Simulating the spectral characteristics of reflection in planar porous structures with antireflection coatings ZnS/DyF$_3$

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Abstract. This paper presents the results of modeling a planar multilayer structure with layers of porous silicon, ZnS and DyF$_3$ coatings by the optical matrix method. It was shown that the optical matrix method, taking into account the model of porous silicon with a variable band gap, which takes into account the porosity gradient, allows us to approximate the course of the curve of the real experiment.

1. Introduction

Porous silicon is a material of particular interest for solar energy, due to its large absorbing surface area. Due to the porous nature (Figure 1), the effective refractive index of porous silicon is lower than that of state material. Simulating the reflective properties of a multilayer structure allows us to identify the optimal parameters of the layers, which lead to a decrease in the reflection coefficient in the entire spectral range under study. In this paper, the reflective properties of a multilayer structure with a porous layer were modeled using the optical matrix method. This approach was used by the authors of [2,3] for structures with a single-layer antireflection coating of porous silicon and showed good agreement with the experiment.

![Figure 1. Cross cleavage of a porous structure [1].](image)

2. Experiment

The porous layer was obtained by electrochemical etching on a silicon substrate in alcoholic solutions of hydrofluoric acid. The thickness of the porous layer of the resulting structure was 10 microns.
ZnS and DyF$_3$ coatings were applied by thermal evaporation in vacuum. The spectral characteristics of the reflection coefficient were studied using a Shimadzu UV-2450 spectrophotometer.

3. The optical matrix method
Along with the traditional calculation, there is a matrix method [4-5], allowing to establish a number of relationships between the input and output parameters of the system using a single matrix of the optical system. The choice of one method or another is dictated by the requirements of the task at hand.

Plane wave interacting with a stack of layers

$$E = E_0 e^{ikr_{-}io\omega}, \quad H = H_0 e^{ikr_{-}io\omega}$$

$$\begin{bmatrix} E_{j-1} \\ H_{j-1} \end{bmatrix} = M_{j-1} \begin{bmatrix} E_j \\ H_j \end{bmatrix} = \begin{bmatrix} \cos \varphi_j & \frac{i}{n_j} \sin \varphi_j \\ in_j \sin \varphi_j & \cos \varphi_j \end{bmatrix} \times \begin{bmatrix} E_j \\ H_j \end{bmatrix}$$

$$\varphi_j = \frac{2\pi}{\lambda} n_j (z_j - z_{j-1}) \text{ - phase thickness of the layer}$$

Border conditions:

$$\begin{aligned} E_0 &= E_0^{(r)} + E_0^{(r)} \\ H_0 &= n_0 E_0^{(r)} - n_0 E_0^{(r)} \quad \text{(3)} \\ E_{(m)}^{(t)} &= 1 \\ H_m &= n_mE_{(m)}^{(t)} = n_m \end{aligned}$$

Transformation matrix:

$$\begin{bmatrix} E_0 \\ H_0 \end{bmatrix} = M_1 M_2 M_3 \cdots M_{m-1} \begin{bmatrix} E_m \\ H_m \end{bmatrix} \quad \text{(4)}$$

Taking into account the boundary conditions:

$$\begin{bmatrix} E_0^{(r)} + E_0^{(r)} \\ n_0 E_0^{(r)} - n_0 E_0^{(r)} \end{bmatrix} = \begin{bmatrix} m_{11} & im_{12} \\ im_{21} & m_{22} \end{bmatrix} = \begin{bmatrix} 1 \\ n_m \end{bmatrix} \quad \text{(5)}$$

Amplitude and energy coefficients of reflection and transmission of a multilayer interference system:

$$r_0 = \frac{E_0^{(r)}}{E_0^{(r)}} = \frac{n_0(m_{11} + in_mm_{12}) - (m_{21} + in_mm_{22})}{n_0(m_{11} + in_mm_{12}) + (n_mm_{22} + im_{21})} \quad \text{(6)}$$

$$R = \frac{|E_-|^2}{|E_+|^2} = |r|^2$$

The main parameters of modeling are shown in Table 1. In all cases, the total thickness of the porous silicon layers was 10 μm, and the refractive index was taken in values between the refractive index of silicon and the refractive index of zinc sulfide [6]. The model [7-8] assumes the formation of nanocrystallites and pores of various sizes in PSi layers. It is supposed that smaller nanocrystallites are located near the surface and their concentration reduces with depth. This causes a porosity gradient.
and, correspondingly, macroscopic dielectric function and refractive index gradients. Therefore, PSi can be considered as a semiconductor with a varying forbidden gap (graded bandgap semiconductors) or, in conformity with our case, as a stack of layers with different refractive indexes increasing towards the inner interface with the silicon substrate.

**Table 1. Simulation parameters**

|        | Si  | por-Si | ZnS | DyF₃ |
|--------|-----|--------|-----|------|
| n      | 3.42| 3      | 2.2 | 1.6  |
| D, µm  | 270 | 10     | 0.056 | 0.13 |

**Figure 2.** (a) Figure with short caption; (b) Figure with short caption.

### 4. Results and discussion

Taking into account the porosity gradient of the structure (Figure 3), several modifications of the model were considered: 1 porous layer, 6 porous layers, 8 porous layers and 10 porous layers. The control graph was the graph of the real experiment. The simulation results are shown in Figure 4.

**Figure 3.** Comparison of the simulation results a multilayer porous structure with a different number of layers and experiment.
By reducing the simulation step, it was possible to achieve some agreement with experiment Figure 4.

Comparing the simulation results with the multilayer porous structure experiment.

From the analysis of the obtained graphs, it can be seen that the representation of porous silicon in the form of 10 layers of the same thickness with a refractive index varying from silicon to air allows us to approximate the course of the curve of the real experiment. However, the discrepancy between the theory and the experiment can be explained by the features of absorption in real porous structures, which were not taken into account sufficiently fully in this model. Similar results were obtained in the works [3].

5. Conclusion
Thus, the resulting model allows us to determine the optimal parameters of the photosensitive structure without the use of complex mathematical calculations, which will further simplify the technological process of creating multilayer solar cells with a low reflection index.

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