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FEATURES OF THE REFRACTIVE INDEX OF POROUS SILICON WITH GRADIENT POROSITY

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1. Introduction

After the detection of intensive photoluminescence of porous silicon (PS) at room temperature in the visible range of spectrum [1], a number of works dedicated to the study of the mechanisms of fabrication of PS as well as of its properties (physical, chemical, photoluminescent, optical, photoelectric, etc.) for different applications of this new material, in particular, for creating new devices (optoelectronic pairs, light-emitting diodes, gas sensors, waveguides, etc.) has sharply increased. This interest is triggered by the unique properties of porous silicon, among which the most important one may be the compatibility of porous silicon fabrication technology with silicon technology, which allows the integration of optical and electric functionalities of new devices in a uniform single crystal chip. Among the numerous possible applications of PS, because of the control capability of its refractive index, of utmost importance is the application of PS as antireflection coating (ARC) for various optical devices and, especially, for silicon solar cells.

The early studies [2-4] have reported on the reduction of optical losses (reduction of reflection) and improvement of photovoltaic characteristics (increase in the short-circuit current and open-circuit voltage without any perceptible changes of the fill factor). Using precisely designed anodization cells and nondestructive drying techniques, it is possible to reduce to a minimum the inhomogeneity of porosity on the surface of a sample. However, even in this case the photoluminescence of porous silicon layers shows a certain amount of inhomogeneity into the depth of the layer; in other words, there is a gradient of porosity with increasing depth within the layer, which is caused by electrochemical etching. In general, porous silicon layers display a negative gradient of porosity, i.e., the porosity is greater on the surface and decreases into the depth of the layer, although PS layers with a positive gradient of porosity are also known. Further in the work [5] it was reported that the formation of the multilayer PS as ARC on silicon solar cells leads to the reduction of the integrated reflection coefficient up to 3.4%, i.e., it equals the value of the well-known two-layer MgF_2-ZnS antireflection coatings.

However, in the above-mentioned works as a rule, the PS layers investigated as antireflection coatings had homogeneous in depth porosity. Based on the pore morphology studies with electron microscope it was assumed that under the known anodization modes the pores had cylindrical forms and, hence, the depth-dependent porosity of the PS layer was considered almost constant. However, in practice it is rather difficult to induce a formation of strictly cylindrical pores and there are always deviations from the strictly cylindrical form in an entire pore. Moreover, PS layers with various gradients of porosity represent both scientific and practical interest. Such PS layers may be created, for example, by changing the anodization current regimes during electrolysis, or by changing the illumination during the process, or by using silicon substrates with a gradient doping with depth of the layers. It is possible to apply PS layers with gradient porosity in silicon solar cells, like a special case of known cascade ($n_0 < n_1 < n_2 < ... < n_{Si}$) antireflection coatings. The advantages of such layers compared with standard cascade multilayer ARC include the simplicity of their fabrication and an opportunity of smooth modifications of the magnitude of the porosity gradient, and consequently of the refractive index $n_{PS}(z)$ as a function of the z coordinate in the depth of the layer.

2. Theory

In the present work the dependence of the refractive index $n_{PS}(z,\lambda)$ of the PS layer upon the depth z of the layer for pores having various geometrical configurations (conic and spherical) (see Fig. 1) is investigated. To simplify the analysis, we assume a) that the porous structure may be represented as distinct identical cells with a certain configuration of pores, as seen in Fig. 1.

