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Photoluminescence of strained germanium microbridges at various temperatures: experiment and modeling

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The results of the experimental study and theoretical simulation of the photoluminescence (PL) spectra of strained germanium microbridges with improved heat sink are reported. It was shown that in the structures under study the main contribution to the PL signal of micro-bridges is provided by the radiative transitions from Γ-valley to the valence band in the whole considered temperature range (from 80 to 300 K). The influence of interference and self-absorption effects on the shape of the PL spectra of Ge microbridges is discussed. It was demonstrated that Ge microbridges with improved heat sink which was achieved due to the adhesion of the bridges to the underlying layers due to capillary forces are not subjected to the additional stretching as the temperature decreases in contrast to the suspended ones.

Keywords: SiGe structures, tensile strained Ge, photoluminescence, simulation of the photoluminescence spectra.

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1. Introduction

An important task of modern optoelectronics is to create an affordable effective source of near-infrared radiation on silicon. One of the solutions to this problem is the use of deformed, stretched, Ge as an active medium. The bulk Ge, which is a non-direct bandgap material, is nevertheless characterized by a small (140 meV at 300 K) energy difference between the values of the width of the direct and indirect bandgap zones [1]. The application of tensile deformation allows you to reduce the energy gap between the direct and indirect zone in Ge down to zero and turn Ge into a straight-band material. According to various estimates given in the literature, Ge becomes straight-band when applying biaxial deformation at the level of $\sim 1.5-2\%$ or uniaxial deformation at the level of $\sim 4.7-6\%$ [2,3]. Achieving such strain values in continuous Ge layers is possible with epitaxial growth on „virtual substrates" with a large lattice parameter, for example, based on buffer layers InGaAs or GeSn [4,5]. However, this approach has a number of disadvantages related both to the complexity of obtaining „virtual substrates" of high crystal quality, and to the limitation on the thickness of defect-free formation of layers of stretched Ge, which is determined by the critical thickness of pseudomorphic growth (units nm). At the same time, the formation of a strongly stretched Ge can be ensured in the local regions of the initial Ge film grown on silicon (in which the initial small biaxial stretching to $\sim 0.3\%$ is formed due to the difference in the thermal expansion coefficients of Ge and Si) — locally deformed Ge structures of various geometries — due to the use of the so-called „stress concentration method" [6]. Earlier it was reported about the observation of stimulated radiation near 1.5 microns at low temperatures under optical pumping in locally deformed Ge structures of geometry „the microbridge" with uniaxial stretching $\sim 1-2\%$ [7] obtained by this method. At the same time, it was clarified that the observation of stimulated radiation at higher temperatures requires higher deformation values in the bridges [7]. Another group reported [8] on the observation of stimulated radiation in the vicinity of 3 microns in the strongly stretched Ge microbridges (stretching $\sim 5.4-5.9\%$). High values of tensile strain were achieved both due to the geometry of the bridges and due to their cooling to low temperatures. The effect of a significant increase in the stretching of the Ge film with a decrease in temperature is also observed in locally deformed Ge structures with biaxial stretching [9]. The increase in the tensile strain in the Ge microstructures obtained by the stress concentration method with a decrease in temperature is caused by an increase and further redistribution of the tensile strain in the Ge film grown on silicon, the occurrence of which is due to the difference in the coefficients of thermal expansion Ge and Si.

It should be noted that the difficulties of observing stimulated radiation in the locally stretched Ge microbridges are largely related to the problem of heat dissipation, which can be solved by adhesion of the locally stretched region to the underlying layers of the substrate [10]. However, the use of this approach may have an impact on the properties of such Ge microbridges and, in particular, on the dependence of their stretching value on temperature. Since the magnitude of the Ge microbridge deformation directly affects the band structure of the material, the analysis of luminescence spectra can help in finding an answer to this question. Earlier in the literature, the photoluminescence (PL) spectra were modeled for structures representing Ge strips [11], and in this type of structures, the amount of deformation did not depend on temperature. As in the case of Ge strips, when modeling the spectra of the Ge microbridges, it is necessary to take into account both the splitting of the subzones of light and heavy holes in the valence band due to elastic stresses [2,3] and the effects of self-absorption in Ge [11,12]. In addition, interference effects can be observed in this type of structures, associated both with the presence of layers with different refractive index and with the geometric parameters of the bridge.

