing beam propagation or reflection is influenced by the random interface texture. Then the reflected light power can be divided into two parts. The direct incident light is scattered into diffused components (diff) in reflection and in transmission, whereas the rest of light does not scatter, and is assigned to the specular components (spec). If the direct incident light is coherent, the specular component in reflection and in transmission has to preserve the coherence. Therefore the wave path and consequently the absorption in the layer can be increased [12]. This is of vital importance in case of active layers of solar cells, i.e. layers where the photovoltaic conversion occurs.

Intentionally created or modified roughness between two layers can by described by the modified amplitude Fresnel coefficients [12], [16], [17], [18] as:

$$\begin{aligned} r^{(spec)}_{k-1,k} &= r^{(0)}_{k-1,k} e^{-\left(\frac{2\pi Z N_{k-1}}{\lambda}\right)^2}, \\ r^{(spec)}_{k,k-1} &= r^{(0)}_{k,k-1} e^{-\left(\frac{2\pi Z N_{k}}{\lambda}\right)^2}, \end{aligned} \quad (7)$$

where the superscripts (0) denote the Fresnel coefficients of smooth interfaces, Z is the root mean square

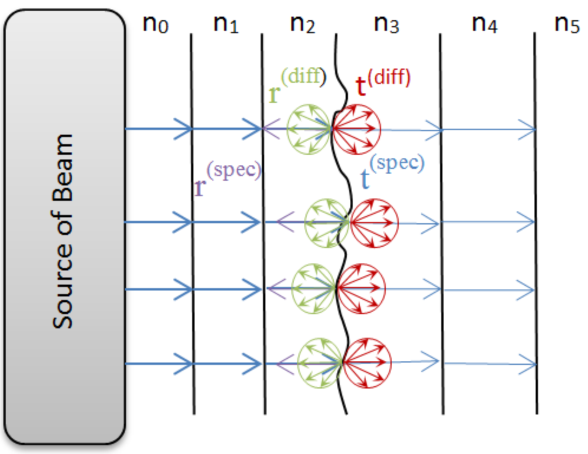


Fig. 1: The wave propagation through a rough interface.

(rms) roughness and N_k is the complex refractive index of k-th layer [12], [16], [17], [18]. The modified coefficients represent the phase differences in the reflected and transmitted beams and are based on the Gaussian distributions of the height irregularities. These coefficients are implemented into the specular part of directed light. The diffused part of light is easily calculable from equation [16], [17], [18]:

$$\begin{aligned} R^{(diff)} &= R^{(0)} - R^{(spec)}, \\ T^{(diff)} &= T^{(0)} - T^{(spec)}, \end{aligned} \tag{8}$$

where $R^{(0)}(T^{(0)})$ is total reflectance (transmittance) at a smooth interface, $R^{(spec)}(T^{(spec)})$ is specular reflectance (transmittance) at a rough interface.

Rms roughness Z is usually obtained from the AFM measurements and is given e.g. by the standard deviation of the values of surface heights of a measured sample area. Then Z is expressed by:

$$Z = \sqrt{\frac{\sum\limits_{n-1}^{N} (z_n - \bar{z})^2}{N-1}}, \tag{9}$$

where $\vec{z}$ is the average of the surface heights within the given area, z_n is the current height value, and N is the number of data points within the given area. More definitions characterizing the surface roughness, for example the mean roughness or the peak-to-valley distance are commonly used, too [21].

In the next part of the simulations of specular reflectance, transmittance or absorptance of solar cell structures with rough interfaces are presented. In these simulations, relevant parts of silicon single junction thin film solar cells are represented by glass substrate, the front TCO electrode, the structure of p-, i- and n-type silicon and the back electrode. As usually p- and n-type layers are much thinner that i-type silicon, therefore these layers were skipped from the simulations.

Then the next simulated structures were as follows CE/ZnO/a-Si/air, where a ZnO layer with the thickness of 300 nm was simulated to be deposited on thick Corning Eagle substrate and followed by a 350 nm thick a-Si layer. This structure was then extended to CE/ZnO/a-Si/c-Si/air, where a new c-Si layer of the thickness of 300 nm was added, or to CE/ZnO/a-Si/c-Si/pc-Si/air, with a new layer of 300 nm of pc-Si. These two last mentioned structures were used to simulate multijunction solar cells that are usually tandem cells consisting of cells of a-Si, pc-Si or c-Si. The intrinsic layers in multijunction solar cells structures have different absorption spectra; it means that a part of solar spectrum is absorbed in one layer and another part in another active layer. The result is that a wider part of solar spectrum can be converted and this makes it possible to achieve a higher efficiency. Multijunction solar cells are very effective solar cells, for which the reported efficiencies are above 40 %, i.e. far higher than for any conventional single junction cells [22]. These efficiencies are achieved mainly for GaAs-based multijunction solar cells.

