ISSN 1063-7826, Semiconductors, 2010, Vol. 44, No. 11, pp. 1480–1485. © Pleiades Publishing, Ltd., 2010.
Original Russian Text © L.V. Krasilnikova, A.N. Yablonskiy, M.V. Stepikhova, Yu.N. Drozdov, V.G. Shengurov, Z.F. Krasilnik, 2010, published in Fizika i Tekhnika Poluprovodnikov, 2010, Vol. 44, No. 11, pp. 1527–1532.

WORKSHOP

Special Features of the Excitation Spectra and Kinetics of Photoluminescence of the $Si_{1-x}Ge_x$:Er/Si Structures with Relaxed Heterolayers

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Submitted April 20, 2010; accepted for publication April 20, 2010

Abstract—Luminescent properties of heteroepitaxial $Si_{1-x}Ge_x$:Er/Si structures with relaxed heterolayers are studied. The results of combined studies of the excitation spectra and kinetics of photoluminescence (PL) are used to single out the components providing the largest contribution to the PL signal of the $Si_{1-x}Ge_x$:Er/Si structures in the wavelength region of 1.54 μm. It is shown that relaxation of elastic stresses in the $Si_{1-x}Ge_x$:Er heterolayer affects only slightly the kinetic characteristics of erbium luminescence and manifests itself in insignificant contribution of the defects and defect–impurity complexes to the luminescent response of the $Si_{1-x}Ge_x$:Er/Si structures. In the excitation spectra of the erbium PL, special features related to the possibility of the rare-earth impurity excitation at energies lower than the band gap of the $Si_{1-x}Ge_x$ solid solution are revealed. It is shown that a peak the width of which depends on the band gap of the solid solution and the extent of its relaxation is observed in the excitation spectra of the erbium-related PL in the $Si_{1-x}Ge_x$:Er/Si structures in the wavelength region of 1040–1050 nm. The observed specific features are accounted for by involvement of intermediate levels in the band gap of the $Si_{1-x}Ge_x$:Er solid solution in the process of excitation of an Er^{3+} ion.

DOI: 10.1134/S1063782610110205

1. INTRODUCTION

The interest in the $Si_{1-x}Ge_x$:Er/Si structures is caused, first of all, by the possibility of development of efficient emission sources on the basis of these structures. It can be shown that introduction of germanium into the active region makes it possible to form an efficient waveguide in structures of this type, the degree of localization of optical modes (Γ) in which is as high as 98% [1]. The highest localization of optical modes in the $Si_{1-x}Ge_x$:Er heterolayers takes place at a high content of germanium and a large thickness of the active region, which is realized in practice only in relaxed $Si_{1-x}Ge_x$:Er/Si structures. In this context, it is of interest to study luminescent properties of the Er^{3+} impurity and special features of luminescent response of the $Si_{1-x}Ge_x$:Er/Si structures with relaxed $Si_{1-x}Ge_x$:Er heterolayers.

In this paper, we report the results of studying the excitation spectra and kinetics of the erbium- and defect-related photoluminescence (PL) in the epitaxial $Si_{1-x}Ge_x$:Er/Si and $Si_{1-x}Ge_x$/Si structures with germanium content varied in the range from 10 to 31%. In the studied structures, the value of residual elastic strains (RES) characterizing the degree of relaxation in the heteroepitaxial layers varied from 82 to 4%.

2. EXPERIMENTAL

The $Si_{1-x}Ge_x$:Er/Si and $Si_{1-x}Ge_x$/Si structures investigated in this study were grown by the method of sublimational molecular-beam epitaxy (MBE) in the GeH_4 ambient [2]. As in the standard method of sublimational MBE, the flux of Er atoms in the case of formation of the active layer was initiated by evaporation of polycrystalline Si source doped with erbium. The samples were grown on the *c*-Si substrates of the KÉF-4.5 brand (*n*-Si:P with the resistivity of 4.5 Ω cm) with the (100) orientation. The process of growth of the $Si_{1-x}Ge_x$ and $Si_{1-x}Ge_x$:Er layers was preceded by formation of a buffer *c*-Si layer with the thickness of ~0.2 μm. The thickness of the cap silicon layer grown on top of the active heterolayers was 100–200 nm. The structural properties and elemental composition of the grown $Si_{1-x}Ge_x$:Er/Si and $Si_{1-x}Ge_x$/Si structures were analyzed by the methods of the X-ray diffraction (XRD) and secondary-ion mass spectrometry (SIMS). As the results of SIMS studies showed, the distribution of the erbium impurity in the $Si_{1-x}Ge_x$:Er

