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Study of the formation mechanisms of Ge terraces on Si(100) during MBE using the RHEED method

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Abstract. In the work, a comparison of the widths of Ge and Si terraces on Si(100) at temperatures in the range from 200 °C to 800 °C was made using diffraction patterns in the [100] direction. The temperatures at which the growth mechanisms for the formation of monoatomic steps of Ge on Si(100) change have been established.

Keywords: molecular beam epitaxy, reflection high-energy electron diffraction, step-flow growth, heteroepitaxy

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Изучение механизмов формирования террас германия на кремнии (100) при МПЭ методом ДБОЭ

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Аннотация. В работе по картинам дифракции в направлении [100] проведено сравнение ширины террас Ge и Si на Si(100) при температурах в диапазоне от 200 °C до 800 °C. Установлены температуры, при которых происходит смена механизмов роста формирования моноатомных ступеней Ge на Si(100).

Ключевые слова: молекулярно-пучковая эпитаксия, дифракция быстрых отраженных электронов, рост по механизму сдвига ступеней, гетероэпитаксия

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Introduction

Modern electronics require increasingly higher performance from components. Nanostructures, due to quantum effects, exhibit unique properties that enhance the capabilities of devices. Silicon, as an affordable semiconductor, is attracting attention in electronics, optoelectronics and solar energy. Germanium with a lattice that differs from silicon by 4.2% makes it possible to create Ge-Si nanostructures, such as quantum wells, wires and dots [1]. The parameters of these nanostructures depend on the synthesis conditions, including temperature, deposition rate, vacuum, and surface angle relative to the crystalline plane of the substrate. The growth of Ge on Si(100) obeys the Stranski–Krastanov mechanism, where the formation of nanoislands begins after the formation of a wetting layer [2]. This process is accompanied by surface changes associated with the movement of steps and the formation of $2\times N$ and $M\times N$ superstructures.

The mechanism of movement of steps during the deposition of Si on Si(100) has not been fully studied, but has theoretical and experimental foundations [3]. The article is devoted to the growth of germanium and silicon on a silicon substrate by the MBE method, specifically to the study of terrace formation at different growth temperatures by the RHEED method.

Materials and Methods

The experiments were carried out on a “Katun-100” molecular beam epitaxy (MBE) installation. The MBE method makes it possible to create pure nanostructures with a minimum number of defects, a sharp heterointerface and specified parameters [4]. After standard pre-epitaxial cleaning of the substrate and application of a 50 nm buffer layer, Ge was deposited on Si(100) at a rate of 0.02 ML/s. The surface morphology was studied by reflection high-energy electron diffraction (RHEED). RHEED is a universal method for obtaining in situ information about a surface and is used by scientists around the world [5]. The substrate was positioned so that the electron beam passed in the [100] direction to the Si(100) surface. Diffraction patterns on a luminescent screen were recorded with a video camera and analyzed using computer programs.

Pre-epitaxial cleaning of the substrate and application of a buffer layer make it possible to eliminate various defects associated with dislocations and impurities; however, atomic steps [6] associated with misorientation will inevitably be present on the surface. As is known, the homoepitaxial growth of Si on Si(100) occurs with the formation of alternating terraces of two types: T_A and T_B terraces with 1×2 and 2×1 superstructures with parallel and orthogonal orientation of dimer rows relative to the edge of the terrace [7]. The growth of Si on Si(100) leads to the fact that each subsequent layer on the terrace turns it into a terrace of the opposite type. At certain temperatures and growth rates, steps can double, and the width of terraces of one type significantly exceeds the width of terraces of another type [8].

When synthesizing Ge on Si(100), the width of the terraces has a great influence on the nucleation of quantum dots on them. Heteroepitaxial synthesis of Ge on Si(100) involves the formation of a wetting layer followed by a transition to 3D growth. In our study, we focused on the mechanisms of wetting layer formation taking into account the presence of monatomic steps on the Si(100) substrate. To do this, after the standard preparation of the plate described above, germanium was deposited onto the Si(100) surface with a misorientation angle of 0.1° at a rate of 0.02 ML/s at different temperatures.

Results and Discussion

In the course of studying the heteroepitaxial growth of Ge on Si(100) using the RHEED method in the [100] direction, the dependences of the ratio of the intensities of the 2×1 and 1×2 reflections ($I_{2\times1}$ and $I_{1\times2}$) on temperature were plotted (Fig. 1). These reflections were located in 1/2 of the

Laue zone. Each point in Fig. 1 corresponds to the maximum ratio of $I_{2\times1}$ to $I_{1\times2}$ during the growth process. The intensity ratio $I_{2\times1}/I_{1\times2}$ corresponds to the area ratio T_B/T_A [3, 9]. For ease of data perception, the "Gauss Fit" approximation method built into the Origin software package was used.

