Photoluminescence of dome and hut shaped Ge(Si) self-assembled islands embedded in a tensile-strained Si layer

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The effect of the growth temperature (T_g) on photoluminescence of Ge(Si) self-assembled islands embedded between tensile-strained Si layers was studied. The observed redshift of the photoluminescence peak of the dome islands with a decrease of T_g from 700 to 630 °C is associated with an increase of Ge content in the islands and with the suppression of smearing of the strained Si layers. The blueshift of the photoluminescence peak with a decrease of T_g from 630 to 600 °C is associated with a change of the type of islands on surface, which is accompanied by a decrease in islands' height. © *2007 American Institute of Physics*. [DOI: 10.1063/1.2756291]

Confinement of charge carriers in low-dimensional Ge/Si heterostructures allows one to increase the efficiency of the radiative recombination and to decrease the temperature quenching of the luminescence signal in Si-based structures. However, in Ge/Si structures grown on Si(001) substrates, the overwhelming part of the band gap offset falls at valence band[1] which allows only holes to be effectively localized in such structures. Three-dimensional localization can be realized in the structures with Ge(Si) self-assembled islands grown on Si(001) substrates (further referred to as Ge(Si)/Si islands). Owing to the type II band alignment, electrons in the structures with Ge(Si)/Si islands can only weakly be confined in Si on the heterojunctions with islands.[2] It has been shown recently[3] that effective confinement of charge carriers of both types can be realized in the new type of Si/Ge heterostructures—Ge(Si) self-assembled islands grown on relaxed SiGe/Si(001) buffer layers and embedded between thin strained Si (ϵ-Si) layers (further referred to as Ge(Si)/ϵ-Si islands). The observed photoluminescence (PL) signal from Ge(Si)/ϵ-Si islands is associated with radiative recombination of holes confined in the Ge(Si) islands and electrons localized in ϵ-Si layers under and above the islands [Fig. 1(a)].[3,4] Effective confinement of electrons in the thin ϵ-Si layers on the heterojunction with an island results in an intensity increase of the PL signal from the islands in the wavelength range of 1.55–2 μm.[3,4] Confinement of electrons in the thin ϵ-Si layers leads to a rise of uncertainty of their coordinates in the k space and, as a result, increases the probability of radiative recombination of charge carriers without phonon assistance. The smaller width of the PL peak from Ge(Si)/ϵ-Si islands compared to the one from Ge(Si)/Si islands can be explained by the prevalence of the nonphonon peak over the phonon-assisted peak in the PL signal from Ge(Si)/ϵ-Si islands.[4]

In our previous work, we have studied the position and width of the PL peak from Ge(Si)/ϵ-Si islands grown at the fixed temperature (650 °C) as a function of the width of the ϵ-Si layers under and above the islands.[3–5] However, it is well known that the size, composition, and shape of Ge(Si)/Si (Refs. 6 and 7) and Ge(Si)/ϵ-Si islands[8] strongly depend on the growth temperature (T_g). For Ge(Si)/Si islands, it was shown that the dependence of the island parameters on T_g essentially affects the position and width of the island-related PL peak.[9–11] In this work, we therefore report on the effect of the growth temperature on the PL from Ge(Si)/ϵ-Si islands.

A series of structures with Ge(Si)/ϵ-Si islands was grown at different T_g in the range from 600 to 700 °C. The structures were grown by molecular-beam epitaxy on $Si_{1-x}Ge_x$/Si(001) (x=20%–30%) relaxed buffer layers with low surface roughness.[12,13] The growth technology of such structures with Ge(Si)/ϵ-Si islands was described elsewhere.[8] All the structures consisted of an unstrained SiGe buffer layer and a thin (2 nm) ϵ-Si layer on which Ge(Si) islands were formed by Ge deposition with equivalent thickness of d_{Ge}=9–12 ML (1 ML ≈0.136 nm). The structures designed for the PL studies had an additional ϵ-Si layer above the islands with the same (2 nm) thickness as the one under the islands and an additional unstrained SiGe cap layer. The sample morphology was studied by an atomic force microscopy (AFM) in the tapping mode ("Solver PRO," NT-MDT, Russia). The PL spectra were measured at 77 K using a Fourier-spectrometer BOMEM DA3.36 and nitrogen-cooled Ge and InSb detectors. The optical pumping was performed by radiation of an ultraviolet HeCd laser (λ =325 nm, P=2.5 mW). The penetration length of this radia-