Parameters of the studied $Si_{1-x}Ge_x$: Er/Si and $Si_{1-x}Ge_x$/Si structures

Structure no.	Germanium content x, %	The heterolayer thickness d_{SiGeEr}, d_{SiGe}, μm	Residual elastic strains RES, %	Doping with erbium
1	11	0.4	82	+
2	23	2.6	6	+
3	31	2.1	9	+
4	26	1.8	4	–

layers is uniform with the Er concentration ~(0.7–5) × 10^{18} cm^{-3}. Structural parameters of the $Si_{1-x}Ge_x$:Er/Si and $Si_{1-x}Ge_x$/Si samples investigated in this study are listed in the table. As can be seen from the table, the thickness of the studied heteroepitaxial layers (d_{SiGeEr}, d_{SiGe}) was varied from 0.4 to 2.6 μm. The content of Ge (x) in the $Si_{1-x}Ge_x$:Er and $Si_{1-x}Ge_x$ layers varied from 10 to 31%; the relative value of residual elastic strains varied from 82 to 4%. Instead of the quantity RES, we can also introduce the related parameter, i.e., the degree of relaxation of the lattice in the heterolayer, R; the latter is defined as $R(\%) = 100 - \text{RES}$.

For studying the excitation spectra and kinetics of PL in the $Si_{1-x}Ge_x$/Si and $Si_{1-x}Ge_x$:Er/Si structures, we used an MOPO-SL (Spectra-Physics) optical parametric generator of light with pumping by a pulsed Nd:YAG laser (duration of excitation-radiation pulses ~5 ns, the repetition frequency of the pulses 10 Hz). The PL signals were detected with nanosecond resolution using an Acton 2300i grating spectrometer, a Hamamatsu photomultiplier based on InP/InGaAs (the working range 0.95–1.7 μm), and a WS 432 (LeCroy) digital oscilloscope. The excitation spectra and kinetics of the erbium- and defect-related PL components were studied in the $Si_{1-x}Ge_x$:Er/Si and $Si_{1-x}Ge_x$/Si structures in the range of wavelengths $\lambda_{ex} = 700$–1300 nm of excitation radiation at temperatures of 16 and 77 K.

3. EXPERIMENTAL RESULTS AND DISCUSSION

In Figs. 1 and 2, we show typical kinetic dependences of the PL signal; these dependences were obtained for relaxed heteroepitaxial $Si_{1-x}Ge_x$:Er/Si structures at various conditions of excitation. As the results of the studies showed, the falloff of the PL signal for the $Si_{1-x}Ge_x$:Er/Si heterostructures at the wavelength of 1.54 μm is characterized by exponential dependence with two decay times. Within the time interval extending to 10 μs, short-time components with the decay times τ ≈ 1 μs contribute significantly to the luminescence response of the $Si_{1-x}Ge_x$:Er/Si

