GaAs epitaxial growth on modified on-axis Si(001) substrates

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Abstract. In this work, the effect of the dose of implantation of Ga atoms into the silicon surface on the epitaxial growth of GaAs was investigated. We demonstrate that the deposition of GaAs occurs mainly on modified areas. Separate crystallites of GaAs with an irregular shape are formed on modified areas at the lowest dose of Ga implantation equal to 1 pC/μm², whereas an increase in the dose of Ga implantation leads to the coalescence of GaAs areas. At a maximum dose of 21 pC/μm², degradation of the morphology and a decrease in the degree of filling of the area are observed, which is also confirmed by an increase in the roughness of the structure.

1. Introduction
The vast majority of modern semiconductor devices are based on silicon. At the same time, the creation of effective light-emitting devices on silicon is difficult due to the fact that silicon is an indirect band gap semiconductor. Therefore, III/V material, in particular GaAs, are used to create photonic devices because of their excellent optical characteristics. Although the integration of highly efficient light emitting sources based on III/V structures with silicon technology remains a difficult task today [1-3], it could allow the creation of photonic integrated circuits compatible with well-established silicon complementary metal oxide semiconductor (CMOS) technology [4-8]. This is expected to combine the advantages of GaAs technology (high-performance laser sources) and Si technology (high-speed information processing).

The preparation of GaAs on silicon devices is complicated due to the presence of a large number of threading dislocations, antiphase domains, and thermal cracks formed during the growth of a polar semiconductor on a non-polar substrate with different lattice constants and thermal expansion coefficients [9-14]. To avoid the formation of dislocations and to provide their self-annihilation, misoriented silicon substrates are used at a tilt angle of 4-7°[9, 12, 15-17], thermal annealing of the substrates over 1000 °C [18-23] and/or the growth of a several microns thick GaAs buffer layer [24-27]. However, these techniques cannot be used because the traditional CMOS technological process is based on the use of misoriented substrates, it is limited in permissible growth temperature, and the high thickness of the buffer layers leads to the formation of thermal cracks. On the other hand, the use of various surface patterning methods allows not only to localize the structure on a certain area of the substrate, but also to reduce the density of dislocations in the growing layers by orders of magnitude while reducing the thickness of the grown nanostructures [28-34]. In this article, the focused ion beam (FIB) method was used to localize and improve the nucleation of the grown structures.
2. Experimental procedure

For growth processes, on-axis Si (001) substrates with preliminary FIB processing were used. Surface modification was carried out by implanting Ga atoms in predetermined areas of the Si substrate. To identify optimal regimes of the FIB procedure, the dose and current of implantation were varied. The epitaxial materials were fabricated using a SemiTEq STE 35 molecular beam epitaxy system with solid-state sources. The removal of native oxide was carried out by annealing the samples in a chamber at 900°C [24]. After removing the oxide, the substrate was cooled to 600 °C and 200 nm of GaAs buffer was deposited at a rate of 0.1 ML/s. The V/III flux ratio was set to 40. To determine the characteristics of the obtained structures, atomic force microscopy (AFM) was used.

3. Results and discussion

Figure 1 shows scanning electron microscopy images of the morphology of GaAs deposited on modified Si areas with implantation current equal to 1 pA and various doses of Ga. At the lowest dose of Ga implantation equal to 1 pC/μm² (Figure 1a), the deposition of GaAs on modified areas occurs as separate crystallites with an irregular shape. An increase in the implantation dose leads to GaAs coalescence and further filling of the areas (Figure 1b, c, d). However, it is worth noting that at the highest dose of implantation, the morphology of the grown nanostructures is deteriorated (Figure 1d). We suggest that this is due to significant damage to the crystal structure of the modified regions during FIB processing.

![Figure 1](image-url)

**Figure 1.** SEM images of the amorphous areas of Si after deposition of 200 nm GaAs with different dose of Ga implanted: (a) 1 pC/μm², (b) 3 pC/μm², (c) 7 pC/μm², (d) 21 pC/μm². The implantation current was 1 pA.
This trend is also observed with an increase in the implantation current and a constant dose of implantation (Figure 2). An increase in the implantation current led not only to a clear deterioration in the morphology of the surface of nanostructures, but also to the formation of whisker nanocrystals (Figure 2(b, d)), which indicates a deterioration in the quality of the epitaxial material and increased defective structure compared to that grown with a lower implantation current.

