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Optical Properties of Porous Silicon *p*-Si (100)

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In this paper the reflectance spectra and transmission spectra of p-Si (100) porous silicon (PS) and silicon wires in the spectral range of 200 ÷ 1800 nm were investigated. Pore size of PS was 5 μm (l_{por} Si layer) and 50 μm (lpor Si layer) with porosity of 45 %, 55 % and 65 %. The length of silicon wires varies from 5.5 μm, to 50 μm with a porosity of 60 %. The decrease in the band gap of p-Si (100) porous silicon and silicon wires which grown on both sides of p-Si (100) as compared to the single crystal p-Si (100) is explained by the quantum-sized effect that occurs in the investigated objects.

Keywords: porous silicon *p*-Si (100), reflectance spectra, transmission spectra, quantum size effect.

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Introduction

At present, there is an increased interest in semiconductor materials that contain nanosized structural elements the presence of which substantially changes the optical, photovoltaic, electrophysical and other properties of semiconductors. Perspective material for modern micro and nanoelectronics is porous silicon. It is known that porous silicon possesses sufficiently effective photoluminescence at room temperature in the visible region of the spectrum. However, mesoporous layers of porous silicon are practically always formed on Omni low substrates, which are not luminescence in the visible region of the spectrum [1] and were confirmed by us in our experiments.

Porous silicon is used for manufacturing light-emitting diodes, photovoltaic converters for solar energy, ultra-high frequency (microwave) instruments, and chemical sensors [1]. Most of the properties of materials that consist of grains of micrometers (nanometer) sizes strongly depend on their specific surface. The specific surface is determined using the formula: $S = \frac{A}{rV}$, where A is the surface area of the particle, V – volume of the particle; ρ – density.

An effective method of increasing the specific surface of the sample is to reduce the size of its grains. Another method of increasing the specific surface S is to make small volumes of volumetric material [2].

Despite the sufficiently large number of domestic and foreign publications on the technology of obtaining, on the structural, luminescent and electrophysical properties of porous silicon, further studies of this material are an actual.

In this paper, in order to obtain data on the energy band structure, the elucidation of physical processes, mechanisms and the nature of the formation of electronic and optical phenomena on the surface and in the near-surface layer and in the volume of this material, the results of the investigation of optical reflection spectra and the transmission spectra of porous silicon p-Si (100) with pores of 5 μm (l_{por} Si layer) and 50 μm (l_{por} Si layer) and porosity of 45 %, 55 % and 65 %, as well as silicon wires with lengths of l_{NW} 5.5 μm, 20 μm and 50 μm and porosity 60% in the spectral range of 200 ÷ 1800 nm.

I. Experiment

Samples of porous silicon (p-Si) with different porosity were made using electrochemical etching of the surface of the plates of monocrystalline (100) - oriented silicon $p+$ - type conductivity (specific resistance 0.01 Om cm, thickness of plates 510 ± 20 microns) in a solution of concentrated hydrofluoric acid (49 % HF in water) and pure ethanol. In the work, the porosity (45 %, 55 %, and 65 %) and the thickness of the porous layer (5 microns, 50 microns) of specimens varied by applying to the plate controlled by the magnitude of the current density and the duration of etching. Silicon nanowires

(NWs) were grown by liquid chemical etching (MAWCE). Formation of Si NWs was carried out in two stages using two solutions. The digestion time ranged from 10 to 60 minutes to obtain a layer of Si NWs of varying lengths of nanowires.

Optical studies (transmission and reflection) were performed in the range 200 - 1800 nm by the two-beam spectrophotometer Shimadzu UV-3600 and in the range of 2 - 25 μm on the Fourier spectrometer of the Perkin Elmer Spectrum BXII. All studies were conducted at room temperature. The resolution of the devices was no worse than 0.01 nm.

II. Results and discussion

In the absence of defects, electrons, holes, phonons, excitons or excitations in a crystal are described by Bloch waves, which can be freely distributed in a crystal. If the crystal is not infinite and there are two infinitely high barriers at a distance L from each other, which may reflect Bloch waves along the z direction, then there is a spatial limitation of the wave data. It is known that the normal oscillations of the oscillating string model with two fixed ends are standing waves of wavelength λ,