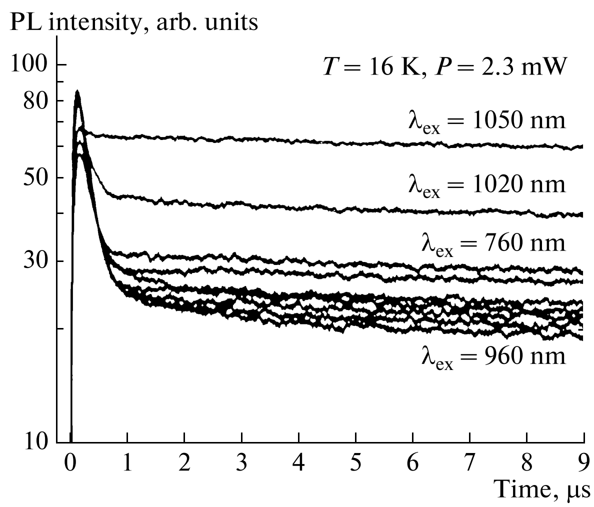

Fig. 1. The PL kinetics in the $Si_{1-x}Ge_x$:Er/Si structure with germanium content 31%, d_{SiGeEr} = 2.1 μm, and RES = 9%. The PL signal was detected at a wavelength of 1.54 μm within the temporal range from 0 to 10 μs (T = 16 K). The measurements were performed in the wavelength range λ_{ex} = 760–1050 nm of the excitation radiation.

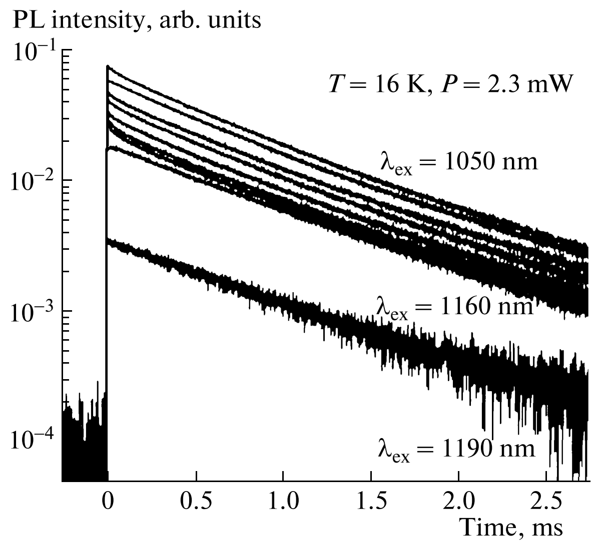

Fig. 2. The PL kinetics for the $Si_{1-x}Ge_x$:Er/Si structure with x = 31%, d_{SiGeEr} = 2.1 μm, and RES = 9%. The PL signal was detected at the wavelength 1.54 μm within the temporal range from 10 to 2.5 ms (T = 16 K). The measurements were performed in the wavelength range λ_{ex} = 750–1190 nm of the excitation radiation.

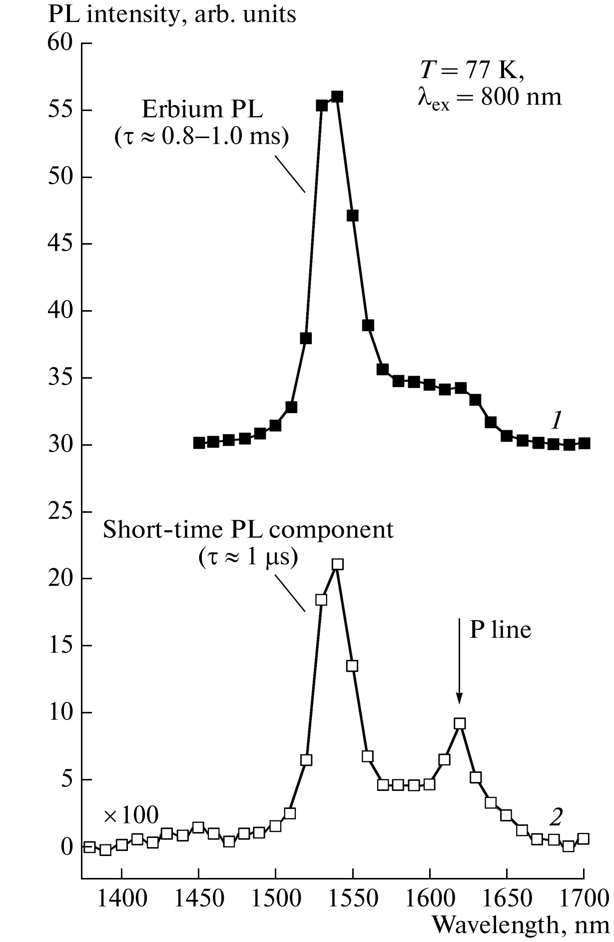

Fig. 3. Photoluminescence spectra for the $Si_{0.69}Ge_{0.31}$:Er/Si structure as obtained from the analysis of kinetics of the photoluminescence signal under conditions of excitation at the wavelength of 800 nm ($T = 77$ K): (*1*) the spectrum of the erbium-related PL component and (*2*) the spectrum of the short-time PL component.

