doi: 10.56761/EFRE2024.N1-P-017001

Influence on the growth of germanium of temperature on silicon

O. Kukenov[*], *V. Dirko, K. Lozovoy, A. Kokhanenko*

National Research Tomsk State University, Tomsk, Russia
[*]*okukenov@mail.ru*

Abstract. This paper presents a study of the initial stage of epitaxial growth of Si and Ge on Si(100) using the reflection high-energy electron diffraction method. Temperature ranges with dominant growth mechanisms and the influence of temperature on the efficiency of elastic stress relaxation are determined. It is shown how the combination of these factors affects the parameters of quantum dots.

Keywords: molecular beam epitaxy, reflection high-energy electron diffraction, silicon, germanium, step-flow, elastic stress relaxation, dimer rows.

1. Major sections

Numerous studies of the heteroepitaxial growth of germanium on silicon show that, under certainconditions, the formation of several morphologically different types of islands is possible in this system with a square and rectangular base [1]. In addition, under certain growth conditions, it is possible to form so called whisker-like quantum dots, which have a very high ratio of length to base with [2]. At the same time, for effective device use it is necessary to create heterostructures with a very narrow size distribution of nanoislands, since this is what provides the best conditions for the manifestation of quantum effects. The homogeneity of the islands critically depends on the growth parameters, such as the growth temperature, the deposition rate of germanium and its amount, as well as the annealing time of the structure after growth. The required size distribution of quantum dots can only be achieved through careful selection and constant monitoring of synthesis conditions.

The Si(100) surface appears in the form of wide terraces separated by steps (terrace edges). The nature of the appearance of terraces follows from the impossibility of creating ideally oriented substrates. Thus, the misorientation of the crystal plane with the cut plane leads to a stepped Si(100) surface. Terraces can be of two types: T_B with perpendicular orientation of dimer rows relative to the step (2x1 superstructure), T_A with dimer rows located on its surface parallel to the edge of the terrace (1x2 superstructure). In the diffraction pattern, the intensity of the reflection 2x1 corresponds to the area of the terrace T_B, and 1x2 – T_A.

In this work, when analyzing the synthesis of Si on Si(100) by reflection high-energy electron diffraction (RHEED) in a wide temperature range, the dependences of the intensity ratio and the ratio of vibration periods 2x1 and 1x2 were plotted (Figure 1).

Based on Figure 1, we can conclude that at temperatures of 200–500 °C, the growth of Si on Si(100) occurs with the formation of two-dimensional islands. This is explained by the fact that the overgrowing of terraces requires the same amount of time, the oscillations do not have a pronounced bimodal character, and the intensity of reflections from the 2x1 and 1x2 superstructures differs slightly. Further, with increasing temperature, the diffusion length of adatoms increases and they reach the edges of the steps. The steps move closer together due to the permeability effect and one terrace becomes larger than the other with a maximum at the point of 550 °C. This leads to a synchronous increase in the three curves shown in Figure 1. At temperatures above 550 °C, the step-flow growth mechanism begins to predominate.

When analyzing the growth of Ge on Si(100), the dependence of the ratio of the intensities of reflections 2x1 to 1x2 on temperature was also plotted (Figure 2) and additionally the dependence of the intensity of the reflection $1/N$ on the growth time (Figure 3) [3].

The dependence presented in Figure 2 is similar to the dependence in Figure 1. The ratio of I_{2x1} to I_{1x2} is also maximum in the region of 550–560 °C. In Figure 3, the obtained dependence makes it clear that with increasing temperature, the efficiency of relieving elastic stresses in the Ge-Si system increases. The diffusion length of surface atoms increases, which increases their chances of occupying the most energetically favorable position. The combination of these quantities determines the dominant growth mechanism of two-dimensional layers at a given temperature. It was found that near a temperature of 550 °C there is a critical point at which monatomic steps of different types are as close as possible, and dimer rows effectively relax elastic stresses in the system. Based on this, a temperature of 550 °C was chosen as the priority temperature for creating quantum dots. To compare the parameters of nanoislands, samples with Ge nanoislands on Si(100) grown at temperatures of 470–600 °C were studied using scanning electron microscopy.

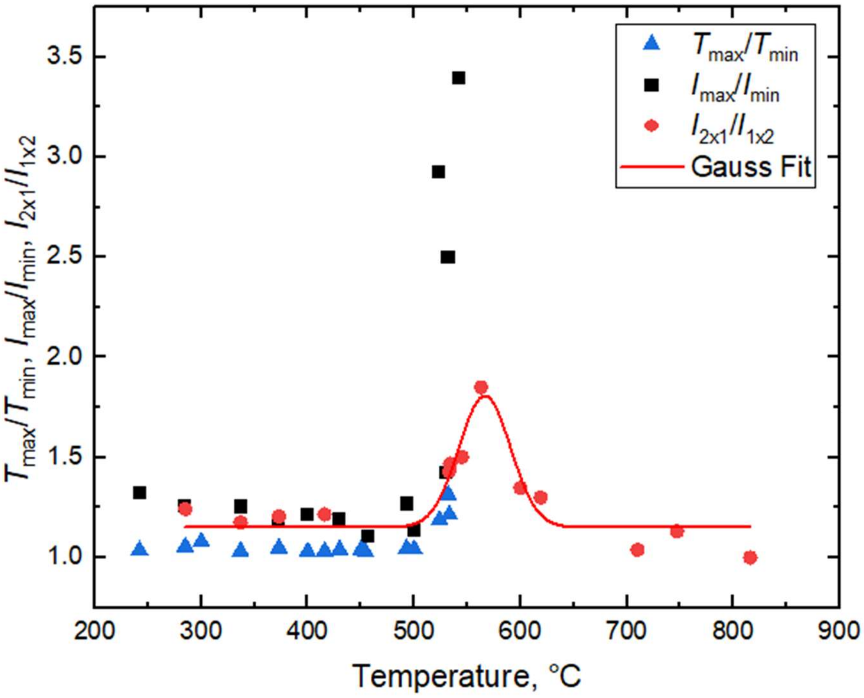

Fig. 1. Temperature dependence of the ratios of periods and intensities of oscillations in the direction [110], corresponding to the formation of different types of steps and ratios of the intensities of reflections 2x1 to 1x2 in the direction [100] (for Si).

