Gradient-Index Antireflecting Coatings for Silicon: Modeling and Optimization

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Abstract – The spectra of Reflectance, Transmittance and Absorbance of inhomogeneous porous silicon and silicon suboxide layers were calculated. We considered the propagation of light in the system of "Si substrate – gradient-index antireflection coating". The computational program was developed to solve the problem of interaction between electromagnetic waves with different type of layered and inhomogeneous media. The medium with inhomogeneous distribution of electrophysical properties is considered as a structure which consists of many of homogeneous ones. In the case of multilayered system, we used a recurrence relation, which binds interference in the system of layers with the interference phenomenon in each sublayer. Fresnel's coefficients were used to calculate the reflection and transmission on the boundaries between sublayers. The complex refractive index of each sublayer was determined according to the effective-medium approximation. We analyzed the influence of the profile of media parameters distribution on the transmission of electromagnetic waves across the system "Si substrate – gradient-index antireflection coating" to find the optimal profile. We show that effective antireflecting coatings can be produced with the use of inhomogeneous layers.

1. Introduction

Surface reflection of a photocell is caused by considerable difference between optical parameters of the photoconverter material and the environment. It may be reduced by applying antireflective interference coatings consisting of one or several homogeneous layers. However, one-layer coating cannot efficiently reduce the reflection in a wide wavelength range because of neighboring interference maxima. A wider spectral range may be obtained either by increasing the number of layers or by using other technical decisions. One of the solutions of the problem is usage of inhomogeneous layers providing better matching of optical parameters of different media [1–4]. It enables to reduce considerably the reflection due to the decrease in the difference between the values of optical parameters of adjacent layers. Usage of an inhomogeneous layer allows suppressing of interference maxima narrowing the spectral range. For absolutely transparent media the reflection decreases as the gradient layer thickness increases and hence transition between media becomes smoother. In real media, it is necessary to take into account the absorption [5] which imposes restrictions on the layer thickness.

2. Calculation procedure

As for electromagnetic waves propagation through inhomogeneous mediums exact decisions are known only for some profiles of medium inhomogeneity, it is expedient to choose one of the approached calculation methods for achievement of greater generality and possibility of modeling anyone of medium parameter distributions in a layer. In the submitted paper, the method of partition of inhomogeneous layer into thin homogeneous sublayers is used because of its greater obviousness [6]. Then the received sequence of thin sublayers is further calculated as usual multilayered system. Furthermore, by variation of parameters of sublayers, the method of partition of a layer into a system of sublayers allows to fit the profile of layer ensuring the best effectiveness.

At calculations the formulas expressing reflection and transparence of sublayers through parameters of the sublayers have been used [7]:

$$r = \frac{r_j + r_{j+1}\ e^{-i2\varphi}}{1 + r_j\ r_{j+1}\ e^{-i2\varphi}},\qquad t = \frac{t_j\ t_{j+1}\ e^{-i\varphi_i}}{1 + r_j\ r_{j+1}\ e^{-i2\varphi_i}}, \tag{1}$$

r_j, r_{j+1}, t_j, and t_{j+1} are the Fresnel coefficients:

$$r_j = -\frac{n_{j-1} - n_j}{n_{j-1} + n_j},\ r_{j+1} = -\frac{n_j - n_{j+1}}{n_j + n_{j+1}},\qquad t_j = \frac{2n_{j-1}}{n_{j-1} + n_j},\ t_{j+1} = \frac{2n_j}{n_j + n_{j+1}}, \tag{2}$$

n_{j-1}, n_j, and n_{j+1} are the refractive indexes (complex) of previous, current and next sublayer; φ_j is the phase shift:

$$\varphi_j = \frac{2\pi}{\lambda} n_j\ h_j\ , \tag{3}$$

h_j is the thickness of current sublayer.

Parameters of sublayers have been determined on an effective medium approximation. There are known some relations linking dielectric constants of a two-component mixture with the percentage of components. In the paper of Aspnes et. al. [8] has been shown that the properties of Si–SiO_2 system are mirrored most adequately with the relation of Bruggeman [9]. Therefore, the model of an effective medium has been chosen just in the form of Bruggeman:

$$f\frac{\varepsilon_1-\varepsilon_{eff}}{\varepsilon_1+2\varepsilon_{eff}}+(1-f)\frac{\varepsilon_2-\varepsilon_{eff}}{\varepsilon_2+2\varepsilon_{eff}}=0, \qquad (4)$$

ε_{eff}, ε_1, and ε_2 are the dielectric functions of the effective medium, components 1 and 2, and f is the volume filling factor of the component 1. At calculations, dielectric constants of silicon [10] and silicon dioxide [11] in a complex form have been used. For calculations of porous silicon parameters has been also used the formula (4). Then silicon dioxide constants were substituted by the unity.