3. Simulations

In this section the simulation results considering rough interfaces between ZnO and silicon layers in the multilayer structures used in single or multiple junction solar cells are presented. In these simulations we suppose ZnO layer used as a TCO layer prepared with various *rms* roughness intentionally. The simulated multilayer structures are composed of CE/ZnO/one or more Si layers (a-Si, c-Si, pc-Si)/air. The thicknesses of ZnO and Si layers were set to be of realistic values. Optical properties (refractive indices and extinction coefficients) of all media involved into simulations were taken from [17].

We simulate specular reflectance $R^{(spec)}$ (transmittance $T^{(spec)}$ of the structures with rough interfaces in a wide spectral region (∼450–1000 nm) that are of interest due to the significant absorption in silicon as a material for thin film solar cells. Knowledge of specular reflectance/transmittance of multijunction solar cells is important because without having an integrated sphere a lot of commercial spectrophotometers measure just specular optical quantities [22], [23], [24]. For the simulations the normal incidence of incident light is considered.

In Fig. 2 we can observe the absorptance of the structure: CE/ZnO(300 nm)/a-Si(350 nm)/c-Si(300 nm) /air, where the roughness was applied only to the interface between ZnO and a-Si layer. The absorptance was calculated from Eq. (6).

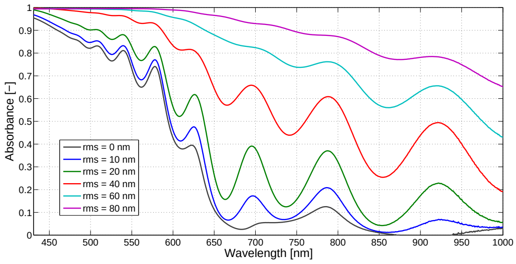


Fig. 2: The influence of interface roughness represented by *rms* on the absorptance, the roughness was applied between ZnO and a-Si layers of the structure: substrate/ZnO/a-Si/c-Si/air.

According to Fig. 2 we can clearly deduce that the absorptance increases with increasing the *rms* roughness. When the interface is flat (*rms* roughness $Z = 0$), the absorptance of the investigated structure is equal to 5 % at the wavelength of 700 nm. By increasing the *rms* roughness to $Z = 40$ nm, the absorptance increases up to ~65 % at this wavelength. In this simulation the maximum *rms* was set up to 80 nm. This results in increasing the absorptance up to ~95 %. From Fig. 2 it is apparent that the integrated absorptance in the investigated spectral region (430–1000 nm) increases significantly too.

Now let us suppose the structure CE/ZnO(300 nm)/a-Si(350 nm)/c-Si(300 nm)/pc-(300 nm)/air. When no roughness was applied the final absorptance of the whole structure at 700 nm was equal to 10 % as it can be seen in Fig. 3. A very interesting change was observed by adding a new layer and increasing the roughness between ZnO and a-Si layer to the value of 20 nm. The absorptance of the structure for this *rms* roughness was increased up to 45 % at 700 nm. By increasing *rms* to the 60 nm the absorptance of the above mentioned structure increased even up to 94 % at 700 nm. Adding a new layer consisted of different materials can explore the influence on the absorption spectra of the whole structure, because different materials have different absorption spectra. Each added layer was supposed to be an active absorbing solar layer (p-i-n structure).

The next characterization of the solar cells is the transmittance representing the percentage of incident light power that is not absorbed in the whole structure. We do not involve the back contact of the structure into transmittance simulations. The Fig. 4 shows the transmittance of the structure CE/ZnO/a-Si/c-Si/pc-Si/air, where the same roughness was applied between ZnO/a-Si layer

These results were compared with the case of no roughness for the comparison. For $rms = 0$ we can

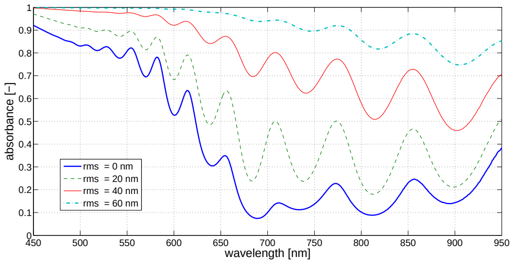


Fig. 3: Absorptance of the structure CE/ZnO/a-Si/c-Si/pc-Si/air, where the same roughness was applied between ZnO/a-Si layer.

observe that the transmittance at the wavelength of 700 nm is approximately 70 % and this is the maximum value of the transmittance of this structure.