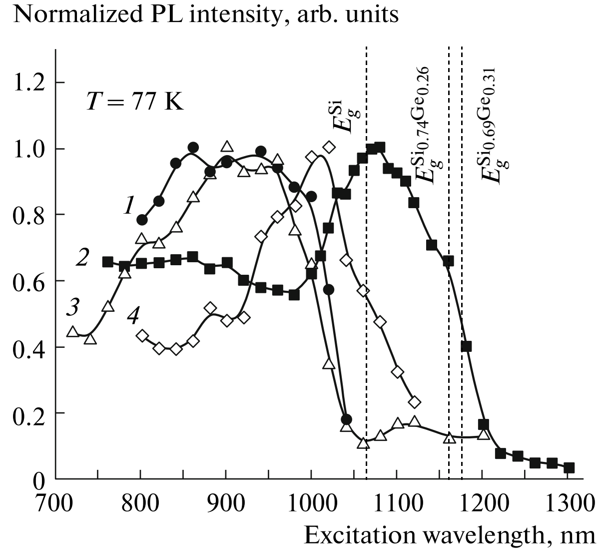

Fig. 4. Normalized spectra of excitation of the defect- and erbium-related PL components in the $Si_{0.74}Ge_{0.26}$/Si and $Si_{0.69}Ge_{0.31}$:Er/Si structures as measured at $T = 77$ K: (*1*) the spectrum of the short-time PL component observed at the wavelength of 1450 nm for the $Si_{0.69}Ge_{0.31}$:Er/Si structure, (*2*) the spectrum of the line of the erbium-related luminescence for the $Si_{0.69}Ge_{0.31}$:Er/Si structure, (*3*) the spectrum of the PL line D1 for the $Si_{0.74}Ge_{0.26}$/Si structure, and (*4*) the spectrum of the P line for the $Si_{0.69}Ge_{0.31}$:Er/Si structure.

structures (Fig. 1). Evidently, the presence of these components in the PL kinetics of relaxed $Si_{1-x}Ge_x$:Er layers can be related to the existence of defects and defect–impurity complexes in the studied structures. In the time range from 10 μs to 10 ms, the components related to the rare-earth erbium impurity make the dominant contribution to the luminescence response of the $Si_{1-x}Ge_x$:Er/Si structures at the wavelength of 1.54 μm. The kinetics of photoluminescence of Er^{3+} ions in the $Si_{1-x}Ge_x$:Er/Si structures with a high degree of relaxation of elastic strains (RES = 6–9%) and a large thickness of the active heterolayer (larger than 1 μm) is described by the decay times (τ ≈ 0.8–1 ms) typical of a rare-earth impurity [3] (Fig. 2). Evidently, these decay times are indicative of an insignificant role of nonradiative recombination channels and slight influence of processes of relaxation of elastic stresses in a $Si_{1-x}Ge_x$:Er layer on temporal characteristics of decay of erbium-related PL. We should also note that the short-time components of the PL signal singled out as a result of studies of the PL kinetics in the time range extending to 10 μs are much lower (by the signal intensity) by several orders of magnitude than the luminescence response of the rare-earth impurity. As an example, in Fig. 3, we show the PL spectra of short-time signal components (τ ≈ 1 μs) and also of the erbium-related PL component (τ ≈ 0.8–1 ms) measured for the $Si_{1-x}Ge_x$:Er/Si structure with $x = 31\%$, $d_{SiGeEr} = 2.1$ μm, and RES = 9%. As can be seen from Fig. 3, at a temperature of 77 K and the wavelength $\lambda_{ex} = 800$ nm of excitation radiation, the PL signal of the erbium component in this sample exceeds the signal of the short-time component by almost three orders of magnitude.