Further, profiles optimal for Silicon substrate matching with the environment have been determined by the method of step-by-step approach. In this method, a certain profile (for example, linear) is chosen as initial and the thickness is given too. Then the profile is subdivided into sections (in our case 50 sections), and the steps in thickness and volume filling factor are defined for each section (in our case $\Delta H = 0.005$ μm and $\Delta f = 0.005$, respectively). Beginning from the first section the refractive index of each sublayer is chosen successively to maximize transmittance. After individual layer optimization, a new index is retained for the use with subsequent layer optimization. Completion of the last sublayer and the whole layer thickness constitutes a pass. The process is then repeated for many passes, starting again with the layer one.

3. Results and discussion

As the modeling example of this procedure application parameters of gradient films consisting of silicon suboxide and porous silicon have been calculated.

The diagram Fig. 1 shows profiles of components distribution for matching by complex refractive index, obtained by using of this method for silicon suboxide. In this case, computer modeling gives preference to the profile where a low refractive index layer (SiO_2), whose thickness is much less than the wavelength (less than 20 nm), is inserted between the areas of the gradient layer and the substrate. Such interlayer does not introduce considerable changes into the interference picture but enables to reduce absorption in the range with the highest extinction. The common coating thickness has made 0.17 μm in the case with a protective glass and 0.165 μm without it.

In the case of using porous silicon the inhomogeneous film should not contain underlayers with very low refractive index and, as consequence, very high porosity. Otherwise the integrity of this film could be broken. The demand for monotonous dependence of the porosity and the related to it volume filling factor from the coordinate will be more strict. Therefore into the program of profile retrieval has been interposed the requirement according to which nonmonotone profiles were expelled.

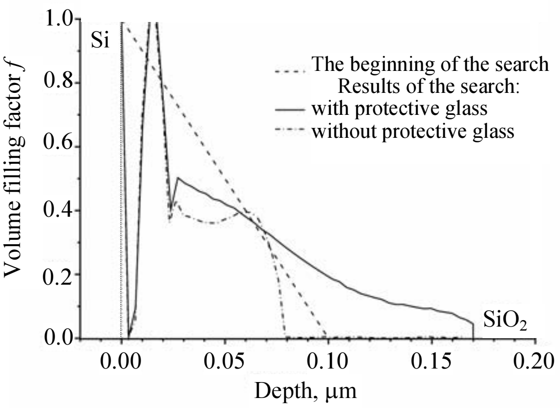

Fig. 1. Matching profiles calculated for SiO_x films

In the calculations was used as the initial the profile described by the formula [4]

$$n(x)=\frac{n_i\,n_s}{n_s-(n_s-n_i)(x/d)}, \qquad (5)$$

where n_i is the refractive index in the region of incidence; n_s is the refractive index of the substrate; d is the layer thickness.

For the antireflective coating consisting of porous silicon was only calculated the version without using the protective glass. The parameters distribution profile gained by this way is shown in Fig. 2.

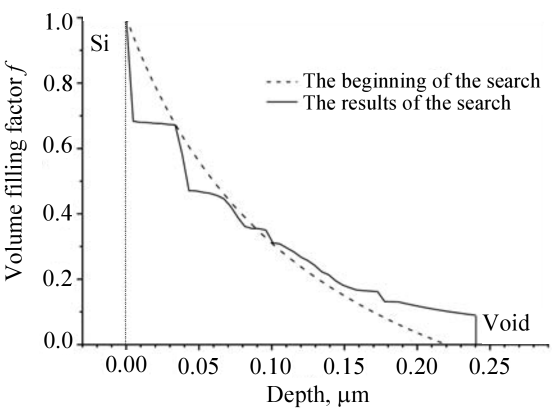

Fig. 2. Matching profile calculated for porous silicon film

As it is evident from Fig. 2 the film describable by the means of this profile is possible to be presented as a combination of quasi-homogeneous and inhomogeneous layers. In this case the common coating thickness has made 0.24 μm. Besides, the volume filling factor lies within the range of 0.1–0.7, which corresponds to the porosity range of 30–90%. It facilitates the task of manufacturing real porous silicon films corresponding to this profile, because technologically it is possible to gain *p*-Si with the porosity laying in these limits.

