Conference materials
UDC 539.27
DOI: https://doi.org/10.18721/JPM.183.217

Determination of the length of the 2×*N* superstructure during the synthesis of Ge on Si(001) at different temperatures

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Abstract. The article is devoted to the study of the length of the 2×*N* superstructure during epitaxial growth of Ge on Si(001) at different synthesis temperatures in the range from 200 °C to 750 °C. The analysis took place during the growth process by reflection high-energy electron diffraction in the direction of [110]. The work makes it possible to evaluate the effectiveness of elastic stress relief due to 2×*N* at the initial stages of growth over a wide temperature range.

Keywords: molecular beam epitaxy, reflection high-energy electron diffraction, relaxation of elastic stresses, 2×*N* superstructure, heteroepitaxy

Funding: The research was carried out at the expense of the grant of the Russian Science Foundation No. 25-12-20004, https://rscf.ru/en/project/25-12-20004/ and the Administration of the Tomsk region.

Citation: Kukenov O.I., Dirko V.V., Lozovoy K.A., Maier X.A., Kokhanenko A.P., Determination of the length of the 2×N superstructure during the synthesis of Ge on Si(001) at different temperatures, St. Petersburg State Polytechnical University Journal. Physics and Mathematics. 18 (3.2) (2025) 91–95. DOI: https://doi.org/10.18721/JPM.183.217

Материалы конференции
УДК 539.27
DOI: https://doi.org/10.18721/JPM.183.217

Определение длины сверхструктуры 2×*N* при синтезе Ge на Si(001) при разных температурах

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Аннотация. Статья посвящена исследованию длины сверхструктуры 2×*N* при эпитаксиальном росте Ge на Si(001) при разных температурах синтеза в диапазоне от 200 °C до 750 °C. Анализ происходил в процессе роста методом дифракции быстрых электронов в направлении [110]. Работа позволяет дать оценку эффективности снятия упругих напряжений за счет образования сверхструктуры 2×*N* на начальных стадиях роста в широком температурном диапазоне.

Ключевые слова: молекулярно-пучковая эпитаксия, дифракция быстрых электронов, релаксация упругих напряжений, сверхструктура 2×*N*, гетероэпитаксия

Финансирование: Исследование выполнено за счет гранта Российского научного фонда № 25-12-20004, https://rscf.ru/project/25-12-20004/ и Администрации Томской области.

Ссылка при цитировании: Кукенов О.И., Дирко В.В., Лозовой К.А., Майер К.А., Коханенко А.П. Определение длины сверхструктуры 2×N при синтезе Ge на Si(001) при разных температурах // Научно-технические ведомости СПбГПУ. Физико-математические науки. 2025. Т. 18. № 3.2. С. 91–95. DOI: https://doi.org/10.18721/JPM.183.217

Introduction

In the world of constantly evolving technologies, increasingly stringent requirements are put forward for electronic components. Despite their miniature size, they must be efficient enough to perform the necessary tasks. The transition to nanoscale structures has opened up the possibility of creating small and, due to the effect of dimensional quantization, efficient components for microelectronics, optoelectronics and many other areas [1, 2]. The main requirements for such structures are their purity, precise size compliance and sharpness of heteroboundaries. The molecular beam epitaxy (MBE) method is well suited for such parameters, allowing the creation of structures of a given thickness with sharp heteroboundaries and a minimum number of defects [3]. The silicon–germanium material system is considered well studied and quite successful. Silicon, due to its availability, has an extensive technological base. Germanium, due to its compatibility with silicon and better electronic properties, is able to significantly improve the characteristics of electronic components created on the basis of Ge–Si [4]. Despite the active development and study of Ge growth processes on Si, there are significant gaps in knowledge that are becoming increasingly noticeable given modern requirements for the quality of nanostructures. One of them is the relaxation of elastic stresses of the germanium layer on silicon. Relaxation of elastic stresses due to a change in the surface morphology occurs during the epitaxial growth of Ge on Si due to a 4.2% lattice mismatch. The relaxation mechanism at the initial stages of growth is the formation of $2\times N$ and $M\times N$ superstructures, and after the formation of the wetting layer is complete, the transition from two-dimensional to three-dimensional growth occurs [5]. This process can be tracked during growth without stopping it using the reflection high-energy electron diffraction (RHEED) method [6]. Epitaxial processes that depend on the growth parameters determine the geometric and electrophysical properties of nanostructures. Therefore, increasing the control of epitaxial synthesis processes will lead to the creation of nanostructures of the required sizes and properties. Based on this, the aim of the work is to determine the length of the $2\times N$ superstructure at different temperatures during epitaxial growth of Ge on Si(001) using RHEED patterns.