The present work is devoted to modeling the PL spectra of the locally deformed Ge microbridges, taking into account all of the above effects, as well as identifying the effect of temperature on the amount of deformation of micro-bridges in which contact with the underlying layers of the substrate was realized due to adhesion, designed to improve heat dissipation.

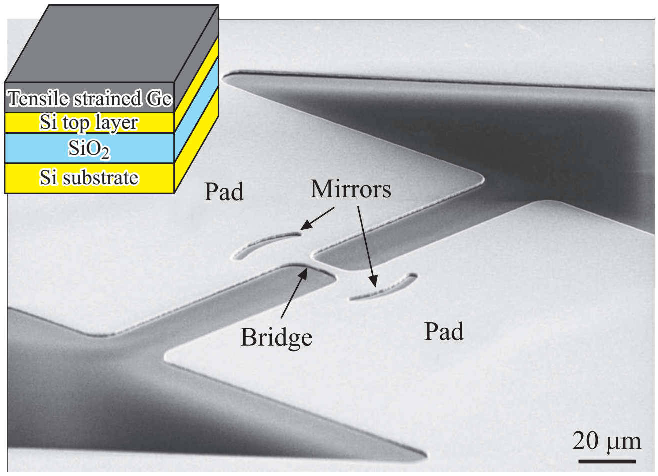

Figure 1. An image from a scanning electron microscope (SEM) of the Ge microbridge under study. The insert shows a schematic representation of the original structure for clarity.

2. Experiment procedure

The initial Ge layers were grown on „silicon−substrates on a−insulator" (SOI) by molecular beam epitaxy. To reduce the density of defects in Ge/SOI layers, the „method of two-temperature growth" with subsequent cyclic annealing in a vacuum chamber [13–15] was used. Further, the *n*-Ge layers 300 nm thick, doped with Sb at the level of $3 \cdot 10^{19}\,\text{cm}^{-3}$ were grown on Ge/SOI buffer layers. As was shown earlier by [1,16–19], this doping level is optimal for achieving at room temperature the maximum intensity of the luminescence signal associated with direct radiative transitions in Ge. When doping Ge with antimony, the method previously developed by the authors, described in [20], was used. According to X-ray diffraction analysis, in the grown Ge films, due to the difference in the coefficients of thermal expansion of Ge and Si, tensile deformation was achieved at the level of 0.2−0.25%.

The creation of locally deformed Ge microstructures in the geometry of the „microbridge" type was carried out using laser maskless lithography, plasma chemical and „wet" selective etching. To increase the intensity of the luminescence signal, bridges were built between fragments of a spherical mirror formed by annular sectors with smoothed corners (see Fig. 1). Such a geometry makes it possible to achieve an increase in the PL signal intensity from the Ge microbridges by providing an optical restriction in the direction along the bridge (in the other two directions it is created due to the limited geometric dimensions of the bridge), i.e., the formation of a microresonator [21]. The improvement of heat removal from the investigated Ge microbridges was carried out due to the adhesion of the active region of the structure to the underlying layers of the substrate due to the action of capillary forces [10]. As it was shown earlier, this approach makes it possible to increase the maximum power of optical pumping (which does not lead to irreversible changes in the microbridges) of the studied structures in ~ 4 times [10]. The process of formation of the investigated Ge microbridges is described in detail in works [10,21]. In contrast to the previous work of the authors [21], in this work, micro-bridges with low (up to 2%) stretching values were created due to resizing, which made it possible to analyze the entire luminescence signal from the microbridges using a multi-channel detector OMA-V based on a ruler InGaAs photodiodes (wavelength range 0.8−2.1 microns (0.6−1.55 eV)).