Figure 2. SEM images of the amorphous areas of Si after deposition of 200 nm GaAs with different dose of Ga implanted: (a) 1 pC/μm², (b) 3 pC/μm², (c) 7 pC/μm², (d) 21 pC/μm². The implantation current was 10 pA.

To find the optimal FIB regime, surface treatment of the nanostructures was investigated by atomic force microscopy, which allowed us to determine the degree of filling of the nanostructures, their roughness and height. Figure 3a shows the dependences of the degree of filling of nanostructures on the implantation dose at two different currents. With a change in the implantation dose from 1 to 3 pC/μm², a sharp increase in the graph is observed, which is explained by the coalescence of initially individual crystallites. Nanostructures obtained in areas treated with a dose and implantation current of 7 pC/μm² and 1 pA, respectively, show the best degree of filling among all other samples. However, a further increase in the implantation dose leads to a decrease in the degree of filling, which, as mentioned above, is associated with a deterioration in the structural quality of nanostructures.

An analysis of the surface roughness showed that with an increase in the dose of implanted Ga from 1 to 7 pC/μm², the roughness of the grown nanostructure decreases (Figure 3b). For
nanostructures grown in areas with an implantation current of 1 pA, a lower surface roughness is observed compared to 10 pA. However, in both cases, with an increase in the implantation dose from 7 to 21 pC/μm², the roughness increases, which confirms the processes of surface and quality deterioration of the grown nanostructures. Of course, the roughness of 23 nm is excessively high, however, growth processes using the nucleation layer and multi-stage buffers will reduce not only the roughness, but also the defectiveness of the structures.

![Figure 3](image)

**Figure 3.** Dependences of the (a) degree of filling, (b) roughness, and (c) height on the dose of implanted Ga at various implantation currents.

As the current and dose of implantation change, the height of the nanostructures also changes (Figure 3c). An increase in the dose and/or current of implantation leads to a decrease in the height of the resulting nanostructure. This is due to the fact that during FIB processing at low doses and implantation currents surface swelling is observed. A further increase in the parameters of the FIB processing modes leads to the volatilization of the substrate material and an increase in the depth of the resulting holes. The study of this effect is important from the point of view of knowing the total height of nanostructures measured not only from the surface of the substrate, but also from the surface of the hole.

4. **Conclusions**

Therefore, we can conclude that there is an optimal dose and current of Ga implantation into the silicon surface at which the best parameters of the grown structures are observed. Despite the fact that
the GaAs buffer is defective, the use of nucleation layers and the technique of multi-stage growth of buffer layers will provide a smooth two-dimensional interface.

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**References**

[1] Tang M, Park J-S, Wang Z, Chen S, Jurczak P, Seeds A, Liu H 2019 *Prog. Quant. Electron* 66 1-18

[2] Ageev O A, Solodovnik M S, Balakirev S V, Eremenko M M 2016 *Phys. Solid State* 58 1045–52

[3] Il'Ina M V, Blinov Y F., Il'In O I, Klimin V S, Ageev O A 2016 Proc. of SPIE 10224 102240U-1–4

[4] Soref R A 1993 *Proc. IEEE* 81 1687–1706

[5] Shiferen L, Aitken R, Brown A R, Chandra V, Cheng B, Riddet C, Alexander C L, Cline B, Millar C, Sinha S, Yeric G and Asenov A 2014 *IEEE Trans. Electron Devices* 61 2271–7

[6] Vahala K J 2003 *Nature* 424 839

[7] Klimin V S, Rezvan A A, Kots I N, Naidenko N A 2018 J. Phys.: Conf. Ser. 1124 071019

[8] Klimin V S, Rezvan A A, Ageev O A 2018 J. Phys.: Conf. Ser. 1124 071020

[9] Grundmann M, Krost A and Bimberg D 1998 *J Vac Sci Technol B Microelectron Nanometer Struct* 9 2158–66