Materials and methods

The experiments were carried out at the "Katun–100" MBE installation. Commercially available Si(001) substrates with a misorientation angle of 0.1° were used. Ge synthesis occurred after pre-epitaxial cleaning of the substrate and application of a 75 nm buffer layer. The germanium deposition rate was the same for all experiments and amounted to 0.02 ML/s.

During the experiment, the surface morphology was determined by the reflection high-energy electron diffraction method. The initial stage of Ge formation on Si(001) is the emergence of the $2\times N$ superstructure. On the surface, long dimer rows of Si are replaced by short rows of Ge. This mechanism of elastic stress relaxation at the initial stage of growth is the most advantageous for this material system [7]. The length of the superstructure can be determined by the $(1/N)$ reflections that appear in the diffraction patterns (Fig. 1) [8].

Fig. 1, *a* shows the diffraction pattern from the Si(001) surface, and Fig. 1, *b* shows the diffraction pattern from the Ge/Si(001) surface. As can be seen, Fig. 1, *b* has additional $1/N$ reflections. The superstructure length was determined as follows. The distance between the (00) and (01) reflections was divided by the distance $(1/N)$ and (01). Thus, taking into account the inversion of scales in reciprocal space, it was determined how many times the new superstructure is larger than the crystal lattice parameter.

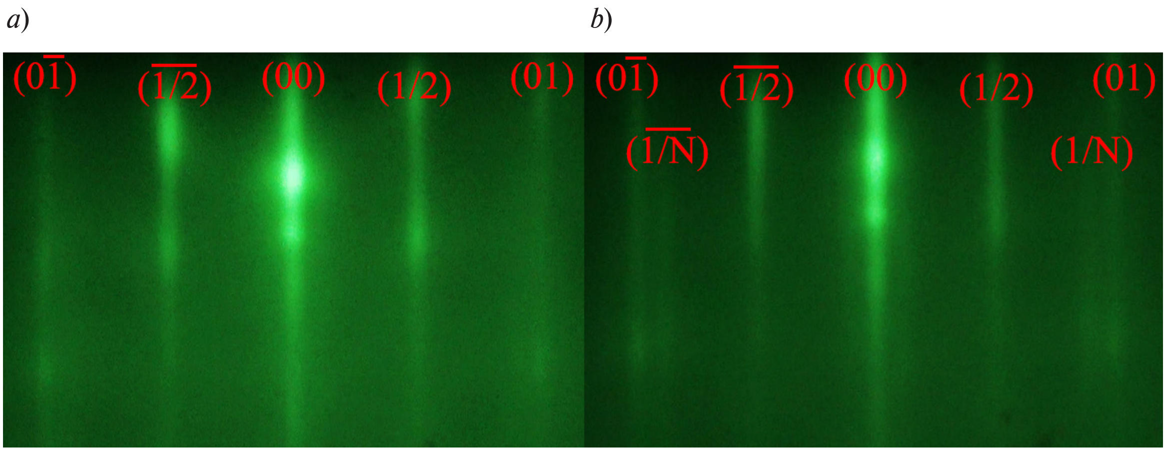

Fig. 1. RHEED patterns from pure Si(001) (*a*) and from Ge/Si(001) (*b*)

Elastic stresses caused by lattice mismatch, at a certain thickness of the two-dimensional germanium layer, can no longer be relieved by the formation of superstructures. At this stage, a stronger relaxation mechanism is activated – three-dimensional growth [9]. The start time of 3D growth is determined by the change in the intensity of the reflex (01) of the RHEED pattern [10]. Fig. 2 shows, as an example, the dependence of intensity (*I*) on amount of material (*n*) during the deposition of Ge on Si (001) at a temperature of 400 °C. Fig. 2 also shows RHEED patterns characteristic of a two-dimensional layer (on the left) and a three-dimensional structure (on the right).