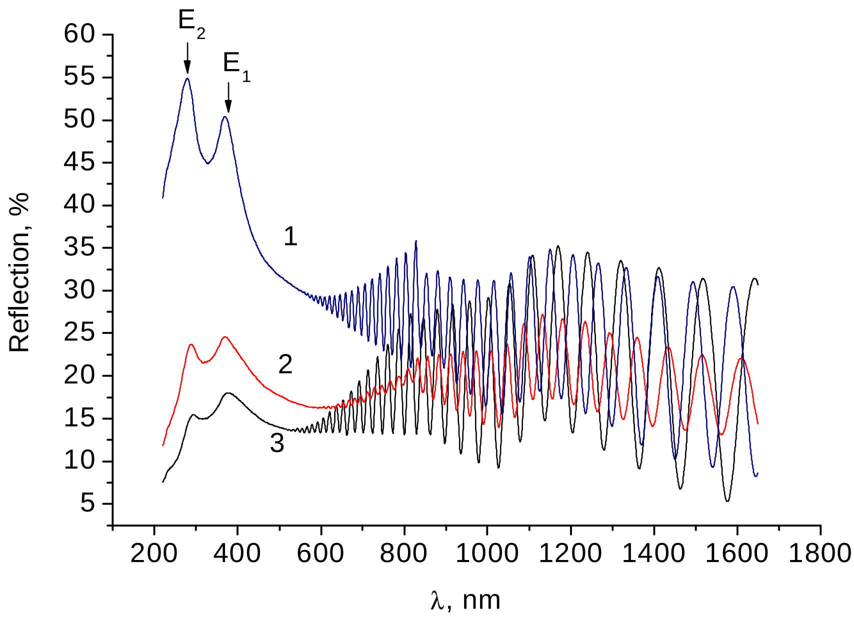

Fig. 1. Reflection spectra of porous silicon at a pore size of 5 μm (lpor Si layer): curve 1 - porosity 45 %; curve 2 - porosity 55 %; curve 3 - porosity 65 %.

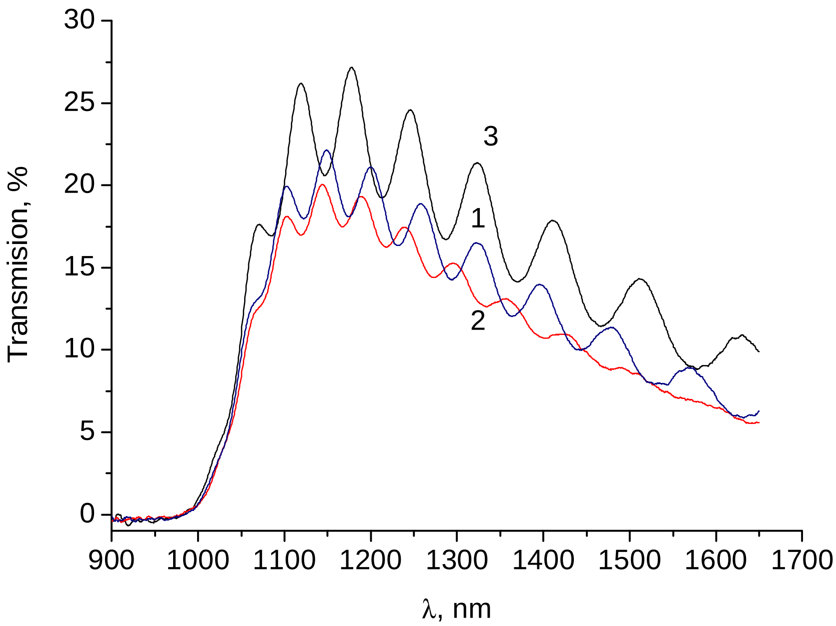

Fig. 2. Transmission spectra of porous silicon at a pore size of 5 μm (lpor Si layer): curve 1 - porosity 45%; curve 2 - porosity 55 %; curve 3 - porosity 65 %.

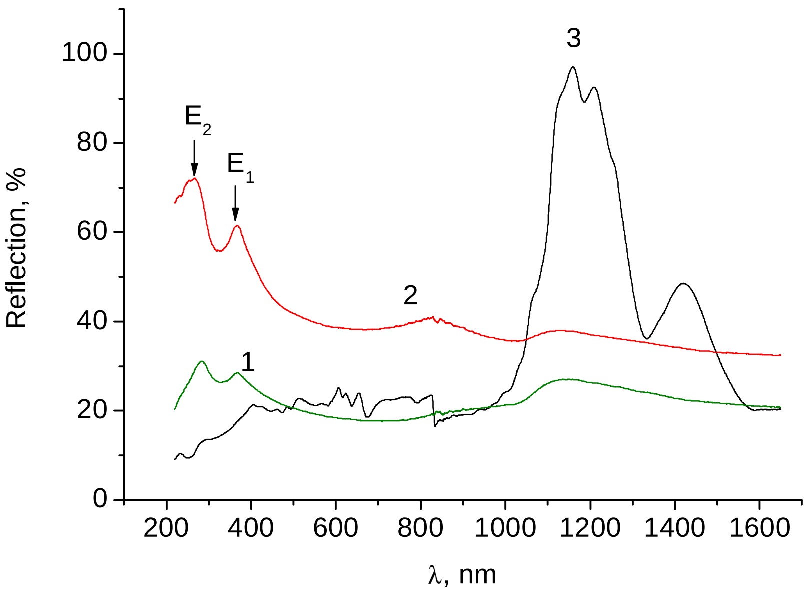

Fig. 3. Reflection spectra of porous silicon at a pore size of 50 μm (lpor Si layer): curve 1 - porosity 45 %; curve 2 - porosity 55 %; curve 3 - porosity 65 %.