Experimental studies of the obtained Ge microstructures were carried out using scanning electron microscopy (SEM), white light interferometry, spectroscopy of Raman scattering (micro-Raman) and micro-photoluminescence spectroscopy (micro-PL). In the study of micro-PL spectra, pulsed radiation of an Nd:YAG laser at a wavelength of 532 nm (repetition frequency — 80 MHz, pulse duration ~ 10 ps) was used to excite the signal. The focusing of the laser beam and the collection of radiation from the surface of the studied structures were carried out using the Mitutoyo Plan Apo NIR 50x lens, which provides the size of the excitation spot on the sample ~ 3 microns. The micro-PL spectra were recorded using an Acton 2300i lattice monochromator and a multichannel detector OMA-V based on a line of InGaAs photodiodes (wavelength range 0.8−2.1 microns). The measurements were carried out at temperatures from 80 to 300 K, for which the sample was placed in a specialized flow cryostat for studies in the micro-PL mode.

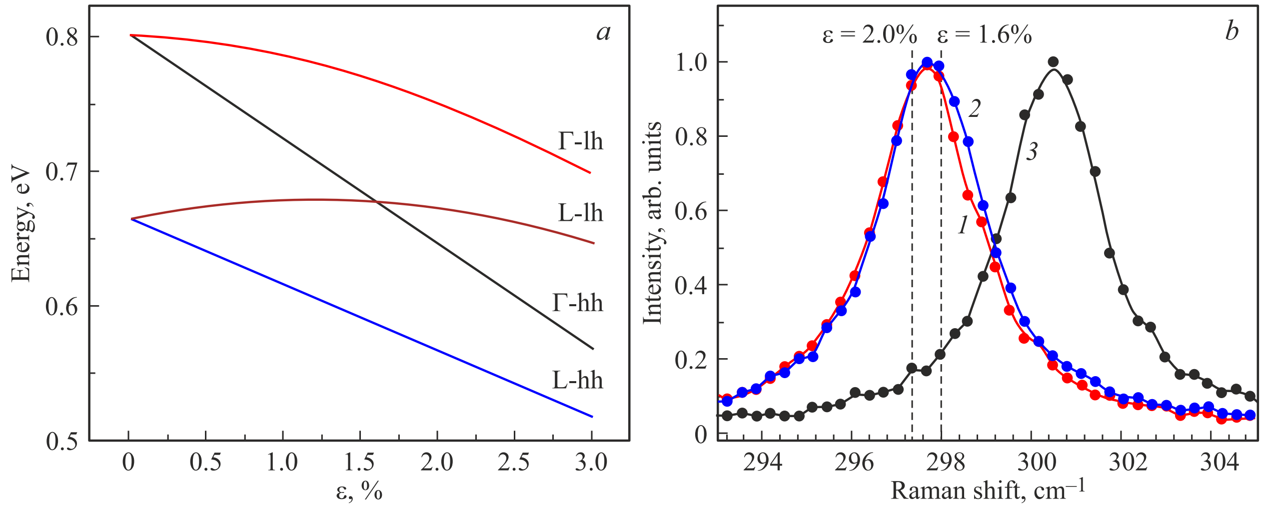

Figure 2. *a* — dependences of transition energies from Γ- and L-valleys to subzones of light (lh) and heavy (hh) holes in Ge depends on the value of uniaxial tension; *b* — LO-phonon lines in the micro-Raman spectrum, taken at the center of the microbridge (*1*), at a distance of 2 microns from the center of the microbridge (*2*) and the peak from the volumetric Ge (*3*). Vertical dotted lines mark the boundaries of the measurement error of micro-Raman and the corresponding boundary values of deformation.

3. Results and discussion

In this work, the PL spectra of the stressed Ge microbridges with a length of 5 microns were studied. As noted above, when stretching germanium, a modification of its band structure is observed — the distance between the minima of Γ- and L-valleys in the conduction band decreases, while the energies of both valleys decrease. In addition, the splitting of the subzones of light and heavy holes also occurs in the valence band. Fig. 2, *a* shows the dependences of the transition energies from Γ- and L-valleys of the conduction band to various subzones in the valence band, calculated using kp-method. We note that the calculations performed give a good agreement with the results of calculations from the literature [2,22]. Due to the splitting of the subzones of light and heavy holes in the valence band during stretching, several components corresponding to different radiative transitions can be observed in the PL signal from deformed micro-bridges from Γ- and L-valleys to these subzones.

