Optically Active Centers in Si/Si$_{1-x}$Ge$_x$:Er Heterostructures Containing Er$^{3+}$ Ions

L. V. Krasilnikova$^a$, M. V. Strepihova$^a$, N. A. Baidakova$^a$, Yu. N. Drozdov$^a$, Z. F. Krasilnik$^a$, V. Yu. Chalkov$^b$, and V. G. Shengurov$^b$

$^a$Institute for Physics of Microstructures, Russian Academy of Sciences, Nizhni Novgorod, 603950 Russia
$^b$Research Physicotechnical Institute, Nizhni Novgorod State University, Nizhni Novgorod, 603950 Russia

Abstract—The basic types of optically active erbium centers that make the major contribution to the photoluminescence signal from the Si/Si$_{1-x}$Ge$_x$:Er heterostructures with the Ge content from 10 to 30% are analyzed in detail. It is shown that the origin of the optically active centers containing Er$^{3+}$ ions correlates with the molar composition of the Si$_{1-x}$Ge$_x$:Er layer and the content of oxygen impurity in the layer. The major contribution to the photoluminescence signal from the Si/Si$_{1-x}$Ge$_x$:Er heterostructures with the Ge content below 25% is made by the well-known centers containing Er$^{3+}$ ions and oxygen. An increase in the Ge content in the Si$_{1-x}$Ge$_x$:Er layer ($x \geq 25\%$) yields the formation of a new type of centers, specifically, the Ge-containing optically active erbium centers unobserved in the Si-based structures previously.

PACS numbers: 71.55.Ht, 78.55.Ap, 78.55.Hx, 78.66.Db, 78.66.Li

DOI: 10.1134/S1063782609070094

1. INTRODUCTION

The Si/Si$_{1-x}$Ge$_x$ structures doped with erbium attract interest due to the possibility of developing an efficient emission source on their basis. Introduction of the Si$_{1-x}$Ge$_x$ layer into silicon allows the formation of an effective waveguide with a high (above 80%) degree of localization of radiation in the active layer [1]. Previously [2], we showed that the external quantum efficiency of photoluminescence (PL) of the Si/Si$_{1-x}$Ge$_x$:Er structures could be as high as ~0.4%, which is comparable to the maximal efficiencies attained in the Si/Si:Er structures without any special treatments of the surface in order to extract radiation. Moreover, for the structures of such a type, it was shown for the first time that it was possible to attain an inverse occupancy of the energy levels of the Er$^{3+}$ ions by optical pumping [3].

Despite the above-mentioned achievements, the Si/Si$_{1-x}$Ge$_x$:Er structures still remain poorly understood in respect to the conditions of formation, the nature, and the structure of optically active centers that involve the Er$^3$ ions and make the major contribution to the PL signal. The effect of the molar composition of the alloy and the content of co-dopants (specifically, oxygen) on the type of optically active erbium centers has not been studied.

In this paper, we report the results of comprehensive analysis of the fine structure of the PL spectra of the Si/Si$_{1-x}$Ge$_x$:Er heterostructures, in which the Ge content in the heterolayer is varied from 10 to 30%. We consider the basic types of optically active centers formed in the materials and show correlation between the types of the centers and the molar and impurity composition of the heterolayer.

2. EXPERIMENTAL

The Si/Si$_{1-x}$Ge$_x$:Er heterostructures studied here were grown by sublimation molecular beam epitaxy (MBE) in a germane (GeH$_4$) atmosphere at the temperature of growth 500°C. The basic feature of this technique is that germanium is supplied to the growing layer owing to pyrolysis of germane. The procedure of growth was described in details elsewhere [4]. As in the case of the standard sublimation MBE technique [5], to dope the layers with the rare-earth impurity, we used polycrystalline silicon doped with erbium. The samples were grown on the (100)-oriented single-crystal silicon (c-Si) substrates (for the substrates, we used $n$-Si:P with $\rho = 4.5\, \Omega\,cm$). The growth of the Er-doped Si$_{1-x}$Ge$_x$ alloy was preceded by the formation of the c-Si buffer layer with the thickness ~0.2 $\mu$m. The thickness of the coating Si layer grown over the active Si$_{1-x}$Ge$_x$:Er heterolayer was 100–200 nm. To analyze the structural parameters and elemental composition of the epitaxial Si$_{1-x}$Ge$_x$:Er layers grown in this manner, we used the techniques of X-ray diffraction (XRD) and secondary ion mass spectroscopy (SIMS). The SIMS data on the elemental composition of the structures showed that the Er dopants were distributed...
in the structures almost uniformly (with no segregation). The erbium dopant concentration in the Si$_{1-x}$Ge$_x$:Er layers was $(0.7–2.0) \times 10^{18}$ cm$^{-3}$. The oxygen concentration was in the range $(2–20) \times 10^{18}$ cm$^{-3}$. The Ge content ($x$) in the structures was varied from 10 to 30%, and the thickness of the heteroepitaxial layers was $d$(Si$_{1-x}$Ge$_x$:Er) = 150–2300 nm. The residual elastic stresses (RES) defined by the degree of relaxation of the heterolayer were in the range from 100 to 1%.

The PL measurements and the analysis of the fine structure of the PL spectra were accomplished by high-resolution Fourier spectrometry. The PL spectra were studied using a BOMEM DA3 Fourier spectrometer, with the resolution as high as 0.1 cm$^{-1}$ in the range of wave numbers from 5000 to 10000 cm$^{-1}$. For the excitation source, we used a Nd:YAG laser emitting at the wavelength 532 nm with the power 200 mW. After propagating through an optical filter, the laser beam was focused with a lens into a spot ~1 mm in diameter at the sample surface. The PL signal was detected with the germanium photoelectric detector, Edinburgh Instruments EO-817A cooled with liquid nitrogen. The PL studies were carried out in the range of temperatures $T = 4.2–150$ K.

### 3. RESULTS AND DISCUSSION

All of the heteroepitaxial Si/Si$_{1-x}$Ge$_x$:Er/Si structures studied here exhibit an intense PL signal at the wavelength 1.54 µm corresponding to the basic radiative transition $^4I_{13/2} \rightarrow ^4I_{15/2}$ in the 4f shell of the Er$^{3+}$ ion. Previously, we showed that, in the structures of this type with the Ge content ~10%, the major contribution to the luminescence response was made by optically active centers and complexes of erbium ions with oxygen [6]. In this study, we present a more comprehensive analysis of the types of Er$^{3+}$-containing optically active centers formed in the Si$_{1-x}$Ge$_x$:Er heterolayers with the Ge content 10–30% and consider the correlation between the types of the centers and the molar and impurity composition of the heterolayer, specifically, the oxygen content in the layer.

Figure 1 shows the PL spectra of the structures in the wavelength range corresponding to intra-atomic transitions in the Er$^{3+}$ ion. The most intense PL lines observed at the wave number 6508 and 6472 cm$^{-1}$ in the spectra of the structures with a high oxygen content (Fig. 1a) coincide in energy position with the first lines of the individual axially symmetric centers containing oxygen and Er$^{3+}$ ions, i.e., the Er–O$1$ centers detected previously in the ion-implanted Si:Er layers.