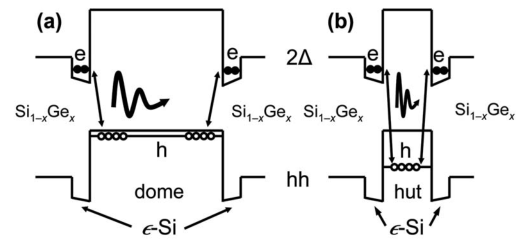

FIG. 1. Schematic band alignment in the structures with Ge(Si)/ϵ-Si (a) dome and (b) hut islands. Positions of the 2Δ electron valleys and the heavy hole bands are shown.

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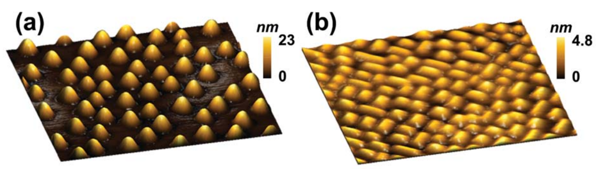

FIG. 2. (Color online) AFM images of the structures with Ge(Si)/ϵ-Si (a) dome islands grown at 660 °C (image size of 1×1 μm^2) and (b) hut islands grown at 600 °C (image size of 500×500 nm^2). The color scale in the images corresponds to the local surface height. Take note of the large difference in z scale of the AFM images.

tion in Si-based structures is as small as ~10 nm. This allowed to generate charge carriers in a thin surface layer of the structures only and to avoid a dislocation-related PL signal from the defect region of the SiGe relaxed buffer.[3,14]

The earlier AFM studies of the growth of Ge(Si) islands on ϵ-Si layers have shown that the dome shaped Ge(Si)/ϵ-Si islands prevail on the surface at T_g in the range of 630–700 °C and d_{Ge}=10–12 ML [Fig. 2(a)].[3,8] The surface density of the islands increases and their size decreases with a decrease of T_g. At the same time, the average Ge content in uncapped Ge(Si)/ϵ-Si dome islands rises from ~70% to ~82% with T_g decreasing from 700 to 630 °C, as was determined by x-ray analysis relying on uniform strained layer approximation.[15,16] According to the AFM studies, a sharp change in islands' morphology occurs around T_g =600–630 °C,[8] while at $T_g \leqslant 600$ °C the hut islands with a much smaller average height than the dome islands dominate on the surface of the structures [Fig. 2(b)]. An array of hut islands was formed by deposition of an equivalent Ge amount of d_{Ge}=8–9 ML.

Similar to the Ge(Si)/Si islands, the dependence of Ge(Si)/ϵ-Si island parameters (size, shape, and composition) on T_g results in characteristic PL spectra. Figure 3 shows the PL spectra from the structures with Ge(Si)/ϵ-Si islands grown at different temperatures. It can be seen that the PL peak from the Ge(Si)/ϵ-Si islands shifts to lower energies as T_g decreases from 700 to 630 °C (Fig. 3). One of the reasons for the observed shift is that with a decrease of T_g, an increase of the Ge content in the dome islands occurs, which is due to a lower diffusion of Si atoms into the islands. The valence band offset on the heterojunction between the ϵ-Si layer and the islands increases with the Ge content in the islands, which in turn reduces the energy of the indirect in