The deformation amount in the microbridges was determined using micro-Raman by the displacement of the LO-phonon line in Ge relative to its position in the undeformed Ge [10]. Fig. 2, *b* shows lines of LO-phonons in micro-Raman spectra taken at the center of the microbridge and at a distance of 2 microns from the center of the bridge, which characterize the Ge deformation inside the excitation spot during the study of micro-PL, as well as the LO-phonon line volumetric Ge. The level of uniaxial deformation in the microbridge is determined from the shift of the LO-phonon line by the formula $\varepsilon = 0.68\Delta\omega - 0.019\Delta\omega^2$ [23] and lies in the range of 1.6–2.0%, considering the recording error the Raman spectrum (vertical lines on Fig. 2, *b*). We note that the deformation of the part of the bridge investigated by the micro-PL method (inside the spot with a diameter of $\sim$ 3 microns) can be considered homogeneous.

Fig. 3 shows the micro-PL spectrum of a microbridge with a length of 5 microns at room temperature (curve *1*). The PL signal of the Ge microbridge is shifted to a region of lower energies relative to the PL signal of the unprocessed region of the structure (curve *2*) corresponding to the radiative transitions from the Γ-valley to the valence band in the weakly stressed initial Ge/SOI film [24]. This displacement is explained by a decrease in the energy of the Γ-valley with an increase in deformation.

As can be seen, the spectrum of the Ge microbridge has a rather complex shape, which is associated both with the presence of components corresponding to radiative transitions into the subzones of light and heavy holes, and with the contribution of interference effects. In particular, modulation in the high-energy part of the spectrum (750–850 meV) corresponds to interference across the Ge bridge with a width of 3 microns.

In order to confidently link the signals observed in the micro-PL spectrum with radiative transitions in the stretched Ge, theoretical modeling of the spectra was carried out, while the elastic stress value $\sim$ 1.8% was taken, corresponding to the position of the maximum point of the line LO-phonon in the micro-Raman spectrum the bridge under study (Fig. 2, *b*). The zone structure of the uniaxially deformed Ge microbridges was calculated in the kp-approx dimension (Hamiltonian 8×8). The values of the band gap width and the values of matrix elements were taken from the work [25], the value of spin-orbital splitting, the Luttinger coefficients and the values of the deformation modules — from the work [26], deformation potentials for electrons — from [27]. The position of the Fermi quasi-levels necessary for modeling the PL spectra was determined taking into account the level of doping of structures ($\sim 3 \cdot 10^{19}\,\mathrm{cm}^{-3}$) and the level of optical pumping. For more information about the modeling of the PL spectra of Ge-doped structures (with a relatively small deformation), see the study [28].

When determining the position of quasi-Fermi levels in the structure, the density of holes as non-basic charge carriers was determined by the level of optical pumping. At the same time, since at the doping level used by donors ($3 \cdot 10^{19}\,\mathrm{cm}^{-3}$), a complete electrical activation of the impurity [18] is observed, the electron density value was chosen by $3 \cdot 10^{19}\,\mathrm{cm}^{-3}$ is greater than the density of photogenerated electron-hole pairs.

With the optical excitation parameters used (wavelength — 532 nm, repetition rate — 80 MHz, average excitation power — 10 MW, spot diameter ~ 3 microns, radiation penetration depth into the structure ~ 20 nm) and without taking into account surface recombination and other non-radiative processes, the concentration of charge carriers generated during the pulse at the depth of excitation penetration can be estimated as $\sim 10^{21}\,\mathrm{cm}^{-3}$. At the same time at the density of charge carriers $\sim 10^{20}-10^{21}\,\mathrm{cm}^{-3}$ the electron diffusion length at room temperature, estimated taking into account the table values of mobility [29] and experimentally determined lifetimes of charge carriers in doped Ge [30], is 200−250 nm, i.e., exceeds the depth of radiation penetration into the structure by an order of magnitude and, consequently, proportionally reduces the density of photoexcited charge carriers. Considering this fact and adjusted for unaccounted non-radiative processes when modeling the spectra of PL Ge microbridges, the density of holes in the structure was taken to be $5 \cdot 10^{19}\,\mathrm{cm}^{-3}$, and the electron density — $8 \cdot 10^{19}\,\mathrm{cm}^{-3}$.