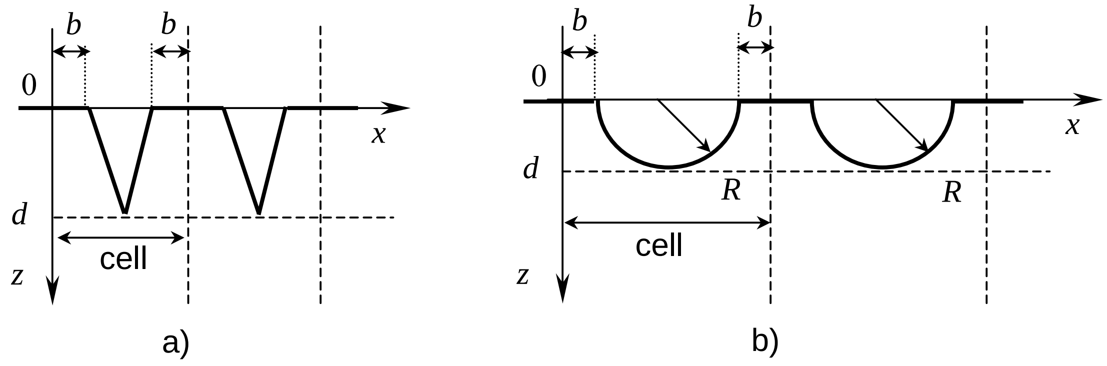

Fig. 1. Schematic illustrations of porous cells with conical (a) and spherical (b) configurations.

The porosity of a material may be defined as

$$p(z) = \frac{S_{por}(z)}{S_0}, \tag{1}$$

where $S_{por}(z)$ is the cross-sectional area occupied by a pore at depth z from the surface, and S_0

is the entire area of the cell surface (Fig. 1). After simple mathematical calculations it is not difficult to obtain the following expressions for the porosity with conical p_c and spherical p_s configurations of pores:

$$p_c(\theta) = \alpha_c(1-\theta)^2, \quad p_s(\theta) = \alpha_s\left(1-\theta^2\right), \tag{2}$$

where $\theta = z/d$, d is the layer thickness, α_c and α_s are some parameters depending on the geometric characteristics of pores (inclination of the cone generator, the radius of the sphere, etc.) (Fig. 1). The parameters α_c and α_s change in the range of $(0 \div 1)$ depending on the above-mentioned geometric characteristics and the configuration of pores.

Depending on the relation of the dimensions of the pores and the wavelength of the incident light there are different models - approximation theories for the description of the optical properties of porous systems. For example, it is known [6] that in those cases when the wavelength of the incident light is considerably more than the typical dimensions of the pores, it is possible to use the model of effective medium, according to which a two-component porous medium may be replaced by a new effective medium with a macroscopic dielectric constant. The task of averaging depends on the micro-topology of the medium and it is frequently complex. Among the enumerated approximations the most suitable for porous silicon is the approximation of Bruggeman as it is indicated in [7]. The optical properties of porous materials in contrast to the continuous samples of the same substances depend also on the microstructures of pores. For the solution of a number of applied problems, in particular, for the deposition of antireflection coatings it is necessary to find substances with specific refraction coefficients at a certain wavelength or a wavelength range. From this point of view, PS layers have an advantage, since