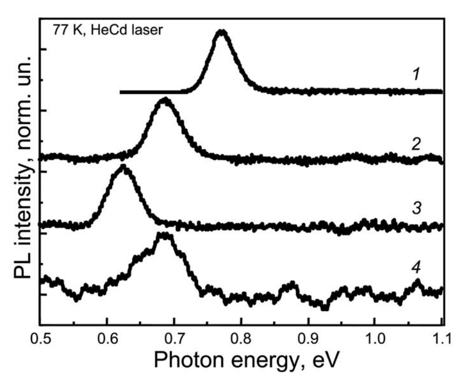

FIG. 3. PL spectra of the structures with Ge(Si)/ϵ-Si islands grown at (1) 700 °C, (2) 660 °C, (3) 630 °C, and (4) 600 °C. The PL spectra are normalized on the maximum of the signal from the islands and shifted in the vertical direction for clarity.

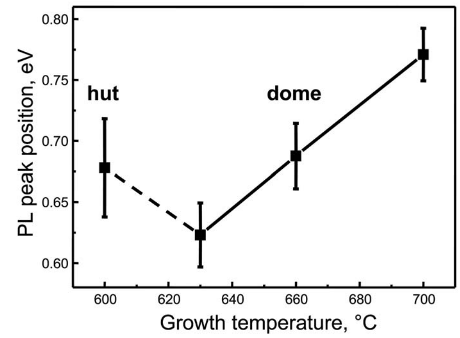

FIG. 4. Experimental dependence of the Ge(Si)/ϵ-Si island-related PL peak position on T_g. The vertical lines show the full width at half maximum of the PL peaks for each T_g. The dashed line corresponds to the transition from dome to hut islands.

real space optical transition [see Fig. 1(a)] and results in shift of the PL peak to lower energies (Fig. 3). It should be noted that the height of the Ge(Si)/ϵ-Si dome islands produced at such growth temperatures of 630–700 °C was higher than 10 nm, which allows us to neglect the effect of quantum confinement on the energy levels of holes in the dome islands. In the Ge(Si)/ϵ-Si dome islands of minimal height (grown at 630 °C) the estimated value of the size quantization energy for holes did not exceed 10 meV.

Another possible reason for the observed redshift of the PL peak is the suppression of diffusion-induced smearing of the thin ϵ-Si layers under and above the islands at lower growth temperatures. Diffusion-induced smearing dependent on T_g can cause thinning of the ϵ-Si layers, which leads to a moving of the electron energy levels in ϵ-Si layers toward the conduction band in the SiGe layers [Fig. 1(a)]. This results in the shift of the island-related PL peak to higher energies with an increase of T_g. A set of structures with larger thickness (3 nm) of the ϵ-Si layers under and above the islands was grown in the range of T_g=630–700 °C in order to determine the influence of smearing of the ϵ-Si layers on the PL peak position. The shift of the island-related PL peak toward lower energies (70–75 meV) with a decrease of T_g from 700 to 630 °C for this set of structures was about two times smaller than that for the structures with the 2 nm thick ϵ-Si layers (145–150 meV) (Fig. 4). Thus the temperature dependence of the Ge(Si)/ϵ-Si dome island-related PL peak position is less strong for the structures with thicker ϵ-Si layers. This is due to the fact that the influence of smearing of the ϵ-Si layers on the energy level of electrons is more pronounced for the thinner ϵ-Si layers.