The calculated PL spectrum obtained for the deformation value 1.8% and concentrations of photoexcited charge carriers $5 \cdot 10^{19}\,\mathrm{cm}^{-3}$, is shown in Fig. 3 (curve *3*). Two peaks in the simulated PL spectrum correspond to radiative transitions into the subzones of light and heavy holes. A comparison of the experimental and calculated spectra (curves *1* and *3* in Fig. 3) shows a noticeable discrepancy both in the position and in the shape of the lines. The observed discrepancy in the position of the experimental and calculated PL spectra is explained by the fact that the modeling did not take into account the effect of the doping level on the position of energy zones in Ge, the so-called „bandgap narrowing“ (BGN) effect — effect of Ge band gap renormalization at high doping levels [28,31,32]. As it was shown earlier [28], at the levels of germanium doping with antimony ($3 \cdot 10^{19}\,\mathrm{cm}^{-3}$), the width of the Ge direct band gap decreases by ~ 30 meV by compared to unalloyed Ge. Taking into account the BGN effect makes it possible to achieve a good agreement of the spectral position of the experimental and calculated spectra (curves *1* and *4* in Fig. 3). The insert to Fig. 3 shows the calculated spectra shifted by the value of BGN, obtained for the boundaries of the range of error in determining the deformation — 1.6 and 2.0%. Good fit is observed for the entire range of errors. Comparing the theoretical and experimental spectra, it can be argued that the two components in the PL spectrum correspond to transitions into the subzones of light and heavy holes.

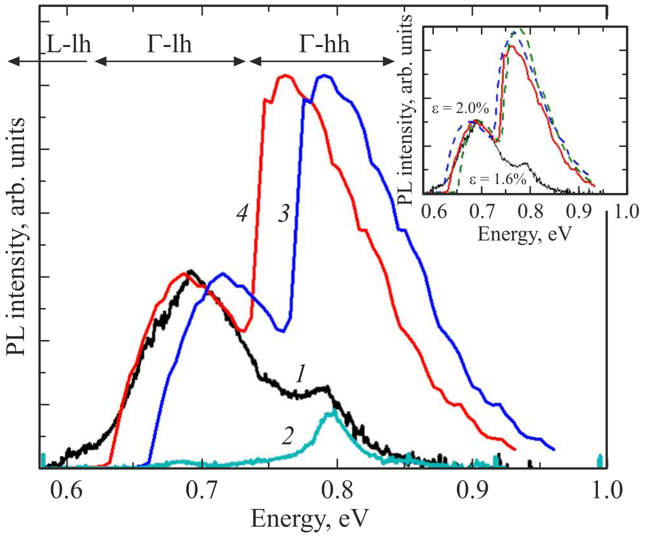

Figure 3. PL spectra of the Ge microbridge 5 microns long (*1*) and the unprocessed region of the structure (*2*) at room temperature, PL spectra obtained as a result of calculations without considering the bandgap narrowing effect (BGN) (*3*) and taking into account the effect of BGN (*4*) for the amount of deformation in the bridge 1.8%. The insert shows the calculated spectra, taking into account the BGN effect, obtained for the amount of deformation in the bridge 1.8%, as well as at the limits of the error range for determining deformation from the Raman spectra — 1.6 and 2.0%.

Nevertheless, even for the calculated spectra taking into account the BGN effect, there is a noticeable discrepancy in the ratio of the intensities of the high- and low-energy parts of the spectrum. In part, this discrepancy may be due to the so-called self-absorption effect in Ge — interband absorption of the PL signal near the direct zone [11,12]. Fig. 4, *a* shows the spectra calculated taking into account (curve *2*) and without taking into account (curve *3*) the self-absorption effect, for deformation 1.8% and taking into account the effect of BGN. Taking into account the effect of self-absorption makes it possible to achieve a qualitative correspondence in the ratio of the intensities of high- and low-energy parts in the experimental and calculated spectra. The remaining differences may be related to the following factors. To assess the effect of self-absorption in Ge layers, only the absorption during the propagation of radiation vertically inside the bridge with its reflection from the lower boundary of the stressed Ge layer in contact with the layer SiO_2 was considered. However, in the studied structures, self-absorption can also occur when radiation propagates along the bridge between the resonator mirrors, and in this case we are talking about absorption in a layer with variable magnitude and type of deformation (uniaxial deformation in the bridge and biaxial — in plates). It should

