Optical properties of dry etched vertically aligned silicon structures with different geometry

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Abstract. In this paper, we study the effect of the height and diameter of vertically aligned silicon structures on their optical properties. Structures with different geometry were formed using nanosphere lithography and dry etching. Nanosphere lithography was realized with 0.9 and 2 μm latex spheres. The etching process was carried out through a formed mask (template) composed of 0.9 and 2 μm latex spheres, respectively. The diameter of the spheres and the etching time determined the size of the formed structures and their optical properties. A significant reduction of the total reflection with height as well as blue shift of the minimum with diameter decrease were observed.

1. Introduction

Nowadays, most solar cells are made of silicon due to its availability and relatively low cost. Further development of photovoltaics requires to increase the efficiency of solar cells and to decrease the price of the produced energy. Thus, new concepts and approaches should be explored. One of the key factors affecting the efficiency of solar cells is the optical losses. They are related to reflection and incomplete absorption in the active layers of a semiconductor material. One of the promising ways to reduce optical losses is the use of vertically aligned silicon structures. Reflection losses can be reduced by varying the structural parameters of the wires, such as periodicity, diameter ($D$) and height ($H$) (Figure 1).

![Figure 1. Schematic of the vertically aligned silicon structures.](image)
It is possible to obtain vertically aligned structures by cryogenic etching [1]. The essence of this method is that the silicon substrate is cooled up to -140 °C. At this temperature, the side surface is passivated due to the formation of a non-volatile SiO2F2 compound. This compound blocks the etching mechanism. Thus, the cryogenic process provides deep and anisotropic etching of silicon [2-4]. Before the dry etching, it is necessary to create a mask (template) on its surface. The most promising way is the formation of a mask using colloidal nanospheres. This allows to avoid the use of complex methods of lithography [5-6].

2. Experimental
At the beginning, 500 nm layer of SiO2 was grown on 4-inch (100) silicon substrate by plasma-chemical deposition with Oxford Instruments PlasmaLab 100 PECVD equipment. N-type silicon wafers (100) with resistivity of 0.06 – 5 Ohm·cm were used.

A mask (template) on the surface of the SiO2/Si substrate was formed using the nanosphere lithography and spin-coating technology. For the formation, 0.9 and 2 μm polystyrene spheres were used. Initial polystyrene solutions were 10 wt. % 0.9 μm and 2 μm spheres in water.

0.9 μm polystyrene spheres solution was separated in centrifuge and diluted in isopropanol/water solution before deposition. The optimal parameters for applying 1 μm spheres are water/isopropanol volume ratio 7/13, solution temperature of 50 °C and drying speed of 1000 rpm.

2 μm polystyrene spheres solution was separated in centrifuge and dilute in isopropanol/water/proplylene glycol solution before deposition. The optimal volume ratio of isopropanol/water/proplylene glycol was 7/2/1. To obtain a close-packed monolayer of 2 μm spheres, a lower drying speed of 700 rpm and a solution temperature of 20 °C were required.

The described parameters provide the maximum coverage of the substrate surface with a monolayer of 0.9 μm (Figure 2, a) and 2 μm (Figure 2, b) polystyrene spheres.

![Figure 2. Optical microscopy image of 0.9 μm (a) and 2 μm (b) polystyrene spheres deposited on SiO2/Si substrate.](image)

Then polystyrene spheres were etched in oxygen plasma to reduce their diameter. Etching was carried out in ICP mode with the following parameters: temperature of -20 °C, ICP power to 1000 W, CCP power was equal to 3 W, pressure to 25 mTorr and O2 flow to 50 sccm. The diameter of the spheres obtained after etching in oxygen plasma will determine the size of the formed wires.

Further, through the formed sphere mask, silicon oxide was removed in CHF3 plasma forming thus a SiO2 hard mask for the subsequent silicon cryogenic etching. SiO2 etching was carried out in a cyclic mode, i.e., the etching steps alternate with the cooling steps. The optimal parameters of the plasma etching SiO2 are temperature of -20 °C, ICP power was set to 700 W, CCP power to 40 W, pressure was set to 3 mTorr, CHF3 flow to 30 sccm and etching time 60 sec.

The final step is the cryogenic etching of silicon at the following parameters: temperature of -140 °C, RF power to 30 W, ICP power to 1000 W, flow SF6/O2 to 50/11 sccm and pressure to 5 mTorr. The etching rate is 1200 nm/min.

Figure 3 shows the structures formed on silicon substrate through a SiO2 mask formed with polystyrene spheres of 2 μm size. The etching time is 5 minutes.
It can be seen from figure 3 that the height of the structures is 6 μm and the diameter is 1.8 μm. The parameters of the structures obtained on different substrates are presented in table 1.

| Sphere diameter, μm | Structure parameter | diameter, μm |
|---------------------|---------------------|--------------|
|                     | height, μm          |              |
| 0.9                 | 8                   | 0.4          |
|                     | 5                   | 0.615        |
|                     | 3                   | 0.6          |
| 2                   | 5.3                 | 1.4          |
|                     | 6                   | 1.5          |
|                     | 6                   | 1.8          |
|                     | 5.9                 | 1.2          |

The spectral dependences of total reflection for different heights and diameters of the silicon wires were obtained by using the integrating sphere ISP-50-8-GT from Ocean Optics. The geometry of the structures strongly effects on their optical properties (Figure 4).

It can be seen from figure 4 (a) that an increase in wire diameter from 1.2 to 1.8 μm leads to an increase in total reflection, especially in the short-wavelength region. In the long-wavelength region,
the inverse effect is observed, the reflection slightly decreases. Thus, a blue shift of the short wavelength edge of the reflection minimum with decrease of the diameter is observed.

Figure 4 (b) shows the spectral dependence of total reflection at three different wire heights. An increase in wire height leads to a decrease in the total reflection of vertically aligned structures.

3. Conclusion
We have studied the optical characteristics of vertically aligned silicon structures in terms of wires diameter and height. It was shown that the optical reflection of the wires arrays is sensitive to their diameter and height. Reflection and, consequently, optical losses can be significantly reduced by varying the geometry of the wires. A relatively low reflection was observed for wires with diameter of 0.4 μm and height of 8 μm, respectively.

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