In Fig. 4, we show the results of studies of the excitation spectra of the short-time component of the PL signal at the wavelength of 1.54 μm; this component may be related to the defects in the $Si_{1-x}Ge_x$:Er/Si structures. For comparison, we also show in Fig. 4 the excitation spectra of the PL erbium component. It can be seen that the excitation spectrum of the short-time PL component for the structure with $x = 31\%$, $d_{SiGeEr} = 2.1$ μm, and RES = 9% (spectrum *1* in Fig. 4) is shifted to shorter wavelengths with respect to the excitation spectrum for the erbium PL (spectrum *2* in Fig. 4). The PL signal of the short-time component with the decay time τ ≈ 1 μs is not observed at energies of the photon of excitation radiation lower than the band gap of the $Si_{1-x}Ge_x$ solid solution. The obtained data are in good agreement with the results of studies of excitation spectra for the so-called P PL line observed in the case of the $Si_{1-x}Ge_x$:Er/Si structures and related to the defect–impurity complexes with involvement of carbon and oxygen (the energy of the radiative transition is 767 meV) [4] and also with the results of studies of the PL excitation spectra for the $Si_{1-x}Ge_x$/Si structures with the relaxed $Si_{1-x}Ge_x$ heterolayer undoped with the erbium impurity; in this case, the PL signal is predominantly related to dislocations. Let us consider these results in more detail by the example of the $Si_{0.74}Ge_{0.26}$/Si and $Si_{0.69}Ge_{0.31}$:Er/Si studied at a temperature of 77 K. In the PL spectra of the $Si_{0.69}Ge_{0.31}$:Er/Si structure measured at the energy of the excitation-radiation photon corresponding to the interband transition, a high-intensity PL peak is observed in the region of the wavelength 1535 nm; this peak is related to the basic radiative transition $^4I_{13/2} \rightarrow {}^4I_{15/2}$ in the 4*f* shell of the Er^{3+} and is characterized by the decay times $\tau \approx 0.8$–1 ms (Fig. 3). The arrow in Fig. 3 (with designation P line) shows the position of the P PL line. The latter P PL line at the wavelength of ~1615 nm is observed in the PL spectra of the $Si_{1-x}Ge_x$:Er/Si structures simultaneously with the PL components peaked at a wavelength of 1540 nm with the decay time of ~1 μs. The decay times of both of these PL components are in the time range extending to less than 10 μs. The $Si_{1-x}Ge_x$/Si structure not doped with erbium was grown with the heterolayer thickness $d_{SiGe} = 1.8$ μm and a high content of germanium in this layer ($x = 26\%$), which, as a consequence, brings about a pronounced relaxation. The value of RES in the grown structure was 4%. The predominant contribution to the PL signal of the $Si_{0.74}Ge_{0.26}$/Si structure is made by the high-intensity PL line at the wavelength of 1550 nm. The observed line (the D1 line) belongs to the well-known set of lines D1–D4 related to dislocations [5–8]. The positions of the D lines in the PL spectra depend on the germanium content in the layer of the $Si_{1-x}Ge_x$ solid solution and shift to lower energies as the Ge content is increased [9]. The position of the line D1 in the PL spectrum of the $Si_{0.74}Ge_{0.26}$/Si structure under consideration is shifted relative to the spectral position of the line D1 in silicon [4] by ~7 meV and correlates with the parameters of the heterolayer under study. The PL excitation spectrum shown in Fig. 4 and obtained for the line D1 (spectrum *3* in Fig. 4) is substantially different from the excitation spectrum of the erbium-related PL component (spectrum *2* in Fig. 4). The positions of the peaks in the PL excitation spectra for both the PL D1 and P lines (spectrum *4* in Fig. 4) are shifted (with respect to the peak observed in the excitation spectra of the erbium-related component) to higher energies. The PL signal associated with the defect–impurity and dislocation-related components for the $Si_{0.69}Ge_{0.31}$:Er/Si and $Si_{0.74}Ge_{0.26}$/Si structures is not observed at the energies of the photon of the excitation radiation lower than the energy corresponding to the band gap of the $Si_{1-x}Ge_x$ solid solution. The observed special features in the spectra of excitation of the short-time PL components at the wavelength of 1.54 μm and correlation of these features with the excitation spectra for the known PL lines of the defect–impurity and dislocation nature and also the spectral position and time-related characteristics evidently testify in favor of the above assumption concerning the defect-related short-time response in relaxed $Si_{1-x}Ge_x$:Er/Si relaxed structures. However, as was already mentioned above, the contribution of these components is much smaller than the luminescence response related to the rare-earth impurity.

