Simulation optical parameters nanowire structures of various shapes.

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Abstract. In this study, three-dimensional fragments of nanowires structures were simulated in which the thread cross sections had a square, triangular and round shape. The theoretical data were compared with the experimental results, described in detail in [1]. The influence of the shape of the filaments on the theoretical course of the reflection curve is also shown.

1. Introduction
Silicon nanowires are a modern and promising nanomaterial of great interest for various fields of science [2-4]. Due to the complex surface, silicon nanowires have unique properties that allow them to be used as an anti-reflective coating for solar cells. Silicon nanowires also have advantageous optical and structural properties that differ from porous silicon. Silicon nanowires created on the surface have micro-nano textures that contribute to the hydrophobicity of the surface. These hydrophobic characteristics can be used in self-cleaning applications. These surfaces can be used for solar energy, in dusty environments [5]. Dust settles on surfaces and partially prevents solar radiation from reaching energy-saving devices such as photovoltaic panels and volumetric receivers, which reduces the performance of the device over time [6]. The spectral characteristics of nanostructures are modelled. At the moment, there are several models that can reliably describe the real course of the reflection curve for nanostructured materials, including silicon nanowires. In this paper, it is shown that the theoretical reflection coefficient depends on the shape of the wires (square, triangular, pyramidal), and one of the simulated structures coincides with the experimental results described in the article [1].

Figure 1. SEM-image of the real structure of nanowires and one of the structures, which is used in the Comsol Multiphysics software package.
2. The method of sample production

Silicon nanowires (SiNW) were manufactured by a two-stage metal-assisted chemical etching method (MACE). A metal-assisted chemical etching method was used, and AgNO3 (99.8%), H2O2 (30% in water), H2SO4 98%, and HF (48%) were used as the chemical etchants. The first step was to deposit silver on the surface of the silicon wafers, and then etching was carried out in an etching solution of HF / H2O2 5 M / 30% of the etchant. The remaining metal particles were removed from the surface with a solution of H2O: HCl: HNO3 for one hour [7-9].

For silicon nanowires of crystalline quality with transverse dimensions from 10 nm and higher, the so-called quantum-size effect for charge carriers is realized, which leads to an increase in the band gap and a shift of the optical absorption edge to the high-energy region. The optical properties of silicon nanostructures with large transverse dimensions will significantly depend on the effects associated with the spatial distribution of local electric fields and caused by light scattering by both individual nanoobjects and their ensembles. The study of such effects in nanostructures in the form of ensembles of silicon nanowires is particularly relevant, since they are easily integrated with microelectronics and sensor devices and materials for various applications, including biophotonics and medicine.

There are a number of practical tasks for creating light-sensitive structures, for which it is necessary to reduce the reflection coefficient at the boundary of two media. Modelling the distribution of the electric field on a filamentous surface allows us to describe physical processes with non-standard surface geometry.

3. Method of simulation

The Comsol Multiphysics software package was used to describe the passage of electromagnetic waves in a nanowire structure consisting of 10 wires with a thickness of 0.05 microns [10]. To solve this problem, a system was chosen in which a part of the silicon substrate is in the air (Fig. 2), so a wave equation was adopted based on an alternating electric field for two media:

$$\nabla \times (\nabla \times E) - k_0^2 \varepsilon_r E = 0$$

By default, the software package already contains the basic optical parameters of the two media for solving the equation. In our case, such media are air and silicon. Simulation of the electric field propagation, carried out in the software package in the optical range (300-1000 nm), allows you to calculate the distribution of the near field.

The boundary conditions under which the condition $n \times E = 0$ is satisfied in this system are the side faces of the bounded air medium. The upper face of this scheme is the plane of the energy flux density of the incident radiation (Fig. 3). It is also necessary to determine the scattering parameters (S-parameter) in terms of the electric field. To convert the picture of the electric field on the "in" port into a scalar complex number corresponding to the voltage in transmission line theory, it is necessary to
decompose the electromagnetic fields on the ports according to their own modes. We assume that the fields are normalized with respect to the integral of the power flow through each port cross-section, respectively. This normalization depends on the frequency. The port excitation is applied using the main eigenmode. The calculated electric field $E$ at the input "in" consists of the excitation and the reflected field. S-parameters are set:

$$S_{\text{in}} = \frac{\int_{\Omega} (E - E_1)E_1}{\int_{\Omega} E_1 \cdot E_1}$$

Figure 3. The plane of incidence of the electric field through the input port in the air environment of the Comsol Multiphysics software package.

Figure 4. Graphs of the dependence of the reflection coefficient on the wavelength obtained in various theoretical models (square, triangular, pyramidal) and practical data: red line – triangular nanowires, blue line – square nanowires, green line – pyramidal nanowires, black line – practical data.

The numerical method for solving this problem was to construct a finite element grid for the entire system. The dimensions of one grid element ranged from 0.1 to 5 microns. The wave optics module has a special periodic state. The periodic condition can identify simple mappings at the boundaries of the source and destination plane of equal form. The destination can also be rotated relative to the source. In this paper, a continuous type of periodic conditions was chosen. The tangential components of the solution variables are equal to the source and destination.
4. Results and discussion
The description of the passage of electromagnetic waves in the structure of nanowires consisting of 25 nanowires with a thickness of 0.2 microns with different shapes (pyramidal, triangular and square) was carried out in the Comsol Multiphysics software package.

Figure 4 shows the results of modelling the dependence of the light reflection coefficient on the length of the incident wave. Electromagnetic radiation passed through a structure with a nanowire, in which the distance between each element of the nanowire system was 0.2 microns. The analysis shows that in the wavelength range from 300 to 800 nm, the minimum reflection coefficient for theoretical models is in different values, but it is the triangular nanowires (Fig.5) are as close as possible to the practical values obtained in [1].

![Figure 4](image.png)

Figure 5. 3D map of light distribution in structures of various shapes nanowires (pyramidal, triangular, square). Matrix 5x5 with a minimum reflection coefficient.

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References
[1] Yilbas B S, Salhi B, Muhammad Y, Al-Sulaiman F, Haider A and Nasser A 2016 Scientific Reports. 6,1 1-13
[2] Li X 2012 Curr. Opin. Solid State Mater. Sci. 16 71–81
[3] Noor M O and Krull U J 2014 Anal. Chim. Acta 825 1–25
[4] Chen L J 2007 J. Mater. Chem. 17 4639–4643
[5] Liu K and Jiang L 2012 Annu. Rev. Mater. Res. 42 231–263
[6] Mani M and Pillai R 2010 Renew. Sust. Energ. Rev. 14 3124–3131
[7] Ma D D D, Lee C S, Au F C, Tong S Y and Lee S T 2003 Science 299 1874–1877
[8] Wu S, Shao Y M, Nie T, Xu L, Jiang Z and Yang X 2015 Nanoscale Res. Lett. 10 325–333
[9] Han H, Huang Z and Lee W 2014 Nanotoday 9 271–304
[10] Hochbaum A I 2005 Nano Letters. 5 457