Conference materials UDC 539.27 DOI: https://doi.org/10.18721/JPM.163.120

Effect of temperature during homoepitaxial growth of Si on Si(100) on the character of reflection high-energy electron diffraction patterns

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Abstract. To create high-quality nanostructures, it is important to understand the surface morphology for given growth parameters. The paper shows the effect of temperature on the ratio of intensities and periods corresponding to the growth of Si steps with different types of superstructure. The analysis was carried out in directions [100] and [110].

Keywords: molecular beam epitaxy, reflection high-energy electron diffraction, step-flow growth of silicon, homoepitaxy

Funding: The reported study was supported by grant from the Russian Science Foundation No. 21-72-10031, https://rscf.ru/project/21-72-10031/.

Citation: Kukenov O.I., Sokolov A.S., Dirko V.V., Lozovoy K.A., Kokhanenko A.P., Analysis of the temperature dependence of homoepitaxial growth of Si on Si by reflection high-energy electron diffraction, St. Petersburg State Polytechnical University Journal. Physics and Mathematics. 16 (3.1) (2023) 112–116. DOI: https://doi.org/10.18721/JPM.163.120

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Материалы конференции УДК 539.27 DOI: https://doi.org/10.18721/JPM.163.120

Влияние температуры при гомоэпитаксиальном росте Si на Si(100) на характер картин дифракции быстрых отражённых электронов

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Аннотация. Для создания качественных наноструктур важно понимать морфологию поверхности при заданных параметрах роста. В работе показано влияние температуры на соотношение интенсивностей и периодов, соответствующих росту ступеней Si с разным типом сверхструктуры. Анализ проводился в направлениях [100] и [110].

Ключевые слова: молекулярно-лучевая эпитаксия, дифракция быстрых отраженных электронов, ступенчатый рост кремния, гомоэпитаксия

Финансирование: Работа выполнена при поддержке гранта РНФ № 11. 21-72-10031, https://rscf.ru/project/21-72-10031/.

Ссылка при цитировании: Кукенов О.И., Соколов А.С., Дирко В.В., Лозовой К.А., Коханенко А.П. Анализ температурной зависимости гомоэпитаксиального роста Si на Si(100) методом дифракции быстрых отраженных электронов // Научно-технические ведомости СПбГПУ. Физико-математические науки. 2023. Т. 16. № 3.1. С. 112–116. DOI: https://doi.org/10.18721/JPM.163.120

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Introduction

The trend towards miniaturization of electronic components was observed in the last century [1]. With a decrease in the size of semiconductors to the order of nanometers, quantum properties begin to actively manifest themselves. By limiting one, two or three directions, quantum wells, filaments or dots, respectively, are obtained, the spectrum of the density of energy states of which differs from that of a bulk semiconductor [2]. It is difficult to imagine the modern world without high-frequency transistors, photoelectronic objects, processors and other devices based on semiconductor nanostructures.

Progress in the field of semiconductor nanoelectronics is inevitably accompanied by stricter requirements for the quality and accuracy of grown nanostructures. The purest epitaxial structures with a minimum number of defects are obtained by molecular beam epitaxy (MBE). The creation of high quality nanostructures is impossible without a precise surface control method. The method of reflection high-energy electron diffraction (RHEED), implemented in the MBE method, has proven to be a universal tool for controlling the surface morphology in the in situ growth of semiconductor nanostructures [3–4].

Obtaining information about the surface during epitaxy is an important task for understanding the processes that occur during growth. Since silicon is the most common material in the semiconductor electronics market, it is receiving special attention. Homoepitaxial growth of Si on Si(100) has been studied for a long time; however, due to the existence of gaps in the understanding of surface processes, they still remain topical [5–6].

Materials and Methods

After chemical cleaning, the Si substrates are placed in an epitaxy chamber, where the pure oxide deposited in the laboratory is thermally cleaned. Silicon substrates inevitably have defects; therefore, it is important to overgrow them with a buffer layer more than 50 nm thick. As a result of pre-epitaxial preparation, a smooth, defect-free surface is obtained.

Homoepitaxial growth of Si on Si(100) occurs with the formation of alternating terraces of two types [6]: T_A and T_B terraces with 1×2 and 2×1 superstructures with parallel and orthogonal orientation of the dimer rows relative to the edge of the terrace (step). After high-vacuum annealing of the Si(100) substrate, Si was synthesized on Si(100) at a growth rate of 0.09 ML/s at various temperatures.

In the course of studying the homoepitaxial growth of Si on Si(100) in the [110] direction, the dependences of the ratio of intensities and the ratio of oscillation periods at low and medium growth temperatures were constructed using the RHEED method. Also, the dependence of the ratio of the intensities of the 2×1 and 1×2 reflections during Si epitaxy on Si(100) in the [100] direction on temperature in its wide range (Fig. 1) was obtained, which is consistent with the data of other authors [7].



