Preparation of Si substrates for monolithic integration of III–V quantum dots by selective MBE growth

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Abstract. A new method for nanopit formation by molecular-beam epitaxy (MBE) on different silicon substrates has been investigated. The dependence of the shape and depth of the nanopits on substrate orientation and doping type has been studied. The samples with an array of nanopits with 25 nm depth and $(2-6) \times 10^8$ cm$^{-2}$ density for subsequent monolithic selective growth of quantum dots (QD) have been created.

1. Introduction

Today the vast majority of integrated circuits are produced by complementary metal-oxide-semiconductor technology based on silicon [1]. The current trend towards decreasing transistor size to increase the density of transistor-per-chip results in a search of an alternative to widely used electrical interconnects [2]. The use of high-speed optical communication is therefore considered as a promising method [3]. Due to the indirect bandgap of silicon, light-emitting devices based on it have very low efficiency [4]. On the other hand, direct-band compounds of III-V materials are widely used in different photonic devices, such as lasers and photo detectors. Thus, the integration of $A_3B_5$ and Si is crucial for the realization of photonic integrated circuits [5].

Recently, a lot of scientific groups have been carrying out research on integrating direct-band compounds of III-V materials and Si [6]. The application of QDs is considered to be promising due to the low sensitivity to crystalline defects, particularly their incorporation as active region directly in silicon substrate [7]. It has been already shown that the utilization of pre-patterned substrate surface can be used to control position and form of QDs on the substrate [5]. Different methods of pre-growth substrate treatment are usually used for patterned surface preparation, such as electron beam lithography and dry chemical etching [4]. These methods provide an opportunity to form an ordered array of nanopits on the substrate surface with certain precision. In the paper [9] it has been shown that subsequent epitaxial growth can be used to synthesize QDs of given composition in the formed array of nanopits. However, existing methods of pre-growth substrate treatment may lead to the increase of the structure cost and degradation of the growth surface and therefore the active region.

Here we report on an investigation for a new method for nanopit formation on silicon surface without pre-growth substrate treatment for subsequent monolithic selective growth of QDs.

2. Results and discussion

All the samples studied were grown by MBE using a Riber Compact EB 200 setup on (001) or (111) Si substrates with n- or p-type doping. For silicon deposition we used a source with electron impact.
Prior to the growth, the silicon substrates were subjected to a cycle of chemical treatment by the Shiraki method [10], which we modified. During the course of chemical treatment, the native oxide overlayer was removed from the substrate surface and a passivating layer of non-stoichiometric SiO$_2$ was formed. Subsequent annealing of the substrate in the MBE growth chamber at 850°C was performed to remove the passivation layer and the remaining traces of chemical compounds. The further growth of Si buffer layer occurred at the substrate temperature of 600°C.

After MBE synthesis of Si buffer layer on (001) substrate we have observed a formation of pyramidal nanopits (figure 1). To study an influence of the buffer layer thickness on the nanopit parameters a series of structures with 15, 30 and 65 nm Si layers has been grown. Parameters of the structures thus obtained have been presented in table 1. According to the data we may have concluded that the depth and size of the nanopits increase with the growth of the buffer layer thickness.

![Figure 1. TEM picture of 25 nm nanopit grown on n-type (001) Si substrate with 65 nm buffer layer.](image)

**Figure 1.** TEM picture of 25 nm nanopit grown on n-type (001) Si substrate with 65 nm buffer layer.

| Buffer layer thickness, nm | Nanopit depth, nm | Nanopit size, nm |
|----------------------------|-------------------|------------------|
| 15                         | 4.6               | 140              |
| 30                         | 8.8               | 171              |
| 65                         | 14                | 185              |

A series of structures with 65 nm buffer layer has been grown on Si substrates with different orientation and doping type. AFM images of the samples have been shown in figure 2. According to the figure 2(a) the use of (111) Si substrate has led to the formation of nanopyramids with 3 nm height instead of nanopits. The images represented in figure 2(b, c) have allowed us to make an assumption that the nanopit formation has occurred on (001) Si substrates without regard to doping type.
However, in the case of p-type substrates the nanopits have formed inside spherical protrusions of 3 nm heights in contrast to the n-type substrates on which such a process have happened right on the surface. The nanopit depth has also differed for n- and p-type doping. The higher values of this parameter have been obtained for samples with n-type substrates (25 nm depth for n-type substrates and 14 nm for p-type). The density of the nanopits has been about $10^8$ for all the samples grown on n-type substrates.

![AFM pictures](image)

**Figure 2.** 10×10 nm AFM pictures of the samples grown on different Si substrates. (a) n-type (111), (b) p-type (001), (c) n-type (001).

According to the paper [11], the formation of the studied nanopits may be caused by the defects of crystal lattice that occur during the chemical substrate treatment. Under certain conditions of liquid chemical treatment of a doped Si substrate, dopant atoms, which are defects of the crystal lattice, turn into places where selective etching predominantly occurs. Any inhomogeneities, such as the presence of oxide or active sites (dopant atoms) on the surface, may lead to the enhancement of the selective (or anisotropic) etching. The hypothesis of the anisotropic nature of the etching is evidenced by the formation of nanopyramids instead of nanopits when changing substrate orientation from (001) to (111), as well as the changes in the nanopit formation when using (001) substrates with different types of doping.

### 3. Conclusions

The new method of chemical preparation of the Si substrate and certain conditions for the growth of the buffer layer by MBE to create an array of nanopits with 25 nm depth and $6 \cdot 10^8$ cm$^{-2}$ density has been developed. The nanopit depth and size have been shown to increase with the growth of the buffer layer thickness. The nanopits of the best shape and maximum depth have been obtained on n-type (001) Si substrate.

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