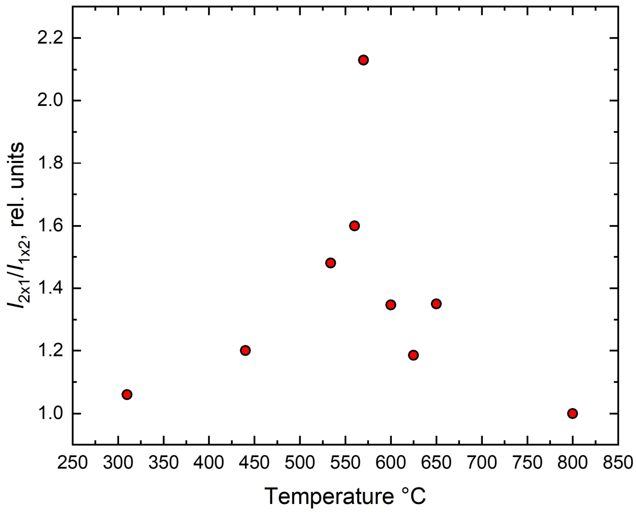

Fig. 2. Temperature dependence of the ratios of the intensities of reflections 2x1 to 1x2 in the direction [100] (for Ge).

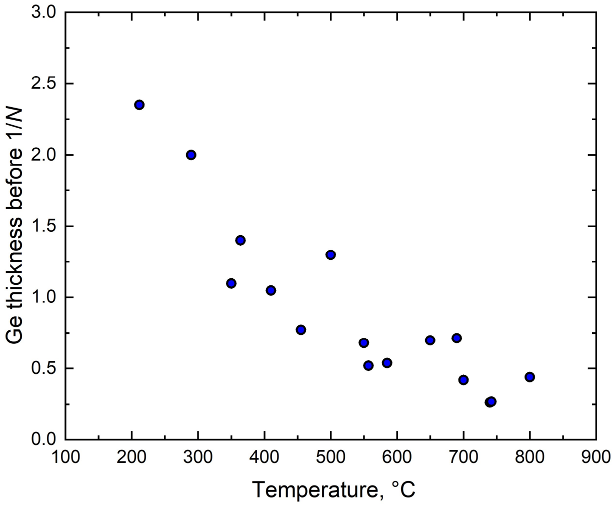

Fig. 3. Temperature dependence of the number of Ge layers before the appearance of 1/*N* in the [110] direction.

It is shown that with such a small change in the growth temperature near the critical temperature, the samples differ significantly in the density of quantum dots per square centimeter and the sizes of nanoclusters: 470 °C – 10^{11} см$^{-2}$; 550 °C – $7{\cdot}10^{10}$ см$^{-2}$; 600 °C – 10^{9} см$^{-2}$. The density of quantum dots decreases sharply with increasing temperature above 550 °C, and their size also increases significantly, making it impossible to observe quantum effects. In addition, the sample grown at 550 °C is distinguished by a large ratio of the length of the base of the islands to their width and a small scatter in the sizes of the islands. Therefore, this point is of great interest for the creation of elongated nanoclusters and quantum wires [4].

2. Conclusion

To summarize, controlling the parameters of quantum dots through understanding epitaxial processes is the key to creating advanced nanophotonics and nanoelectronics devices. The work shows that the formation of Si and Ge terraces on the Si(100) surface occurs in a similar way. And the efficiency of relaxation of elastic stresses proceeds more efficiently with increasing temperature. Experiments have shown that the combination of these factors affects the density of quantum dots. Additionally, the shape of the quantum dots was studied, and at 550 °C the nanoislands have an elongated shape. Studies have shown that temperature is a determining factor for the occurrence of epitaxial processes, which directly affect the parameters of quantum dots.

Acknowledgement

The work was supported by the Russian Science Foundation and Tomsk State University Development Program (Priority 2030)

3. References

[1] L.V. Arapkina, and V.A. Yuryev, Classification of Ge hut clusters in arrays formed by molecular beam epitaxy at low temperatures on the Si(001) surface, *Physics-Uspekhi*, vol. **53**, 289–302, 2010, doi: 10.3367/UFNr.0180.201003e.0289

[2] J. Tersoff, and R.M. Tromp, Shape transition in growth of strained islands: Spontaneous formation of quantum wires, *Physical Review Letters*, vol. **70**, 2782–2785, 1993, doi: 10.1103/PhysRevLett.70.2782

[3] V.V. Dirko, K.A. Lozovoy, A.P. Kokhanenko, and A.V. Voitsekhovskii, High-resolution RHEED analysis of dynamics of low-temperature superstructure transitions in Ge/Si(001) epitaxial system, *Nanotechnology*, vol. **33**, 115603, 2022, doi: 10.1088/1361-6528/ac3f56

[4] K. Liu, I. Berbezier, L. Favre, et al., Self-organization of SiGe planar nanowires via anisotropic elastic field, *Physical Review Materials*, vol. **3**, 023403, 2019, doi: 10.1103/PhysRevMaterials.3.023403