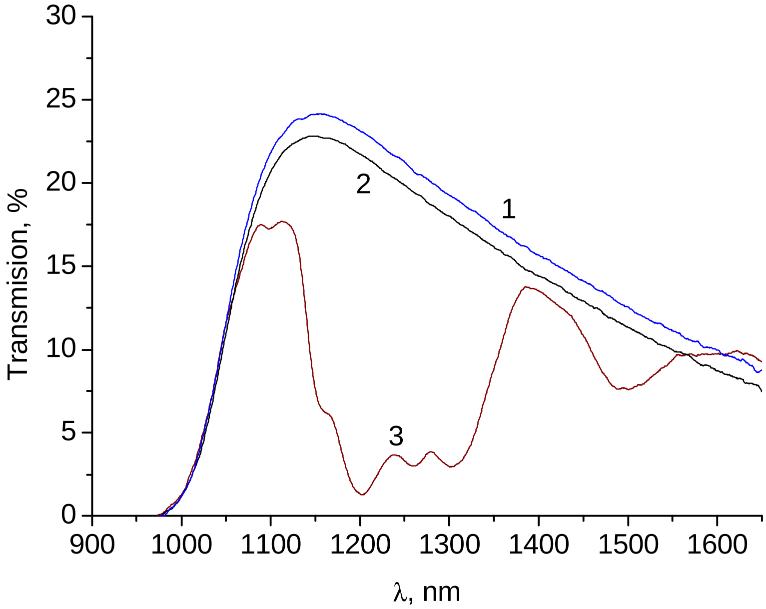

Fig. 4. Transmission spectra of porous silicon at a pore size of 50 μm (lpor Si layer): curve 1 - porosity 45 %; curve 2 - porosity 55 %; curve 3 - porosity 65 %.

which takes discrete values:

$$l_n = \frac{2L}{n},\ n = 1, 2, 3\ldots \qquad (1)$$

For a free particle with an effective mass, the motion of which in a crystal in the z direction is limited by non-penetrating barriers (barriers with infinite potential energy), the values of the wave vectors k_z of the Bloch wave are allowed to look like:

$$k_{zn} = \frac{2p}{l_n} = \frac{np}{L},\ n = 1, 2, 3\ldots \qquad (2)$$

The energy of the ground state in comparison with the crystal's state without restriction increases or decreases by the value of [3]:

$$\Delta E = \frac{\mathbf{h}^2 k_{z1}}{2m^*} = \frac{\mathbf{h}^2 p^2}{2m^* L^2}. \qquad (3)$$

Figures 1 and 2 shows the spectra of optical reflection and transmission of porous silicon at a pore size of 5 μm (l_{por} Si layer) with a different porosity *x*, which varies within 45% ≤ x ≤ 65%.

As shown in Figure 1, in the high-energy region of the spectrum, two peaks of E_1 and E_2 of monocrystalline silicon p-Si (100), corresponding to energies of 3.35 eV ($E_1(\Lambda_1^C - \Lambda_3^V)$ [4]) and 4.465 ($E_2(\Lambda_1^C - \Lambda_5^V)$),