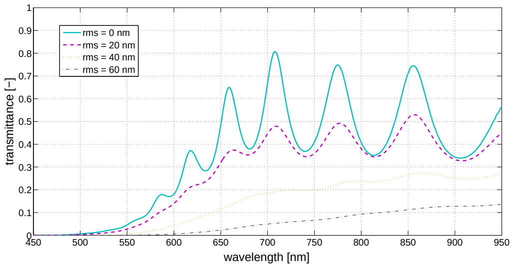


Fig. 4: Transmittance of the structure CE/ZnO/a-Si/c-Si/pc-Si/air, where the same roughness was applied between ZnO/a-Si layer.

Changing the *rms* on ZnO/a-Si interface to 20 nm causes a significant decrease of the transmittance from 70 % at the wavelengths in the vicinity of 700 nm to the 45 % in this wavelength region. Interesting in this case is to monitor the impact of the changing roughness on the transmittance of the structure. In this simulation we used the maximum value of interface roughness $rms = 60$ nm and we could see the whole structure change in transmittance in the wavelength region about ~700 nm to about 5 %. This result manifests that the influence of the change of the interface roughness at the ZnO/a-Si interface may significantly improve the final transmittance of the structure.

The reflectance of the whole structure is also dependent on the surface roughness of the individual layers. This is related to the whole concept of light trapping that was explained above. The aim is to achieve the smallest reflectance to achieve the best light trapping. This can be accomplished by changing the roughness of the interface, in this case at the interface of ZnO/a-Si. In Fig. 5 the impact of roughness on the reflectance of the structure can be seen. As we can observe from the plots, the maximum reflectance at the wavelengths in the vicinity of 830 nm is 55 % at the zero roughness. By changing the interface roughness to 20 nm we can observe the decrease in reflectance in the wavelength region of ∼830 nm to the value of ∼47 %. In applying *rms* roughness of 40 nm the observed reflectance of the whole structure at the wavelength of ∼830 nm decreases up to 25 %, and in case of the *rms* equal to 60 nm, there is the decrease of the reflectance is even more significant (to the values < 10 %). From these simulations it is seen that the change of ZnO/a-Si interface roughness has a great impact on the overall reflectance. Thus we can predict better light trapping scheme when setting the proper interface roughness.

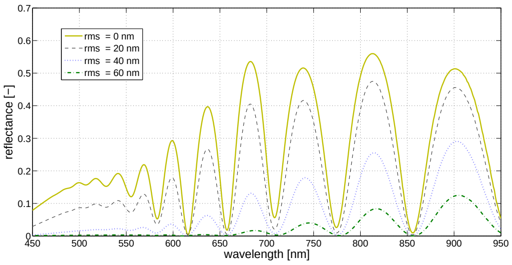
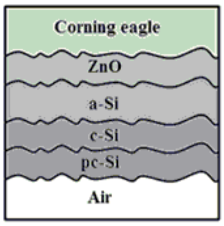


Fig. 5: Reflectance of the structure CE/ZnO/a-Si/c-Si/pc-Si/air, where the roughness was applied between ZnO/a-Si layer.

In the next course of simulations, we applied the interface roughness of the same value to all investigated layers. We focused on simulating the absorptance spectra of the structure composed of five layers CE/ZnO(300 nm)/a-Si(350 nm)/c-Si(300 nm)/ pc-Si(300 nm)/air. Absorptance spectra are of course dependent on the used material, therefore in Fig. 6 also the absorptance spectrum of the structure without any interface roughness is depicted. From Fig. 6 very low values of the absorptance at the wavelengths from ∼650 nm to ∼750 nm can be observed. The roughness expected at each interface of the investigated structure modifies the absorption spectrum and can enhance the absorption across the spectrum. Maximum absorptance of light is achieved at $rms = 40$ nm and in the wavelength region in the vicinity of ∼450 nm approaches to ∼100 %.

The following numerical study shows how the absorptance of the structure CE/ZnO/a-Si/c-Si/pc-Si/air evolves due to the interface roughness applied gradually to various interfaces. Figure 7 illustrates the effect of interface roughness on the final absorptance of the whole structure with $rms = 60$ nm, which is the maximum roughness used in all previous simulations. The resulting graph was obtained by relocating subsequently the rough interface from the first CE/ZnO interface up to the last pc-Si/air interface. In this procedure the roughness was expected to be applied only to one interface while other interfaces were anticipated as smooth. Hence the impact of one rough interface in a multilayer structure with relocated position can be seen in Fig. 7.



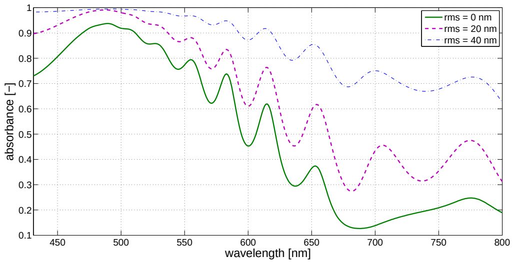


Fig. 6: Absorptance of the structure CE/ZnO/a-Si/c-Si/pc-Si/air, where the same roughness was applied to each layer.

