Theoretical optimization of the photolithography through array of 1.2 μm silica microspheres

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Abstract. Interest in heteroepitaxy of III-V compounds on Si has been growing rapidly in recent years due to the potential of the optoelectronic components integration on silicon. However, most of the semiconductor compounds conventional in optoelectronics cannot be easily integrated on Si substrates due to the formation of the lattice defects. In this paper, we consider the fabrication of the mask consisting of the ordered nanoscale holes with the use of microsphere photolithography for selective epitaxial growth – promising approach for nanostructures fabrication on mismatched substrates. We have carried out the calculation of electromagnetic wave absorption in the photoresist layer through 1.2 μm microspherical silica lenses. The theoretical optimization of the photoresist thickness parameter allowed to obtain a value at which the minimum holes diameter in the photoresist is achieved. These data are necessary for carrying out the process of lithography through microspherical lenses to create a patterned growth mask.

1. Introduction
There are three main problems in the technology of A3B5 semiconductor compounds synthesis on Si: high dislocations density due to the mismatch of the growing material lattice with the substrate, formation of antiphase domains due to the presence of polar/non-polar interface and lattice cracking due to the difference in thermal expansion coefficients between two materials [1]. Due to the large surface area/volume ratio, low dimensional structures can be used to suppress the mentioned effects. Self-assembled nanostructures are easy to synthesize, can have different morphology providing versatility of their properties and can be grown with a variety of materials providing control over their electronic properties. In recent years there has been an increasing demand on mass production of ordered and periodic nanostructures since such nanostructures have found wide application in many high-performance devices, such as LEDs [2], photodetectors, data storage elements, nanoantennas, photonic crystals [3].

Arrays of highly ordered nanostructures can be achieved by several methods [4], such as immersion lithography [5], electron beam lithography [6], focused ion beam lithography [7], deep ultraviolet lithography (DUV) [4], nanoimprint lithography [8] and other less developed methods. The main flaw of these methods is their limited application, mostly governed by the low manufacturing capability on large scale due to the high cost or low production capacity. Thus, today, there is a need of new cheaper and high-performance methods development that will allow manufacture of periodic and highly
ordered arrays of nanostructures over large areas [9]. One of the promising approached is the microsphere photolithography [10, 11]. This work is aimed at development of the fabrication technique of the mask with nanometer-sized openings, acting as windows in the oxide layer obtained by the photolithography on a Si substrate surface for the selective area epitaxy. It is assumed that the use of nano-sized openings in the oxide layer allows to obtain planar structure or ordered array of nanostructures, without dislocations and the formation of antiphase domains at the heterojunction between Si and the semiconductor material [12]. We performed the numerical calculation of the electromagnetic wave propagation and absorption in the photoresist of different thickness covered with SiO$_2$ 1.2 μm microlenses to study correlation between the size of the openings and the photoresist thickness.

2. Modeling
We carried out 3D simulation of the plane incident electromagnetic wave propagation through SiO$_2$ microspherical lenses into the positive photoresist layer. The modeled structure consists of Si substrate with a 50 nm layer of silicon oxide, covered with a photoresist layer and array of hexagonally ordered microspheres with a diameter of 1.2 μm. The choice of the sphere diameter was governed by their commercial availability. The simulation was performed in the CST Microwave Studio. The package uses differential forms of the Maxwell equations for the calculation. Using the calculation in the time domain, the absorption of the electromagnetic field in the photoresist layer with different thickness was studied.

The results of the numerical calculations showed that the depth of the radiation penetration into the resist and the quality of focusing (diameter of the exposed area) depend on the photoresist thickness and on the wavelength used. For the simulation, the wavelength of the plane incident wave of 405 nm and 365 nm was considered, corresponding to the radiation used for the photoresist exposure.

It was established experimentally that when using a positive photoresist thickness of less than 200 nm, there is instability of its thickness. It leads to a variation in the mask pattern size. Thereby, the calculation was carried out with the photoresist thickness in the range from 200 to 500 nm with a 50 nm step. Figure 1 (a - e) shows the electromagnetic wave absorption efficiency in the photoresist layer.