Fig. 1. Dependences of the intensity of reflections 1×2 and 2×1 (*a*) on time, and (*b*) on the coordinate at a growth temperature of 600 °C

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In the analysis of the surface during growth by the RHEED method in the [110] direction, a bimodal nature of intensity oscillations was observed (Fig. 2). It lies in the fact that there are two alternating maxima of different intensity, each of which corresponds to its own period of oscillations.



Fig. 2. Change in the intensity of diffraction patterns over time near the central reflex "00" during the synthesis of Si on Si(100) in the direction of the electron beam [110] at a growth temperature of 450 $^{\circ}$ C

A larger intensity maximum corresponds to the growth of the T_B terrace with a 2×1 superstructure orientation, which corresponds to the arrangement of dimer rows perpendicular to the step edge. A smaller intensity maximum corresponds to the growth of the T_A terrace with the 1×2 superstructure orientation, which corresponds to the arrangement of dimer rows parallel to the step edge [6, 8, 9, 10].

Results and Discussion

In the course of studying the homoepitaxial growth of Si on Si(100) in the [110] direction, using the RHEED method, the dependences of the ratio of intensities and the ratio of oscillation periods at low and medium growth temperatures were plotted, and the temperature dependence of the ratio of the intensities of the 2×1 and 1×2 reflections in the [100] direction upon epitaxy of Si on Si(100) was obtained in wide range of temperatures (Fig. 3).



Fig. 3. Temperature dependence of the ratios of periods and intensities of oscillations in the direction [110], corresponding to the formation of different types of steps and ratios of the intensities of reflections 2×1 to 1×2 in the direction [100]

At low temperatures (200-500 °C) in the [110] direction intensity oscillations with time were studied. The ratio of the oscillation periods corresponding to the 2×1 and 1×2 superstructures slightly differs from 1 and averages 1.05. This means that the formation of one steps takes 5% more time than the formation of another. Therefore, at a constant growth rate (0.09 ML/s), the ratio of the time of formation of the steps will be equal to the ratio of the areas of the steps. Since the ratio of the areas of the steps is close to 1, the rate of convergence of the steps in

this temperature range is minimal. Consequently, the mechanism of growth due to the shift of steps is practically not manifested, and the terraces are overgrown due to the formation of twodimensional islands, and consequently the roughness changes. When an atom hits the surface, its path length is not always enough to reach the edge of the terrace, and most often adatoms meet each other and form two-dimensional islands [6]. The intensity of oscillations corresponding to the formation of different types of terraces in this temperature range differs by 1.22 times. In addition to the width of the steps, the intensity depends on the reflection coefficient, which shows the efficiency with which electrons are reflected from the surface of terraces of different types. In the [100] direction, the intensities of the 2×1 and 1×2 reflections differ by a factor of 1.21 and do not depend on the reflection coefficients of the terraces, since all dimers are located at an angle of 45° to the direction of the electron beam.

At the temperatures of 500-560 °C, the ratio of the periods increases with increasing temperature, which indicates the convergence of steps. The mechanism of growth of layers becomes not only due to formation of islands, but also due to a shift of steps. Some of the adatoms reach the edge of the terrace and are built into the step, while the other part of the adatoms collide with each other, forming two-dimensional islands. Judging by the magnitude of oscillations in the analysis of RHEED in the [110] direction, roughness is present, but it is not as pronounced as at low temperatures.

At the temperatures of 560-600 °C, bimodal oscillations obtained by the RHEED method in the [110] direction are not observed, but transform into oscillations with a doubled period. The intensity ratio of the 2×1 to 1×2 reflections in the [100] direction decreases with increasing temperature. We assume that this is due to the fact that the energy of adatoms becomes sufficient not only to overcome the A-type step, but also to overcome the B-type step. Thus, the converged steps begin to move apart as the temperature rises.

At the temperatures of 600–850 °C, oscillations are not observed, since all adatoms reach the edge of the terraces and the roughness is minimal. The intensity of the 1×2 and 2×1 reflections in the [100] direction is practically the same.

Conclusion

An analysis of the data obtained by the RHEED method in the [110] direction from experiments on the homoepitaxial synthesis of Si on Si(100) by the MBE method have shown that the ratio of the oscillation intensities corresponding to the formation of different types of terraces depends not only on their width, but also on different reflection coefficients.

When analyzing the synthesis of Si on Si(100) in the [100] direction, the ratio of the intensities of the 2×1 and 1×2 reflections is not affected by the reflection coefficients, since all dimers are located at an equal angle relative to the electron beam. However, the intensity can be affected by various features of diffraction patterns (for example, background illumination, diffraction lines from the volume of a substance, etc.), which complicates the analysis of growth processes.

When synthesizing Si on Si(100) and analyzing it by the RHEED method in the [110] direction, the ratio of the oscillation periods is determined by the time of complete filling of the atomic layers, which is not affected by the features of the diffraction patterns and the difference in reflection coefficients.

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Received 13.07.2023. Approved after reviewing 31.08.2023. Accepted 01.09.2023.