Blueshift of the PL peak from Ge(Si)/ϵ-Si islands was observed for a decrease of T_g from 630 to 600 °C (Figs. 3 and 4). A similar blueshift of the island-related PL peak was reported earlier for structures with Ge(Si)/Si islands and with a decrease of growth temperature from 600 to 550 °C.[9] As in the case of Ge(Si)/Si islands[9] we associate the observed blueshift of the PL peak of the Ge(Si)/ϵ-Si islands with a drastic change in islands' morphology, namely, with the transition from dome to hut islands, which occurs in the interval of T_g=600–630 °C.[3,8] This transition is accompanied by a significant decrease in the average height of the Ge(Si)/ϵ-Si islands: from 15 nm for the dome islands grown at 630 °C to 2–3 nm for the hut islands grown at 600 °C (Fig. 2).[8] Because of this significant decrease in the islands' height, the quantization effects become essential in the structures with hut islands not only for the electrons in the ϵ-Si layers but also for the holes localized in the islands. As a result, the energy level of the holes in the hut islands is being pushed out toward the valence band in the ϵ-Si layers [Fig. 1(b)], which increases the energy of the indirect in real space optical transition and results in the observed blueshift of the PL peak. The discussion of the possible reasons why the dome-hut transition for Ge(Si)/ϵ-Si islands occurs at higher temperatures than for Ge(Si)/Si islands is beyond the focus of this work and can be found elsewhere.[8]

It has been observed that, just as the position, the width of the PL peak from Ge(Si)/ϵ-Si islands depends on the type of the islands: the PL peak from Ge(Si)/ϵ-Si hut islands is wider than the one from Ge(Si)/ϵ-Si dome islands (Figs. 3 and 4). The width of the PL peak from Ge(Si) islands is determined by the dispersion of many parameters of the islands, such as their size, shape, composition, and elastic strain. The additional parameter that affects the width of the PL peak from Ge(Si)/ϵ-Si islands is the thickness of the ϵ-Si layers under and above the islands. Among all of the parameters, the difference between dome and hut Ge(Si)/ϵ-Si islands falls mostly at the size and homogeneity of the islands. The structures with arrays of Ge(Si)/ϵ-Si dome islands embedded between tensile-strained silicon layers are characterized with low dispersion of the island size ($<10\%$) [Fig. 2(a)]. Besides that, as was mentioned above, the size of the dome islands weakly affects the energy level of holes in the islands. As a result, the width of the PL peak from the Ge(Si)/ϵ-Si dome islands is rather small (full width at half maximum is 45–55 meV) (Figs. 3 and 4) and may be determined by inhomogeneity of the composition[17] and elastic strain of the islands. Ge(Si)/ϵ-Si hut islands grown at 600 °C have lager size dispersion in comparison to the dome islands (Fig. 2). Taking into account the smaller average height of the hut islands, the large dispersion of the island size causes significant spreading of the hole level energies in the hut islands, which results in substantial broadening of the PL peak (up to 80 meV) from the Ge(Si)/ϵ-Si hut islands (Figs. 3 and 4).

As was mentioned above, due to localization of electrons in the thin ϵ-Si layers, the width of the PL peak from Ge(Si)/ϵ-Si dome islands at low excitation levels is considerably smaller than the width of the PL peak from Ge(Si)/Si islands.[3] As a result, the observed shift of the PL peak from Ge(Si)/ϵ-Si islands with changing T_g was larger than the width of the PL peaks (Figs. 3 and 4). The dependence of the PL peak position on T_g obtained for the Ge(Si)/ϵ-Si islands goes in line with a previously observed similar dependence for the structures with Ge(Si)/Si islands,[9] in which the width of the island-related PL peaks was comparable with the shift of the PL line due to the change of the growth temperature.

In conclusion, we have studied the growth temperature dependence of the position and width of the PL peak from Ge(Si) islands embedded in a tensile-strained Si layer. It has been shown that the redshift of the PL peak from the Ge(Si)/ϵ-Si islands observed with the growth temperature decreasing in the interval of 700–630 °C is associated with an increase of the Ge content in the dome islands and with suppression of smearing of the ϵ-Si layers under and above the islands. The revealed blueshift of the Ge(Si)/ϵ-Si island-related PL peak with a decrease of the growth temperature from 630 to 600 °C is caused by the change of the island type from dome to hut that occurs in this temperature interval and is accompanied by a significant decrease in the average height of the islands. As a result, the energy levels of holes in the hut islands are pushed out towards the valence band in the ϵ-Si layers, which increases the energy of optical transitions related with islands. The observed increase in the width of the PL peak from the Ge(Si)/ϵ-Si hut islands, as compared with the Ge(Si)/ϵ-Si dome islands, is caused by the larger size dispersion of the hut islands.