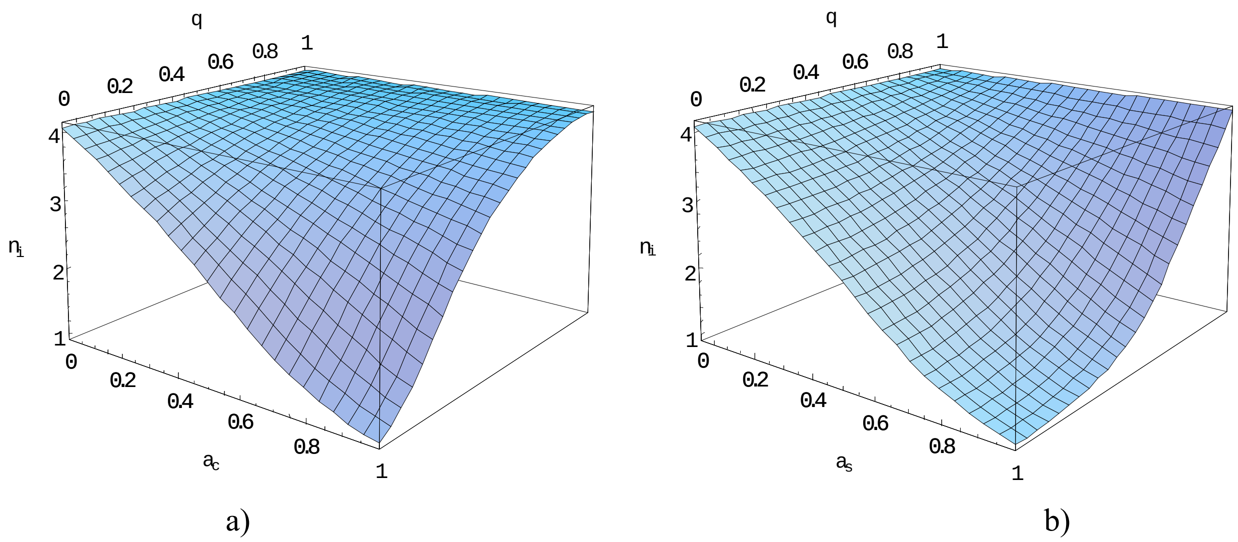

Fig. 2. PS refractive index dependence on θ and $\alpha_{C;S}$ for the conical (a) and spherical (b) pores.

by changing the porosity it is possible to vary the refractive index of a material in a wide range (from $n = n_{air} \cong 1$ to $n = n_{Si} = 3.5$). Therefore it is important to reveal the interrelation between the refractive index and porosity.

In Bruggeman's model the porosity and refractive index for PS layers are related by the formula

$$p = 1 - \left[\frac{(1 - n_{PS}^2)(n_{Si}^2 + 2n_{PS}^2)}{3n_{PS}^2 (1 - n_{Si}^2)} \right], \tag{3}$$

where n_{PS} and n_{Si} are the PS layer and single-crystal silicon refractive indices, depending on the wavelength of the incident light. Solving equation (3) relative to n_{PS}, one obtains

$$n_{PS} = \frac{1}{2} \sqrt{[3p_i(1 - n_{Si}^2) - (1 - 2n_{Si}^2)] + \sqrt{[3p_i(1 - n_{Si}^2) - (1 - 2n_{Si}^2)]^2 + 8n_{Si}^2}} \,. \tag{4}$$

As it is clear from expressions (2) and (4), the effective refractive index n_{PS} depends on the configurative parameters of the pores. In particular, the value of n_{PS} changes into the depth of the layer, i.e., there is a gradient of the refractive index into the depth of the layer.

Three-dimensional graphs of the dependences of refractive indices $n_{PS}(\theta, \alpha_{C;S})$ plotted using the program "Mathematica" based on equation (4) are presented in Fig. 2. Numerical calculations were carried out at $n_{Si} = 4.08$, when the wavelength of the incident light equals 550 nm.

3. Conclusion

The refractive index PS has a nonlinear dependence on θ and $\alpha_{C;S}$, as shown in Fig. 2. Moreover, the dependence $n_{PS}(\theta)$ displays a stronger nonlinearity than the dependence $n_{PS}(\alpha_{C;S})$. As the functional analysis shows, the region of nonlinearity of $n_{PS}(\alpha_{C;S})$ is located in the range $0.6 \le \alpha_{C;S} \le 1$. It is important to note that this nonlinearity grows with an increase in the refractive index n_{Si}, which is observed in the ultraviolet region of the dispersion law of the refractive index of the single-crystal silicon. We conducted our calculations with a fixed value of the refractive index $n_{Si} = 4.08$; however, if we consider the dispersion $n_{Si} = n_{Si}(\lambda)$, in the same way it is possible to find $n_{PS}(\theta, \alpha_{C;S})$ for any wavelength. Thus, we calculated the refractive index n_{PS} for inhomogeneous (with a gradient) PS layers, taking into account the dispersion law and the configurations of pores and using the approximation of effective medium. The theoretical results obtained can be used to solve, among others, the problem of reflection of light from the surface of silicon solar cells with antireflection coating from porous silicon with a gradient porosity.

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