Analysis of the 7x7 to 5x5 superstructure transition by RHEED in the synthesis of Ge on Si (111) in an MBE installation

V V Dirko, K A Lozovoy, A P Kokhanenko and O I Kukenov
Tomsk State University, Faculty of Radiophysics, 36 Lenin av., Tomsk 634050, Russia
E-mail: vovenmir@gmail.com

Abstract. In this paper, we consider the 7x7 to 5x5 superstructure transition during the synthesis of Ge epitaxial layers on a Si (111) surface in its temperature range from 250 to 700 °C. This transition is investigated by reflection high-energy electron diffraction (RHEED). As a result, the dependences of the critical thickness of the 7x7 to 5x5 superstructure transition on the substrate temperature are obtained for the first time.

1. Introduction
Optoelectronics is one of the rapidly developing scientific and technical areas. Its development was due to the fact that a person acquires 80% of information through vision, which allows the use of optoelectronic devices in various systems of information transmission, processing, reception, storage, display. And due to the wide variety of materials used, there are various optoelectronic technologies, means of information transmission through optical channels, converters of optical cure into energy, optical computer technology, etc. Creation of optoelectronic devices on nanoheterostructures allows one to significantly improve existing technologies and to obtain a new class of perfect devices due to quantum mechanical effects [1–4].

One of the main methods of obtaining nanoheterostructures for optoelectronics is the method of molecular beam epitaxy (MBE). In turn, the formation of epitaxial layers is impossible without determining the main factors influencing the synthesis of the formed nanoheterostructures. One such factor is the growth of epitaxial films. The method of reflection high-energy electron diffraction (RHEED) belongs to the "in situ" methods, i.e. it allows one to analyze the state of the substrate surface during the synthesis of materials [5-7].

Pure silicon surfaces with (100) and (111) crystallographic orientations are traditionally used for germanium epitaxy. In this paper, the processes of epitaxial germanium growth on the surface of Si (111) are studied, since this surface is less studied [8, 9]. The obtained temperature dependences of the crystal structure parameters from the RHEED method will be used in modeling the synthesis of Si/Ge structures in the generalized kinetic model [10, 11].

2. The experiment
The synthesis of Ge on a Si (111) substrate was carried out in a high-vacuum molecular beam epitaxy unit "Katun-100". All experiments were carried out at a vacuum level of 10⁻⁹ Torr. Changes in diffraction patterns were recorded by a digital camera with Full-HD resolution and a high sensitivity matrix. Before the experiment, the silicon wafer was subjected to pre-epitaxial preparation, which includes chemical purification from the factory silicon oxide with subsequent application of a thin laboratory oxide. After that, the plate was subjected to thermal annealed at 1000 °C for 10 minutes in
an epitaxy chamber; the complete cleaning of the plate was characterized by the display of a 7x7 superstructure for Si (111). This was followed by the growth of a Si buffer layer with a thickness of about 50 nm.

Using the method of reflection high-energy electron diffraction, the thickness of the Ge layer was measured during the 7x7 to 5x5 superstructure transition at the temperatures of the Si (111) substrate in the range from 250 to 700 °C. The video camera recorded changes in the intensity of the diffraction patterns with subsequent processing of the video file.

3. Results and discussion

Figures 2, 3 and 5 present the images of the main moments of change in diffraction patterns during the 7x7 to 5x5 superstructure transition.

For the above profile, the substrate temperature corresponds to 700 °C, and the germanium deposition rate was 0.04 Å/s.

In the synthesis of Ge on Si (111), growth occurs according to the Stransky-Krastanov mechanism, when at the beginning the germanium layer repeats the superstructure of Si(111) with a superstructure...
of 7x7, as evidenced by elongated reflexes in the diffraction pattern (figures 1 and 2). Due to the 4% mismatch of the lattice constants between Si and Ge, there is a change in the surface layer (figure 3) and a complete 7x7 to 5x5 superstructure transition (figures 4 and 5). Figure 6 shows the profile of the change in diffraction patterns taken in the direction of transition of the superstructure 7x7 to 5x5 and is indicated in figures 2, 3 and 5 by a dashed line.

It can be seen from the profile that the transition of the superstructure does not occur instantly, but after some time. Figure 7 shows the dependence of the thickness of the germanium film with a 7x7 superstructure at the transition to a 5x5 superstructure on the temperature of the Si (111) substrate. Also, figure 8 shows the values of the critical thickness of the 2D germanium layer during the transition to 3D growth depending on the temperature of the Si (111) substrate.

Thus, at low temperatures, the transition of the superstructure occurred at a germanium layer thickness of about 4.7 Å. With increasing temperature, the thickness of the germanium layer with a superstructure of 7x7 increased and reached was 8.2 Å at a temperature of 600 ⁰C. In this case, the complete transition of the superstructure occurred at a single atomic layer of germanium.

4. Conclusions
Thus, the paper presents the results of a study of the 7x7 to 5x5 superstructure transition during the synthesis of Ge on a Si (111) substrate by the method of reflection high-energy electron diffraction. The dependences of the 7x7 to 5x5 superstructure transition at different temperatures of the silicon substrate were obtained. The critical thickness of the stressed heteroepitaxial layer Ge [10, 11] and a change in the parameter of an elementary two-dimensional cell during the growth of Ge on Si (111) were also determined during the experiments.

Acknowledgements
The reported study was funded by RFBR, project number 19-32-90195.

References
[1] Wirths S, Buca D and Mantl S 2016 Prog. Cryst. Growth Characteriz. Mater. 62 1
[2] Zaima S, Nakatsuka O, Taoka N, Kurosawa M, Takeuchi W and Sakashita M 2015 Sci. Technol. Adv. Mater. 16 043502
[3] Izhnin I I, Fitsych O I, Voitsekhovskii A V, Kokhanenko A P, Lozovoy K A and Dirko V V 2018 Opto-Electron. Rev. 26 195
[4] David T, Aqua J-N, Liu K, Favre L, Ronda A, Abbarchi M, Claude J-B and Berbezier I 2018
[5] Wu J, Chen S, Seeds A and Liu H 2015 *J. Phys. D: Appl. Phys.* **48** 363001
[6] Aqua J, Berbezier I and Favre L 2013 *Phys. Rep.* **522** 59
[7] Pchelyakov O P, Dvurechenskii A V, Nikiforov A I, Voitsekhovskii A V, Grigor’ev D V and Kokhanenko A P 2011 *Russ. Phys. J.* **53** 943
[8] Lozovoy K A, Kokhanenko A P and Voitsekhovskii A V 2018 *Nanotechnology* **29** 054002
[9] Yoshida R, Tosaka A and Shigeta Y 2018 *Surf. Sci.* **671** 43
[10] Lozovoy K A, Kokhanenko A P and Voitsekhovskii A V 2015 *Phys. Chem. Chem. Phys.* **17** 30052
[11] Lozovoy K A, Kokhanenko A P and Voitsekhovskii A V 2016 *Appl. Phys. Lett.* **109** 021604
[12] MacLeod J M, Psiachos D, Stott M J and McLean A B 2006 *Phys. Rev. B.* **73** 241306