Let us consider specific features observed in the excitation spectra of the PL signal related to the rare-earth impurity. The results of studying the excitation spectra of the erbium-related PL in the $Si_{1-x}Ge_x$:Er/Si epitaxial structures with the Ge content in the range from 10 to 31% are shown in Fig. 5. Arrows there indicate the position of the band gap for the $Si_{1-x}Ge_x$:Er heterolayers with corresponding values of *x*. The variation in the germanium content in the range 10–31% corresponds to variation in the band gap of the heterolayer from 1.13 eV ($x = 10\%$) to 1.04 eV ($x = 31\%$). It is of interest that, in all studied $Si_{1-x}Ge_x$:Er/Si structures with $x = 10$–31%, an appreciable signal corresponding to the erbium-related PL is observed both under conditions of interband excitation and in the case where the energy of photon in the excitation radiation is significantly lower than the band gap of the $Si_{1-x}Ge_x$ solid solution. In the wavelength range 1040–1050 nm, a peak is observed in the excitation spectra of erbium-related PL of the $Si_{1-x}Ge_x$:Er/Si structures. A similar peak in the excitation spectra of erbium-related PL was observed at the wavelength ~1040 nm for the Si:Er/Si structures [10–12]. As the band gap of the $Si_{1-x}Ge_x$ solid solution and the value of RES are decreased, the width of the maximum in the excitation spectra of the erbium-related PL for the $Si_{1-x}Ge_x$:Er/Si structures changes. As the band gap of the $Si_{1-x}Ge_x$ solid solution is varied from 1.13 eV ($x = 10\%$) to 1.04 eV ($x = 31\%$), the width of the maximum in the excitation spectra of erbium-related PL at the level 0.5 of its height increases from 85 to 142 meV. As structural parameters of the $Si_{1-x}Ge_x$ heterolayers is changed, the degree of their approach to structural perfection also changes. The largest (in the set of studied structures) width of the maximum in the wavelength range 1040–1050 nm in the excitation spectra of the erbium-related PL is observed in structures with practically complete relaxation of elastic stresses. The