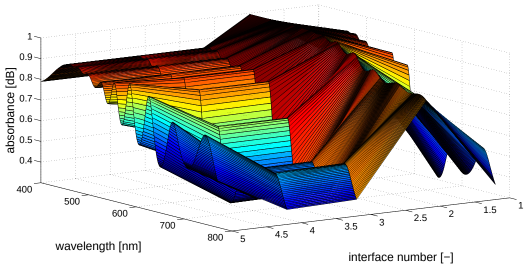


Fig. 7: Absorptance of the structure CE/ZnO/a-Si/c-Si/pc-Si/air by the roughness sequentially applied to each interface.

In this respect it is also interesting to compare the absorptance spectra of different materials used to create the structures. Wavelength-dependent absorptances of different materials deposited on the same substrate but with the same roughness are illustrated in Fig. 8. The value of $rms = 20$ nm was used for all spectra simulations. For the comparison the absorptance of the structure without roughness at all interfaces was included into the plot. Different behavior of different materials of the same roughness can be observed. The increase of the light path caused by rough interfaces of materials with different absorption abilities leads to the observed differences.We conclude that *rms* roughness improves predominantly the absorptance at wavelengths > 600 nm.

As we have already shown adding new layers or increasing the interface roughness may cause pronounced modifications in final structure characteristics. Therefore we have summarized absorptances, reflectances and transmittances averaged in the wavelength region of 430–1100 nm. The comparison of some of investigated structures with various rms values is given in Tab. 1.

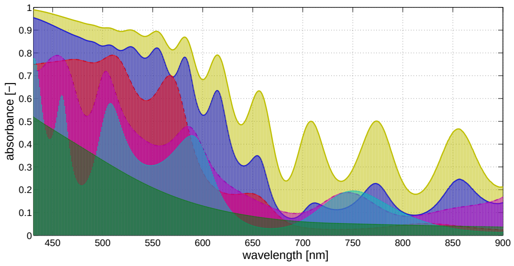


Fig. 8: The absorptance spectra for each material used in the structure CE/ZnO/a-Si/c-Si/pc-Si/air with the applied roughness.

Tab. 1: Average values of absorptance, transmittance and reflectance for the structures no. 1–7 (specified below the table) in the wavelength region of 430–1100 nm.

Str. No.	Absorptance [%]	Transmittance [%]	Reflectance [%]
1	21.15	44.64	34.21
2	25.26	43.24	31.51
3	39.55	35.93	24.53
4	33.37	39.87	26.77
5	72.55	20.47	6.98
6	52.89	28.98	18.12
7	74.7	16.7	8.59

1. CE/ZnO(300 nm)/a-Si(350 nm)/air, without interface roughness.

2. CE/ZnO(300 nm)/a-Si(350 nm)/c-Si(300 nm)/air, without interface roughness.

3. CE/ZnO(300 nm)/a-Si(350 nm)/c-Si(300 nm)/pc-Si(300 nm)/air, without interface roughness.

4. CE/ZnO(300 nm)/a-Si(350 nm)/c-Si(300 nm)/pc-Si(300 nm)/air, *rms* = 20 nm between ZnO and a-Si.

5. CE/ZnO(300 nm)/a-Si(350 nm)/c-Si(300 nm)/pc-Si(300 nm)/air, *rms* = 60 nm between ZnO and a-Si.

6. CE/ZnO(300 nm)/a-Si(350 nm)/c-Si(300 nm)/pc-Si(300 nm)/air, *rms* = 20 nm between all layers of the structure.

7. CE/ZnO(300 nm)/a-Si(350 nm)/c-Si(300 nm)/pc-Si(300 nm)/air, *rms* = 40 nm between all layers of the structure.

In this respect highest absorptances and consequently better light trapping can be achieved by the structures no. 5 and 7 representing multijunction solar cells with rough interfaces with interface roughness applied to ZnO or all layers

4. Conclusion

This paper deals with the analysis of the impact of roughness of the interface between all or selected pairs of layers of multilayer structures representing single or multijunction solar cells. The aim of this work was to determine the effect of interface Gaussian roughness on the transmittance, reflectance and absorptance in the investigated structure. A wide course of simulations concerning the structure composition and *rms* roughness has shown clearly that a proper and comprehensive evaluation of all conditions of locating rough interfaces and specific roughness values favor the increase in absorptance of light in the structure. Our numerical experiments have confirmed the knowledge on beneficial roughness of ZnO surface. Moreover we found out that rough interfaces of all layers could be also effective but the exact interface roughness must be properly selected.

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