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[1] Chris G. Van de Walle and Richard M. Martin, Phys. Rev. B **34**, 5621 (1986).
[2] O. G. Schmidt, K. Eberl, and Y. Rau, Phys. Rev. B **62**, 16715 (2000).
[3] M. V. Shaleev, A. V. Novikov, A. N. Yablonskiy, Y. N. Drozdov, D. N. Lobanov, Z. F. Krasilnik, and O. A. Kuznetsov, Appl. Phys. Lett. **88**, 011914 (2006).
[4] A. V. Novikov, M. V. Shaleev, A. N. Yablonskiy, O. A. Kuznetsov, Yu. N. Drozdov, D. N. Lobanov, and Z. F. Krasilnik, Semicond. Sci. Technol. **22**, S29 (2007).
[5] M. V. Shaleev, A. V. Novikov, A. N. Yablonskiy, O. A. Kuznetsov, Yu. N. Drozdov, and Z. F. Krasilnik, Semiconductors (to be published).
[6] G. Capellini, M. De Seta, and F. Evangelisti, Appl. Phys. Lett. **78**, 303 (2001).
[7] O. G. Schmidt, C. Lange, and K. Eberl, Phys. Status Solidi B **215**, 319 (1999).
[8] N. V. Vostokov, Yu. N. Drozdov, Z. F. Krasilnik, O. A. Kuznetsov, D. N. Lobanov, A. V. Novikov, and M. V. Shaleev, Semiconductors **40**, 229 (2006).
[9] N. V. Vostokov, Z. F. Krasil'nik, D. N. Lobanov, A. V. Novikov, M. V. Shaleev, and A. N. Yablonskiy, Sov. Phys. Solid State **46**, 60 (2004).
[10] M. W. Dashiell, U. Denker, C. Müller, G. Costantini, C. Manzano, K. Kern, and O. G. Schmidt, Appl. Phys. Lett. **80**, 1279 (2002).
[11] V. Yam, Vinh Le Thanh, Y. Zheng, P. Boucaud, and D. Bouchier, Phys. Rev. B **63**, 033313 (2001).
[12] N. V. Vostokov, Yu. N. Drozdov, Z. F. Krasil'nik, O. A. Kuznetsov, A. V. Novikov, V. A. Perevoshchikov, and M. V. Shaleev, Russian Microelectronics **34**, 203 (2005).
[13] N. V. Vostokov, Yu. N. Drozdov, Z. F. Krasil'nik, O. A. Kuznetsov, A. V. Novikov, V. A. Perevoshchikov, and M. V. Shaleev, Phys. Solid State **47**, 42 (2005).
[14] N. Usami, K. Leo, and Y. Shiraki, J. Appl. Phys. **85**, 2363 (1999).
[15] N. V. Vostokov, I. V. Dolgov, Yu. N. Drozdov, Z. F. Krasil'nik, D. N. Lobanov, L. D. Moldavskaya, A. V. Novikov, V. V. Postnikov, and D. O. Filatov, J. Cryst. Growth **209**, 302 (2000).
[16] A. Hesse, J. Stangl, V. Holý, T. Roch, G. Bauer, O. G. Schmidt, U. Denker, and B. Struth, Phys. Rev. B **66**, 085321 (2002).
[17] U. Denker, A. Rastelli, M. Stoffel, J. Tersoff, G. Katsaros, G. Costantini, K. Kern, N. Y. Jin-Phillipp, D. E. Jesson, and O. G. Schmidt, Phys. Rev. Lett. **94**, 216103 (2005).