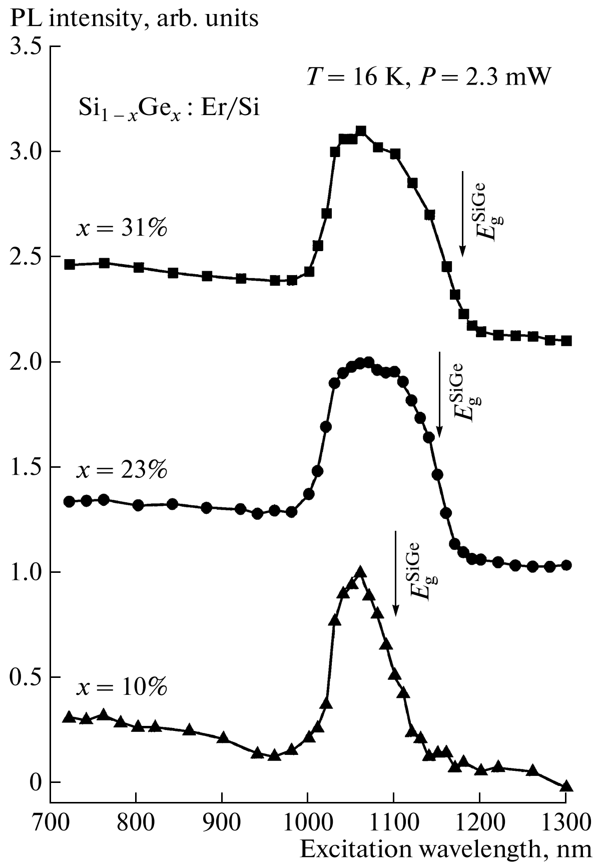

Fig. 5. The excitation spectra for the erbium-related PL in the $Si_{1-x}Ge_x$:Er/Si structures with the germanium content varied in the range from 10 to 31%. Arrows indicate positions of the band gap for the $Si_{1-x}Ge_x$:Er heterolayers. In calculations of the band gap, the content of germanium in the heterolayer, the degree of relaxation, and temperature (T = 16 K) at which measurements were performed were taken into account.

occurrence of the signal of erbium-related luminescence in the case of excitation with photons with energies lower than the band gap of the $Si_{1-x}Ge_x$ solid solution and an increase in the width of the maximum observed in the excitation spectra of the erbium-related PL can be attributed (similarly to [10]) to the existence of impurity–defect complexes (related, in particular, to implantation of erbium ions) or defect-related levels in the band gap of the semiconductor and their involvement in the process of excitation. In this case, absorption of photons with an energy $h\nu_{ex} < E_g$ can bring about excitation of electrons from the valence band directly to energy levels in the band gap and subsequent nonradiative recombination of these electrons with energy transfer to Er^{3+} ions. This hypothesis is supported by the above-described interrelation between the width of the maximum observed in the excitation spectra of the erbium-related PL and the degree of relaxation of elastic stresses in the $Si_{1-x}Ge_x$:Er/Si heterostructures. In this context, it is still unclear why the region of drastic increase in the intensity of the erbium-related photoluminescence in the Si:Er/Si structure in the range of wavelengths of excitation radiation 1000–1050 nm (corresponding to the approach to the edge of the band gap in silicon) coincide with that in a $Si_{1-x}Ge_x$:Er/Si structure. Evidently, this issue requires additional detailed studies.

4. CONCLUSIONS

This, in this study, we investigated luminescent properties of the $Si_{1-x}Ge_x$/Si and $Si_{1-x}Ge_x$:Er/Si heteroepitaxial structures with the range of residual strains from 82 to 4%. The results of combined studies of the kinetics and excitation spectra of photoluminescence (PL) are used to single out the components that make the dominant contribution to the luminescence signal in the $Si_{1-x}Ge_x$:Er/Si structures in the region of the wavelength 1.54 μm. We revealed the components related to the rare-earth impurity, to defects, and to the defect–impurity complexes, which exist in the relaxed $Si_{1-x}Ge_x$ and $Si_{1-x}Ge_x$:Er layers. It is shown that, in the $Si_{1-x}Ge_x$:Er/Si structures with a high degree of relaxation (RES ≈ 6–9%) and the layer thickness on the order or larger than 1 μm, the PL components related to the presence of defects and defect–impurity complexes make only an insignificant contribution to the PL signal.

The results of the performed studies show that, in the $Si_{1-x}Ge_x$:Er/Si structures, an appreciable signal of the erbium-related PL is observed both in the case of the interband excitation and in the case in which the energies of the photon of the excitation radiation are much lower than the band gap of the $Si_{1-x}Ge_x$ solid solution. A maximum in the wavelength range of 1040–1050 nm is observed in the excitation spectra of the erbium-related PL for the $Si_{1-x}Ge_x$:Er/Si; the width of this maximum increases as the band gap of $Si_{1-x}Ge_x$ decreases and as the degree of heterolayer relaxation increases. The observed specific features of excitation spectra for the erbium-related PL are supposedly related to the involvement of intermediate levels in semiconductor's band gap in the excitation processes of the Er^{3+} ion.

ACKNOWLEDGMENTS

We thank B.Ya. Ber for SIMS studies of the structures.

This study was supported by the specific program "Scientific and Scientific–Pedagogical Brainpower in Innovative Russia" for 2009–2013.

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Translated by A. Spitsyn