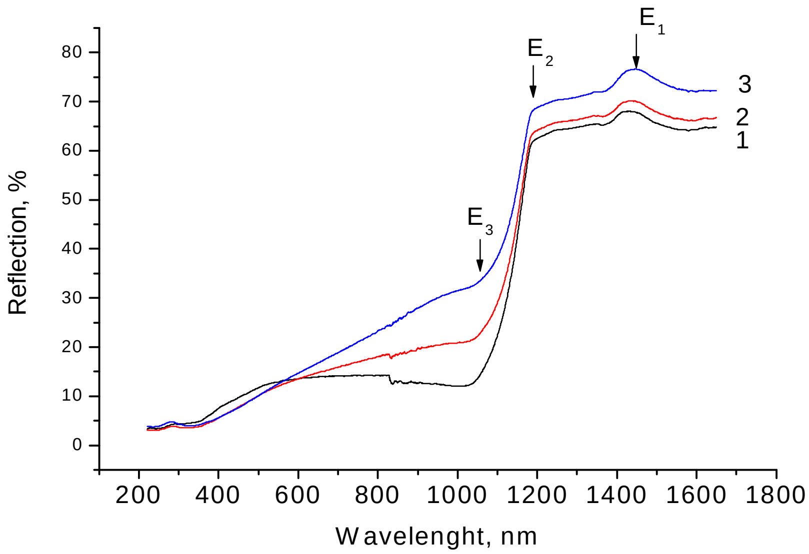

Fig. 5. Reflection spectra of silicon wires: curve 1 - l_{NW} = 5.5 μm; curve 2 - l_{NW} = 20 microns; curve 3 - l_{NW} = 50 microns. Sample porosity is 60 %.

respectively, appear [4]. In the low-energy region of the reflection spectrum of porous silicon p-Si (100), an interference pattern is observed, which is due to the SiO_x and SiO_2 oxides (Fig. 1) and the porosity of the monocrystalline p-Si (100).

With increasing porosity, the intensity of high-energy peaks E_1 and E_2 decreases.

According to the literature [5], the thickness of the transition layer SiO_x is 0.6 nm. The oxide coatings of a real surface of silicon are amorphous films whose thickness varies in the range of 0.5 - 7 nm [6, 7].

Figure 3 shows the spectra of optical reflection of porous silicon at a pore size of 50 μm (lpor Si layer) with different porosity. As can be seen from Fig. 3, peaks E_1 and E_2, at a porosity of 55 %, correspond to energies of 3.396 eV and 4.469 eV respectively (these are the peaks of p-Si (100) monocrystalline silicon). At porosity 45 % peaks E_1 and E_2 correspond to energies of 3.396 eV and 4.375 respectively. At a porosity of 65 % in the low-energy region of the spectrum two peaks with energies of 1.025 eV and 1.07 eV, respectively, appeared.

Figure 4 shows the optical transmission spectra of porous silicon at a pore size of 50 μm (lpor Si layer) with a porosity of 45%, 55% and 65%.

As can be seen from Figures 3 and 4, the reflectance and transmission spectra at 45% and 55% porosity are similar to those of monocrystalline silicon. As is known [8], the main parameter of porous material is the porosity index. It determines which part of the volume of the material is occupied by pores. When this volume is small, the properties of such a material are close to the properties of monocrystalline silicon, which is observed in our case. At high porosity rates, the material acquires new unique properties. In the reflection and transmission spectra with a porosity of 65 %, maxima and minima are observed in the range 1000 - 1500 nm, respectively. Such an effect can be used to create new optoelectronic devices.

Figure 5 shows the optical reflection spectra of silicon nanowires in the wavelength range $\lambda = 0.2$ - 1.8 μm with lengths of nanowires l_{NW}, varying in the range l_{NW} = 5.5 μm - 50 μm. Sample porosity is 60%. The optical reflection spectra are identical on both sides (silicon nanowires are formed on both sides of the p-Si (100)).

In Figure 5, three energy positions E_1; E_2; E_3 are shown that corresponding to energies of 0.862 eV; 1,046 eV and 1,198 eV respectively. With an increase in the length of silicon nanowires the reflection coefficient ***R*** in the range of 0.2 - 1.8 μm wavelengths increases.

Conclusions

According to experimental data and calculations, the reduction in the width of the band gap of p-Si (100) and silicon wires compared to the single crystal p-Si (100) is explained by the quantum-sized effect that occurs in the investigated objects. It is shown that the energy spectra of the investigated structures strongly depend on their specific surface. The possibility of controlling the energy spectrum using the technology of fabricating structures is analyzed.

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Оптичні властивості пористого кремнію *p*-Si (100)

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В даній роботі представлені результати дослідження оптичних спектрів відбивання пористого кремнію p-Si (100) при розмірі пор 5 мкм (l_{por} Si шару) та 50 мкм (l_{por} Si шару) при пористості 45 %, 55 % та 65% і кремнієвих ниток довжиною l_{NW} 5,5 мкм, 20 мкм та 50 мкм із пористістю 60 % в спектральному діапазоні 200 ÷ 1800 нм та спектрів пропускання досліджених зразків. Зменшення ширини забороненої зони пористого кремнію p-Si (100) і кремнієвих ниток, вирощених з обох сторін p-Si (100) в порівнянні із монокристалом p-Si (100) пояснено квантоворозмірним ефектом, який виникає в досліджуваних об'єктах.

Ключові слова: пористий кремній p-Si (100), спектри відбивання, спектри пропускання, квантоворозмірний ефект.