The diagrams in Figs. 3 and 4 represent losses for the reflection and absorption in the films. In the short-wave part of a spectrum increment of an absorption loss is observed.

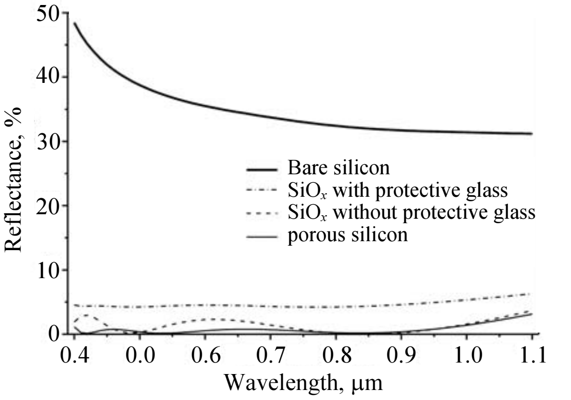

Fig. 3. Reflectance of the gradient-index antireflection coatings

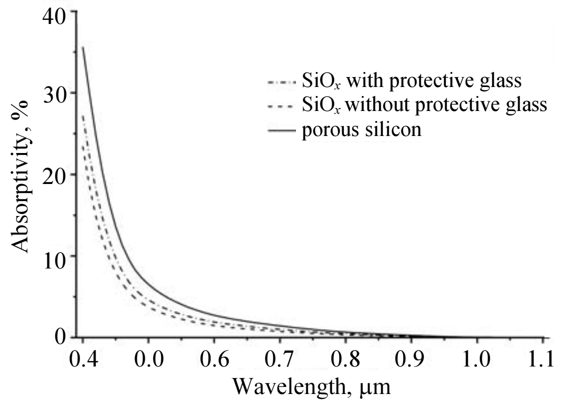

Fig. 4. Optical absorptivity of the gradient-index antireflection coatings

It is related to a tall magnitude of the absorption index of silicon in this spectral range. The average absorption over the range 0.4–1.1 microns in a SiO_x layer has made 2.5% in the case of usage of a protective glass and 2.0% without glass.

Medial reflection losses of 4.6% with a glass (in view of 4% of reflection from the frontal surface of the glass) and 1.3% without glass. Total losses have made 7.1% in the case of usage of protective glass and 3.3% without glass. In the case of using the porous silicon, the reflection and optical absorption averaged over the range have made 0.74 and 3.44% accordingly. Total losses in this case have made 4.18%.

In the Figure 5 are shown dependences of optical transparence of the coating mirroring its effectiveness.

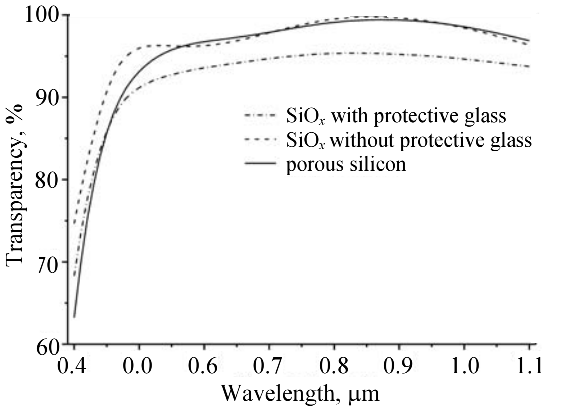

Fig. 5. Transparency of the gradient-index antireflection coatings

Medial passage of a layer over the range 0.4–1.1 microns is 92.9% in the case of using a SiO_x protective glass, and 96.7% without glass and 95.82% with using an inhomogeneous layer of porous silicon as the antireflection coating.

4. Conclusions

In this work is shown, that application gradient-index antireflection coatings make it possible to increment the semiconductor solar cells efficiency as the result of decreasing of reflection losses in a wide range wavelengths. As a gradient-index coating consists of one material with a variation of parameters on the depth, it is possible to gain such coating in an integrated technological process. In the case of using of silicon suboxide the transmittance of gradient antireflective coating can be increased by introduction of a thin (less than 20 nm) underlayer with low refractive index (SiO_2) between a substrate and the gradient layer. Such underlayer does not introduce considerable changes into the interference picture but enables to reduce absorption in the wavelength range with the highest extinction. In the case of using *p*-Si it is possible to use a distribution profile restricted to technologically realizable porosities. Thus, using the inhomogeneous films in a construction of an antireflective coating can raise their efficiency without any essential complication of production.

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