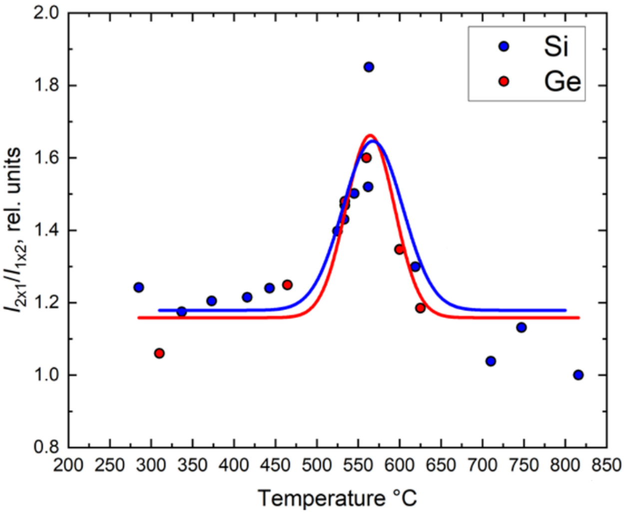

Fig. 1. Temperature dependences of the ratio of $I_{2\times1}$ to $I_{1\times2}$ during the synthesis of Si on Si(100) and Ge on Si(100)

Previously, the mechanism of formation of atomic steps by the RHEED method was studied during homoepitaxial growth of Si on Si(100). At growth temperatures from 200 to 500 °C, the atoms have an insufficient diffusion length to reach the step edges. The growth mechanism due to step displacement is practically not manifested, and the terrace overgrowth occurs due to the formation of two-dimensional islands. In the growth temperature range of 800–625 °C, each atom reaches the step edge and the growth is step-flow. And in the range from 500 to 625 °C, a transient process occurs [9].

As can be seen from Fig. 1, the temperature dependences of the intensity ratio during the growth of Ge and Si on Si(100) are similar. At temperatures of 200–500 °C, the atoms have a diffusion length that is insufficient to reach the terrace edges, since the terrace width ratio remains practically unchanged. In the temperature range of 500–550 °C, an increase in the terrace width ratio is observed, which indicates that one type of terrace (T_B) is overgrown faster than the other (T_A). This feature, as in the case of homoepitaxial growth of Si on Si(100), is caused, firstly, by the fact that the diffusion length of Ge atoms is sufficient to reach the terrace edges; secondly, atoms reaching the edge of the T_B terrace rich in kinks are easily embedded in it, and atoms at the smooth edge of the T_B terrace with a small number of kinks travel a longer path along the step before they find a kink; and, finally, in this temperature range, there is an effect of type A step permeability, when atoms can overcome the smooth A step and continue their path along the T_B terrace [9–10]. Therefore, near 550 °C, a critical point is observed at which one terrace significantly exceeds the other in area. After a temperature of 550 °C, the width of the terraces begins to equalize with increasing temperature. The steps move away because at the edge of the T_A step, Ge atoms with a large diffusion length can meet each other, thereby forming a new kink and accelerating the mechanism of incorporation of Ge atoms into a step of this type. As an alternative explanation, it can be assumed that after 550 °C, the atoms have enough energy to overcome the edge of the T_B terrace.

As shown by the similarity of the graphs in Fig. 1, the same growth mechanisms take place during epitaxial growth of two-dimensional Si and Ge layers on Si(100). In addition, the coincidence of the maxima of the two curves indicates that the diffusion length of Ge on Si(100) at a temperature of 550 °C is close to the diffusion length of Si on Si(100). Undoubtedly, at later stages of growth the processes become more complicated due to the presence of elastic stresses in the Ge/Si(100) system and the emergence of $2\times N$ type superstructures on the surface of the epitaxial layer during the deposition of several monolayers of germanium.

Conclusion

The formation mechanisms of Ge terraces on the Si(100) surface with a misorientation angle of 0.1° are complex. In general, during the growth of Ge/Si(100), the transition from the island mechanism of layer growth to the degree shift mechanism occurs at similar temperatures as during the growth of Si/Si(100) with a critical point of about 550 °C. The processes of terrace formation become more complicated with the emergence of elastic stresses in the system. The formation of the $2\times N$ superstructure affects the intensity of the 2×1 and 1×2 reflections. This leads to difficulties in their interpretation. Despite the fact that the heteroepitaxial growth of Ge on Si(100) has been studied for a long time, some processes still remain unexplored. The results of this work are of a fundamental research nature. Studying the processes of formation of nanostructures based on Ge and Si will undoubtedly improve the quality of creating nanostructures with specified parameters for optoelectronic devices.

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