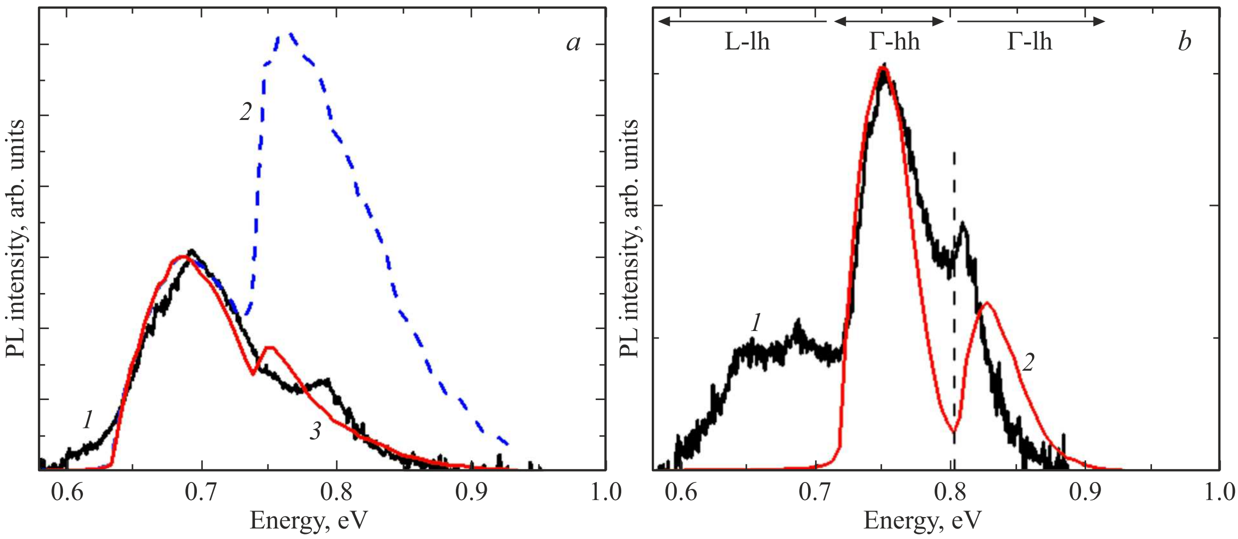

Figure 4. *a* — the PL spectrum of the Ge micro bridge measured at room temperature (*1*), and the calculated PL spectra without considering (*2*) and taking into account (*3*) the effect of self-absorption in Ge at the level of deformation 1.8% (with considering the BGN effect). *b* — the PL spectrum of the Ge microbridge, measured at a temperature of 80 K (*1*), and the calculated PL spectrum for a temperature of 80 K (*2*) at deformations 1.8% taking into account the effects of BGN and self-absorption in Ge.

also be noted that the intensity of the PL signal in the high-energy part of the simulated spectrum is determined by the density of photoexcited charge carriers in the structure, for which a rather rough estimate was made in our case. At the same time, as noted above, interference effects resulting from the reflection of radiation both from the side walls of the bridge and from the lower layer SiO_2 contribute to the appearance of the PL spectrum of the Ge microbridges. The combination of these factors leads to the complexity of modeling the PL spectra of the Ge microbridges, especially in the high-energy region, however, the approach used allows us to qualitatively simulate the PL spectrum of the Ge microbridges and confirm the connection of the observed signals with radiative transitions from the Γ-valley to the subzones of light and heavy holes. A more „smooth" increase in the intensity of the PL signal at the low-energy edge of the experimental spectrum in comparison with the calculated one is explained by the presence of impurity states in Ge, the existence of which was not taken into account during modeling. In addition, a weak signal associated with radiative transitions from the L-valley is also observed in the low-energy (near 0.6 eV) part of the PL spectrum of the Ge microbridges, part of which is outside the sensitivity range of the receiver.