![Figure 1(a, b, c, d, e). Absorption of the incident wave having the wavelength of $\lambda = 405$ nm in the positive photoresist covered with ordered array of 1.2 μm SiO$_2$ microlenses on a Si substrate coated with a 50 nm layer of SiO$_2$: (a) 200 nm, (b) 250 nm, (c) 300 nm, (d) 350 nm, (e) 500 nm.](image_url)
The black contours correspond to the minimum light intensity required for exposure of the photoresist. As can be seen, the profiles of these contours have maxima due to the interference of the incident and reflected from the silicon substrate waves. Analyzing the contours we obtain values of the top and bottom (on the boundary with the oxide layer) exposed area diameter and evaluate their dependencies on the resist thickness shown in Figure 2. The black curve in Figure 2 corresponds to the projected area diameter in the top region. The red curve shows the area diameter in the bottom. From Figure 2 it can be seen that for a wavelength of 405 nm the optimum thickness of the photoresist is 200 nm, and the corresponding size of the holes in the photoresist should be about 180 nm.

The modeling was also carried out for the incident wave length of 365 nm. The thickness of the photoresist was varied from 200 to 500 nm with a step of 50 nm. Figure 3 shows the light absorption for several photoresist thicknesses. It can be seen that at small thickness of the photoresist (200 nm), the exposed area increases. At large thicknesses (from 300 nm), the diameter of the exposed area also increases. At the same time, the power required to expose the photoresist increases 2 times when the thickness increases from 200 nm to 400nm. The radiation with a power used for 200nm resist exposure is completely absorbed in the 400nm photoresist and cannot pass through the photoresist layer.

Figure 2. Plot of the exposed area diameter of the positive photoresist layer on its thickness, for the exposure wavelength of 405 nm, “top region” is the diameter of the exposed area on the surface of the photoresist, "Bottom region" is the diameter of the exposed region of the resist near the surface of the SiO₂ layer.

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Figure 3(a, b, c, d, e). Absorption of the incident wave having the wavelength of $\lambda = 365$ nm in the positive photoresist covered with ordered array of 1.2 $\mu$m SiO$_2$ microlenses on a Si substrate coated with a 50nm layer of SiO$_2$: (a) 250 nm, (b) 200 nm, (c) 300 nm, (d) 350 nm, (e) 500 nm.

The dependence of the positive photoresist exposed area diameter as a function of its thickness is presented in Figure 4. Analyzing the results presented in the graph, it can be seen that for a wavelength of 365 nm, the photoresist thickness of 250 nm corresponds to the minimum focusing region of the incident radiation. With these parameters, the size of the holes should be as small as 170 nm.
Figure 4. Plot of the exposed area diameter of the positive photoresist layer on its thickness, for the exposure wavelength of 365 nm, “top region” is the diameter of the exposed area on the surface of the photoresist, "Bottom region" is the diameter of the exposed region of the resist near the surface of the SiO$_2$ layer.
3. Conclusion
In this work, we have studied numerically propagation of the electromagnetic wave with a wavelength of 405 and 365 nm and its focusing under array of microspherical lenses in the volume of varied thickness positive photoresist. The 50nm silica sublayer that can be used as a mask material for selective epitaxy is taken into account in the model.

According to the calculated data, it was obtained that at a wavelength of 405 nm a layer of positive photoresist with a thickness of 200 nm is suitable for the most efficient focusing of SiO$_2$ by microspherical lenses with a diameter of 1.2 μm. In this case, the diameter of the openings in the developed photoresist can be as small as 180 nm. For the wavelength of 365 nm, the optimum value of the photoresist thickness was 250 nm, while the size of the holes in the photoresist should be about 180 nm.

The obtained calculated data allows to determine the parameters of the photolithography process for fabrication of the photoresist pattern having subwavelength features. The results are aimed at creation of a large scale mask with ordered nano holes in the oxide layer for epitaxial synthesis of A3B5 semiconductor nanostructures on Si.

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