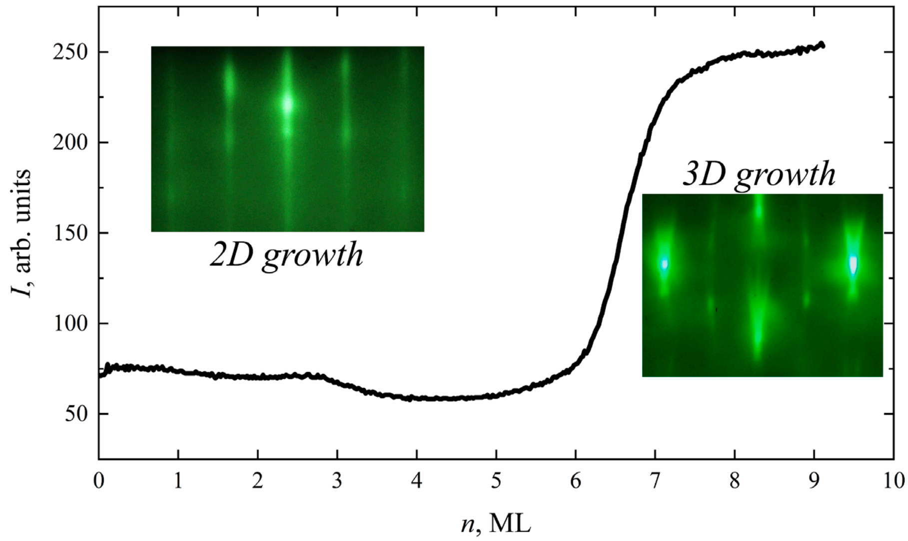

Fig. 2. Dependence of intensity of reflex (01) of RHEED pattern

Knowing the growth rate and the time of transition from two-dimensional to three-dimensional growth, it is possible to determine the thickness of the wetting layer, i.e. the critical thickness, above which germanium grows on silicon with the formation of three-dimensional islands.

Results and discussion

Based on the results of the analysis of experiments on the deposition of Ge on Si(001), carried out at different substrate temperatures in the range from 200 °C to 750 °C, the dependence of the superstructure length (*N*) on the synthesis temperature (Fig. 3, *a*) and the dependence of the critical thickness ($n_{critical}$) of the wetting layer on the growth temperature (Fig. 3, *b*) were constructed.

The dependence of the length *N* on temperature in Fig. 3, *a* can be divided into three temperature ranges. In the first range of 200–350 °C, a decrease in the number *N* is observed. This can

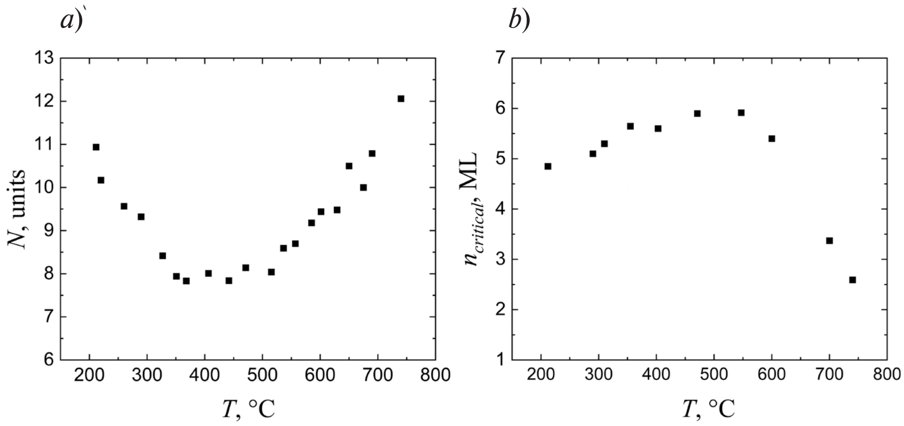

Fig. 3. Dependence of 2x*N* superstructure length (*a*) and critical thickness of the wetting layer (*b*) on growth temperature

be explained by the destruction of dimer chains due to the intensification of thermal vibrations of atoms. A decrease in the number *N*, in turn, indicates that with an increase in temperature, a more complete relaxation of elastic stresses in the system occurs due to the appearance of a larger number of dimer vacancies. In the second range of 350–500 °C, the length of the superstructure $2\times N$ remains constant. This can occur because the highest degree of relaxation accessible to this mechanism (the formation of dimer vacancies) has been achieved, or such a number of vacancies ($N = 8$) completely removes all stresses at these temperatures. In the third range of 500–750 °C, the length of the dimer rows begins to grow. This character of the dependence is explained by a set of processes. A more effective mechanism for the relaxation of elastic stresses is now the formation of $M\times N$ superstructures [11, 12] and the transition to 3D growth, as evidenced by a decrease in the critical thickness of the wetting layer (Fig. 3, *b*). An increase in temperature increases the rate of diffusion into the bulk of the substrate, thereby reducing the Ge concentration on the surface, which reduces the stresses in the system and leads to an increase in the length of the dimer rows [13, 14].

Conclusion

In this work, the reflection high-energy electron diffraction method was used to obtain a detailed dependence of the average size of the $2\times N$ superstructure on temperature in the range of 200–750 °C, which allows us to judge the mechanisms of elastic stress relaxation at the initial stages of Ge synthesis on Si(001). At growth temperatures from 200 °C to 350 °C, the efficiency of stress relaxation in the system is determined by the diffusion length of adatoms. At temperatures of 350–500 °C, maximum stress relaxation occurs, which is achieved by the formation of a 2×8 superstructure. In the temperature range from 500 °C to 750 °C, the length of the dimer series begins to be affected by factors associated with the emergence of $M\times N$ superstructures, accelerated transition to 3D growth, and diffusion of Ge atoms into the Si(001) substrate.

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Received 25.08.2025. Approved after reviewing 25.09.2025. Accepted 25.09.2025.