Conference materials UDC 538.9 DOI: https://doi.org/10.18721/JPM.163.122

Effect of plasma-chemical treatment of Si(001) substrates on the subsequent epitaxial growth of GaAs

M.M. Eremenko[™], L.S. Nikitina, J.Yu. Jityaeva

E.A. Lakhina, V.S. Klimin, O.A. Ageev

Southern Federal University, Taganrog, Russia ☐ eryomenko@sfedu.ru

Abstract. In this work, we investigated the effect of plasma-chemical treatment of silicon substrates on the subsequent epitaxial growth of GaAs. It is shown that a change in processing modes did not lead to a strong change in the root-mean-square roughness of the initial silicon surface. It was found that under the same growth conditions GaAs is formed on substrates differently depending on the silicon treatment mode: from individual crystallites with nanowires to a structure intergrown from individual crystallites. It is shown that a change in the annealing temperature significantly affects the resulting surface morphology.

Keywords: molecular beam epitaxy, silicon, GaAs, monolithic integration, plasma-chemical treatment, scanning electron microscopy

Funding: Работа выполнена при финансовой поддержке Министерства науки и высшего образования Российской Федерации; государственное задание в области научной деятельности No. FENW-2022-0001.

Citation: Eremenko M.M., Nikitina L.S., Jityaeva J.Yu., Lakhina E.A., Klimin V.S., Ageev O.A., Effect of plasma-chemical treatment of Si(001) substrates on the subsequent epitaxial growth of GaAs, St. Petersburg State Polytechnical University Journal. Physics and Mathematics. 16 (3.1) (2023) 122–127. DOI: https://doi.org/10.18721/JPM.163.122

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Материалы конференции УДК 538.9 DOI: https://doi.org/10.18721/JPM.163.122

Влияние плазмохимической обработки подложек Si(001) на последующий эпитаксиальный рост GaAs

М.М. Ерёменко ⊠, Л.С. Никитина, Ю.Ю. Житяева,

Е.А. Лахина, В.С. Климин, О.А. Агеев

Южный федеральный университет, г. Таганрог, Россия □ eryomenko@sfedu.ru

Аннотация. В настоящей работе исследовано влияние плазмохимической обработки кремниевых подложек на последующий эпитаксиальный рост GaAs. Показано, что смена режимов обработки не приводила к сильному изменению среднеквадратичной шероховатости исходной поверхности кремния. Установлено, что при одних и тех же условиях роста наноструктуры GaAs формируются на кремниевых подложках поразному в зависимости от режима обработки кремния: от отдельных кристаллитов с нанопроволоками до структуры, сросшейся из отдельных кристаллитов.

Ключевые слова: молекулярно-лучевая эпитаксия, кремний, GaAs, монолитная интеграция, плазмохимическая обработка, сканирующая электронная микроскопия

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Финансирование: Работа выполнена при финансовой поддержке Министерства науки и высшего образования Российской Федерации; государственное задание в области научной деятельности № FENW-2022-0001.

Ссылка при цитировании: Ерёменко М.М., Никитина Л.С., Житяева Ю.Ю., Лахина Е.А., Климин В.С., Агеев О.А. Влияние плазмохимической обработки подложек Si(001) на последующий эпитаксиальный рост GaAs // Научно-технические ведомости СПбГПУ. Физико-математические науки. 2023. Т. 16. № 3.1. С. 122–127. DOI: https:// doi.org/10.18721/JPM.163.122