As noted above, earlier in the literature, the effect of increasing the stretching of the free-hanging Ge bridges during cooling (with a decrease in the measurement temperature from 300 K to the cryogenic temperature region) was described [8] due to the difference in the coefficients of thermal expansion of Ge and Si is similar to cooling from growth/annealing temperatures to room temperature during the formation of the structure. Since the redistribution of elastic stresses occurs during the microbridges creation in the Ge film (and their increase in the narrowing area of the bridge), when cooling free-hanging structures, this process of stress redistribution is also possible [8]. However, unlike the work of [8], the present work investigated structures in which, after all the stages of their formation, there was a mechanical contact between the Ge bridge and the underlying layers of the substrate. This circumstance may prevent further redistribution of elastic stresses in an already formed structure, as it happens in structures that are stretched Ge strips [11].

In order to check the presence of the effect of additional stretching of the microbridges during cooling in structures in which adhesion of locally stretched regions to the lower layers of the substrate was implemented to improve heat dissipation during the microbridges formation, their micro-PL spectra were studied in the temperature range 80−300 K. Fig. 4, *b* shows the PL spectrum of the microbridge at a temperature of 80 K (curve *1*). The decrease in temperature is accompanied by a shift of the PL signal of the Ge bridges to the region of higher energies caused by a temperature change in the width of the Ge band gap, as well as a decrease in the intensity of the PL signal by ~ 2 times, which is explained by a decrease in the population of the Γ-valley. Another significant difference between the low-temperature spectrum and the spectrum obtained at room temperature is the observation of a sufficiently intense signal in the range of 0.6−0.7 eV, which may be associated with radiative transitions from the L-valley. The increase in the contribution of indirect transitions to the overall PL signal with a decrease in temperature is explained by a decrease in the relative population of higher-energy states and an increase in the lifetime of carriers in the structure, contributing to an increase in the probability of slow processes corresponding to indirect transitions. The small modulation observed in this range may be related to the interference of radiation across the Ge bridge with a width of 3 microns. A similar modulation was noticeable in the range of 750−850 meV (Fig. 3 and 4, *a*) in the spectra recorded at room temperature.

For a temperature of 80 K, a theoretical simulation of the PL spectrum was also carried out: the curve *2* in Fig. 4, *b* corresponds to the calculated spectrum obtained for the deformation value 1.8%, taking into account the effects of BGN and self-absorption in Ge. It can be seen that for low temperature, the calculated and experimental spectra show good fit in terms of the spectral position of the edge of the signals associated with radiative transitions into the subzones of light and heavy holes. The mismatch of the spectra in the high-energy part, as well as in the case of an experiment at room temperature, may be due to the more complex nature of self-absorption, as well as to the influence of interference processes that occur when radiation passes across the bridge and through the bridge vertically with reflection from the lower layer SiO_2.

A similar simulation of the spectra was carried out at other temperatures (160 and 220 K). In almost all cases, taking into account the BGN effect, a good agreement of the position of the PL signals associated with the transition to the subzones of light and heavy holes was observed in the experimental and calculated spectra obtained at the same strain value at all temperatures. The temperature measurements and modeling of the spectra allow us to state with confidence that in structures with the Ge bridges, in which adhesion of locally stretched regions to the lower layers of the substrate was realized during their formation in order to improve heat dissipation, there is no significant increase in the magnitude of their stretching during cooling, which is associated with the absence of stress redistribution in the Ge film from-due to the mechanical contact of the bridges and the substrate. This fact should be taken into account in the future when carrying out work to achieve stimulated radiation in structures with the Ge bridges.

4. Conclusion

As a result of the study of the luminescent properties and modeling of the PL spectra of the locally stretched Ge microbridges formed on SOI substrates with adhesion to the underlying layers, it is demonstrated that in the studied structures in the entire temperature range considered (from 80 to 300 K), the main contribution to the signal of the PL microbridges is made by a signal associated with radiative transitions from the Γ-valley to the valence band. A good correspondence between the simulated and experimental PL spectra at different temperatures was obtained. It has been demonstrated that the presence of a mechanical contact between the Ge microbridge and the underlying layers of the substrate, implemented to improve heat dissipation, prevents further redistribution of elastic stresses in the structure, and this type of Ge microbridges does not undergo noticeable additional deformation during cooling.

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Conflict of interest

The authors declare that they have no conflict of interest.

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