[10] Chen S, Li W, Wu J, Jiang Q, Tang M, Shutts S, Elliott S N, Sobiesierski A, Seeds A J, Ross I, Smowton P M, Liu H 2016 *Nat. Photonics* 10 307–11

[11] Klimin V S, Rezvan A A, Ageev O A 2018 J. Phys.: Conf. Ser. 1124 022035

[12] Mitsuo K and Toshio U 1987 *Jpn. J. Appl. Phys.* 26 L944

[13] Chernenko N E, Balakirev S V, Eremenko M M, Solodovnik M S 2019 *J. Phys.: Conf. Ser.* 1410 012007

[14] Barrett C S C, Atassi A, Kennon E L, Weinrich Z, Haynes K, Bao X-Y, Martin P, Jones K S 2019 J. Mater. Sci. 54 7028–34

[15] Morii H, Tachikawa M, Sugo M and Toth Y 1993 *Appl Phys Lett* 63 1963–65

[16] Bogumilowicz Y, Hartmann J M, Cipro R, Alcotte R, Martin M, Bassani F, Moeyaert J, Baron T, Pin J B, Bao X, Ye Z and Sanchez E 2015 *Appl Phys Lett* 107 212105-1

[17] Mitsuo K and Toshio U 1987 *Jpn. J. Appl. Phys.* 25 L285

[18] Aspnes D E and Ihm J 1986 *Phys Rev Lett* 57 3054–7

[19] Ageev O A, Solodovnik M S, Balakirev S V, Eremenko M M, Mikhailin I A 2016 *J. Phys.: Conf. Ser.* 741 012012

[20] Balakirev S V, Solodovnik M S and Ageev O A 2018 *Phys. Status Solidi B* 255 1700360

[21] Sakamoto T and Hashiguchi G 1986 *Jpn J Appl Phys* 25 L78–80

[22] Eremenko M M, Balakirev S V, Chernenko N E, Ageev O A, Solodovnik M S 2019 *J. Phys.: Conf. Ser.* 1410 012045

[23] Kots I N, Kolomietsev A S, Lisitsyn S G, Polyakova V V, Klimin V S, Ageev O A 2019 *Russian Microelectronics* 48(2) p 72-79

[24] Chen S, Li W, Wu J, Jiang Q, Tang M, Shutts S, Elliott S N, Sobiesierski A, Seeds A J, Ross I, Smowton P M, Liu H 2016 *Nat. Photonics* 10 307–11

[25] Mikhailin I A, Balakirev S V, Eremenko M M, Chernenko N E, Solodovnik M S 2019 *J. Phys.: Conf. Ser.* 1410 012051

[26] Bolkhovityanov Yu B and Pchelyakov O P 2008 *Physics Uspekhi* 51 (5) 437–56

[27] Balakirev S V, Solodovnik M S, Eremenko M M, Konoplev B G, Ageev O A 2019 *Nanotechnology* 30 505601
[28] Wan Y, Li Q, Geng Y, Shi B, Lau K M 2015 *Appl. Phys. Lett.* B **107** 081106
[29] Balakirev S V, Eremenko M M, Mikhaylin I A, Klimin V S, Solodovnik M S 2018 *J. Phys.: Conf. Ser.* **1124** 022018
[30] Wang Z, Tian B, Pantouvaki M, Guo W, Absil P, Van Campenhout J, Merckling C and Van Thourhout D 2015 *Nat. Photon.* **9** 837–842
[31] Ageev O.A., Solodovnik M.S., Balakirev S.V., Eremenko M.M 2016 *J. Vac. Sci. Technol. B* **34** 041804
[32] Wang Z, Tian B, Paladugu M, Pantouvaki M, Le Thomas N, Merckling C, Guo W, Dekoster J, Van Campenhout J, Absil P and Van Thourhout D 2013 *Nano Lett.* **13** 5063–9
[33] Solodovnik M S, Balakirev S V, Eremenko M M, Mikhaylin I A, Avilov V I, Lisitsyn S A, Ageev O A 2017 *J. Phys.: Conf. Ser.* **917** 032037
[34] Balakirev S V, Eremenko M M, Chernenko N E, Ageev O A, Solodovnik M S 2019 *J. Phys.: Conf. Ser.* **1410** 012059