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Introduction

Improving the technology of data processing and transmission today is one of the key tasks in modern micro and nanoelectronics. Modern silicon processors and metal-oxide-semiconductor technology easily cope with data processing [1]. However, silicon is an indirect-gap semiconductor, and this greatly complicates the creation of effective light emitting devices on its basis necessary for information transmission. Therefore, devices based on A3B5 materials are responsible for transmitting information due to their outstanding optical properties. Integration of a light emitting source directly on a silicon substrate will not only reduce the final cost of such devices, but also reduce power consumption while increasing bandwidth throughput [2]. However, the growth of a polar semiconductor on a nonpolar substrate leads to the formation of antiphase domains [3-5]. Also, the growth of GaAs on Si(001) leads to a large number of threading dislocations, which are obtained due to the difference in the lattice constants of both materials [4, 6, 7]. Therefore, to date, many methods have been explored for the formation of III-V semiconductors on silicon in order to reduce the resulting dislocation density and eliminate antiphase domains in the final structures [3-11]. One of such methods is the creation of a "soft substrate" for subsequent epitaxial growth [11]. As an alternative to this method, we propose the creation of a developed surface morphology by plasma-chemical processing which, as expected, will allow the subsequent nucleation of monolithically integrated GaAs nanostructures on Si(001).

Materials and Methods

The epitaxial growth of GaAs on Si(001) substrates with plasma-chemical treatment was studied using a SemiTEq STE35 MBE setup with solid-state sources. Plasma-chemical processing was carried out in combined fluoride plasma in the modes of chemical polishing (CP) and reactive ion etching (RIE). The constant parameters during plasma-chemical treatment were: pressure in the reactor (10 Pa), temperature of the process (25 °C), treatment time (30 s), fluorine-containing gas flow (10 cm³/min), argon flow (60 cm³/min). The capacitively coupled plasma source power was 15 and 95 W, inductively coupled plasma source power was 500 and 400 W, and the voltage was 5 and 38 V for processing in the CP and RIE modes, respectively. After processing, the silicon samples were scanned by atomic force microscopy (AFM) to determine the root-mean-square (RMS) surface roughness. According to the scan results, it was revealed that the RMS roughness of the untreated original surface was 0.171 nm, while after processing in fluoride plasma in CP and RIE modes, the RMS roughness was 0.295 and 0.312 nm, respectively. After treatment, the samples were placed in a growth chamber, where they were preliminarily annealed at 600 and 800 °C for 60 minutes. After annealing GaAs was deposited with a thickness of 200 nm and with a growth rate of 0.25 ML/s at a temperature of 600 °C.

Results and Discussion

The results of experimental studies (Fig. 1) demonstrate differences in the final morphology of the grown nanostructures pre-annealed at 600 °C. It is shown that GaAs nanocrystallites with periodically occurring GaAs nanowires grow on a sample with RIE treatment (Fig. 1, *a*). It should be noted that the nanowires grow in the <111> direction at an angle of 54.7° to the substrate surface. These results allow us to state that the nanowires obtained during the growth process inherit the structure of the silicon substrate.

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Fig. 1. SEM images of GaAs structures grown at T = 600 °C, H = 200 nm, V = 0.25 ML/s on silicon substrates with different processing modes and their AFM profilograms: (a, c) RIE, (b, d) CP. The pre-annealing temperature was T = 600 °C

Studies of epitaxial growth on samples treated in fluoride plasma in the CP mode and annealed at 600 °C showed that a change in the processing mode led to an increase in density and the formation of a GaAs structure intergrown from individual crystallites (Fig. 1, b). It is important to note that there is no growth of GaAs nanowires on the surface. It is likely that such a change in the morphology and mode of epitaxial growth is associated with an increase in the intensity of GaAs nucleation processes on the Si surface with a shift towards two-dimensional growth, which leads to suppression of the growth of GaAs nanowires. We assume that such a change in the growth process is associated with the influence of the geometric parameters of the relief that forms on the surface of the silicon substrate after RIE and CP plasma-chemical processing. According to the AFM profiles of the silicon surface obtained after plasma-chemical treatment (Fig. 2), it is clearly seen that their shape is noticeably different in the cases of RIE and CP modes.



Fig. 2. AFM profilograms of the silicon substrate: after processing in the RIE mode (*a*), after processing in the CP mode (*b*)

On the silicon surface after plasma-chemical treatment in the CP mode, more pronounced peaks of the silicon substrate material are observed than in the RIE mode, the geometric parameters of which contribute to more intense nucleation and coalescence of GaAs nanocrystallites.

Next, samples with GaAs structures were examined by AFM (Fig. 1, c, d). Based on the obtained results, the degree of filling of the Si surface with the GaAs epitaxial material was estimated, which was 67% for samples obtained during growth on substrates treated in the RIE mode and 94.8% when treated in the CP mode. From a quantitative point of view, it is inadequate to judge the roughness of the structures grown on samples processed in the RIE mode, in view of the presence of a large number of individual crystallites. However, the values of RMS roughness (55.5 nm for RIE vs. 37.6 nm CP) make it possible to indirectly judge that when the regime of plasma-chemical processing was changed, the average difference in height of the grown GaAs decreased.

Fig. 3, *a*, *b* shows the SEM images of the GaAs structures grown on the Si(001) substrate preliminarily annealed at 800 °C. It is shown that there was a significant change in the surface morphology compared to the samples obtained by annealing at a temperature of 600 °C (Fig. 1). When processing samples in the RIE mode, no growth of individual GaAs crystallites is observed, as in the case of growth with annealing at 600 °C. Also, the resulting structure is similar to the



Fig. 3. SEM and AFM images of GaAs structures grown at T = 600 °C, H = 200 nm, V = 0.25 ML/s on silicon substrates with different processing modes: (a, c, d) RIE, (b) CP. The pre-annealing temperature was T = 800 °C

structure grown by annealing at 600 °C with CP treatment, except that the intergrown crystallites are more elongated in length. An increase in the length of nanocrystals can indirectly indicate the inheritance of the substrate structure by the grown GaAs nanostructures. When samples are treated in the CP mode, after growth, the presence of nanowires of small size (about 140 nm on average) is observed on the surface. The reason for the parasitic growth of GaAs nanowires remains unclear. It should be noted that nanowires are oriented in accordance with the structure of the substrate and grow in the direction in four directions [-111], [111], [-1-11] and [1-11].

As in the previous case, the samples at the next stage were scanned by the AFM method (Fig. 3, c, d). From the results obtained, it was found that the degree of surface filling with the

material was 95% for the RIE mode of plasma-chemical processing. The RMS surface roughness was 34.87 nm, which is even less than the value obtained after scanning the surface of the sample annealed at 600 °C and processed in the CP mode. Comparative analysis of the AFM profiles (Fig. 1, c and Fig. 3, d) also confirms that the crystallite size increased on the sample with RIE treatment and annealing at 800 °C (larger peak size and lower peak frequency). We attribute this behavior, as mentioned earlier, to the influence of the substrate structure on the grown GaAs structures. In view of the presence of arrays of nanowires on the surface of the structure grown on samples treated in the CP mode, AFM studies were not carried out.

Conclusion

In conclusion, it can be said that a change in the regime of plasma-chemical treatment of Si and/or the temperature of preliminary annealing significantly affects the subsequent epitaxial growth of GaAs, despite the fact that the RMS surface roughness of the samples after treatment differ little from each other. A change in the processing modes from RIE to CP on samples annealed at a temperature of 600 °C led to a change in the growth mode (from growth with nanowires to two-dimensional growth), while, as with growth on samples annealed at 800 °C, an opposite trend was observed. An increase in the pre-annealing temperature also led to a decrease in the roughness of the resulting structure.

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THE AUTHORS

EREMENKO Mikhail M. eryomenko@sfedu.ru ORCID: 0000-0002-7987-0695

NIKITINA Larisa S. larnikitina@sfedu.ru ORCID: 0000-0001-7397-8630

JITYAEVA Julia Yu. zhityaeva@sfedu.ru ORCID: 0000-0002-5961-407X LAKHINA Ekaterina A. lakhina@sfedu.ru ORCID: 0000-0002-9326-2418

KLIMIN Viktor S. kliminvs@sfedu.ru ORCID: 0000-0002-9794-4459

AGEEV Oleg A. ageev@sfedu.ru ORCID: 0000-0003-1755-5371

Received 13.07.2023. Approved after reviewing 25.07.2023. Accepted 26.07.2023.