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

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We report photoluminescence (PL) studies of Ge(Si) self-assembled islands embedded into a tensile-strained Si layer grown on smooth relaxed $Si_{0.75}Ge_{0.25}/Si(001)$ buffer layers subjected to chemical-mechanical polishing. The intense PL from Ge(Si) islands embedded into a strained Si layer compared to the PL from islands grown on unstrained Si(001) is associated with efficient confinement of electrons in a strained Si layer on the heterojunction with islands. The observed dependence of the island PL peak position on thickness of strained Si layer confirms the validity of the model for real-space indirect optical transition between electrons confined in the strained Si layer, and holes localized in islands. © *2006 American Institute of Physics*.
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The interest in the $Si_{1-x}Ge_x/Si$ heterostructures is associated with their potential use for Si-based optoelectronic devices.[1] However, due to the indirect band nature in k space of Ge and Si the luminescence intensity in $Si_{1-x}Ge_x/Si$ heterostructures is rather low. One way to increase efficiency of the radiative recombination in indirect band heterostructures is through confinement of charge carriers of both signs in a small area of space. In order to realize effective two–dimensionally (2D) localizations of charge carriers of both signs, Usami *et al.* used structures with a single pair of a tensile-strained Si layer and a compressive-strained $Si_{1-x}Ge_x$ layer grown on a relaxed $Si_{1-y}Ge_y$ ($x > y$) buffer layer.[2] However, the common drawback of $Si_{1-x}Ge_x/Si$ heterostructures with QWs is that the charge carriers in QW structures are confined only in one direction and can diffuse freely to large distances in the plane of growth and, as a result, nonradiatively recombine on defects, such as dislocations, impurity centers, etc. Effective three-dimensional (3D) space confinement of holes can be realized in structures with Ge(Si)/Si(001) self-assembled islands. Due to effective hole 3D confinement a photoluminescence (PL) signal in the structures with Ge(Si) self-assembled islands was observed up to room temperature by several groups.[3–6] However, only holes are effectively localized in Ge(Si) islands, while the electrons are only weakly confined in Si on the heterojunction with an island[7] [Fig. 1(a)]. Weak confinement of electrons is one possible reason for the low PL intensity from Ge(Si)/Si(001) islands.

In order to realize effective confinement of electrons on heterojunction with island, embedding Ge(Si) islands in a tensile-strained Si (ϵ-Si) layer grown on a relaxed $Si_{1-x}Ge_x/Si(001)$ buffer layer can be used.[8] The ϵ-Si layer is an effective potential well for the electrons[9] and embedding of Ge(Si) islands in the ϵ-Si layer will essentially increase the depth of the potential well for the electrons on the heterojunction with island [Fig. 1(b)]. Besides, the Ge(Si) islands embedded in the ϵ-Si layer can be easily built in strain-balanced SiGe planar microcavities.[10] In earlier published works[8] devoted to the PL of structures with Ge(Si) islands and ϵ-Si layer the patterned substrates were used for growth and ϵ-Si layer was deposited only above islands which complicated the analysis of PL results. Besides, the PL signal observed in Ref. 8 and associated with islands was located in the energy region in which PL signal is usually connected with a wetting layer.[11]

In this work we investigated the growth and photoluminescence of Ge(Si) self-assembled islands built in the middle of ϵ-Si layer deposited on relaxed $Si_{1-x}Ge_x/Si(001)$ buffer layers having small surface roughness. Intensive island-related PL signal [about an order higher in comparison with the PL from Ge(Si) islands grown on the unstrained Si(001) substrate] was observed in the investigated structures. The dependence of the island-related PL peak position on the thickness of ϵ-Si layer was observed, which confirms that the expected energy band alignment is realized.

The investigated structures were grown by the solid source molecular beam epitaxy (MBE) on smooth relaxed $Si_{0.75}Ge_{0.25}/Si(001)$ buffer layers subjected to chemical-mechanical polishing (CMP).[12] The root-mean-square (rms) roughness of the surface of the GeSi buffers did not exceed 0.5 nm. and the threading dislocation density was less than 3.10^4 cm^{-2}. Structures for study of the growth of Ge(Si) self-assembled islands consisted of a 100-nm-thick SiGe layer matched with the top layer of relaxed SiGe buffer and ϵ-Si layer of 2–3 nm thickness on which Ge(Si) self-assembled islands were formed. The islands were produced by deposition of Ge with the equivalent thickness $d_{Ge}=8–12$ ML. The structures for the PL measurements were capped by ϵ-Si with the same thickness as that of the ϵ-Si layer under the islands, and by 80 nm of unstrained SiGe layer. The temperature of the Ge and ϵ-Si layers growth was varied in a range $T_g = 550–700$ °C. The sample morphology was determined by "Solver PRO" atomic force microscopy (AFM) in the tapping mode. The x-ray diffraction measurements were per-

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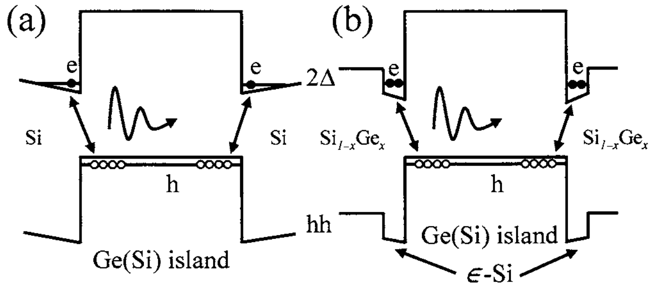

FIG. 1. Schematic band alignment in structures with (a) Ge(Si)/Si(001) and (b) Ge(Si)/$Si_{1-x}Ge_x$ islands embedded in ϵ-Si layer.

formed on a two-crystal diffractometer DRON-4. The PL spectra were recorded by a Fourier-spectrometer BOMEM DA3.36 at 77 K. A cooled InSb detector was used for registration of the PL signal. PL was excited by yitrium–aluminum–garnet (YAG) ($\lambda=532$ nm) and HeCd ($\lambda=325$ nm) lasers.

The AFM investigations have shown that growth of Ge(Si) islands on relaxed SiGe buffer layers [further referred to as Ge(Si)/$Si_{1-x}Ge_x$ islands] is qualitatively equivalent to growth of Ge(Si) islands on Si(001) substrates [further referred to as Ge(Si)/Si islands] (Fig. 2). Two types of island, pyramid and dome, are formed on surface at growth temperatures $T_g \geq 630$ °C and a small amount of Ge deposition [Fig. 2(a)]. The surface density of Ge(Si)/$Si_{1-x}Ge_x$ dome islands is increased, whereas the surface density of pyramids is decreased with an increase of d_{Ge}. The structures with Ge(Si)/$Si_{1-x}Ge_x$ dome islands having narrow size distribution (dispersion of the island sizes <10%) were obtained at $T_g \geq 630$ °C and $d_{Ge}=11$–12 ML [Fig. 2(b)].

In similarity to the Ge(Si)/Si islands growth, the hut islands become the dominating type of Ge(Si)/$Si_{1-x}Ge_x$ islands on surface at low temperatures [Fig. 2(c)]. The AFM investigations have shown that the change in the dominating islands type from dome to hut in the case of Ge(Si)/$Si_{1-x}Ge_x$ island growth takes place at $T_g=600$–630 °C, which is a little higher than in the case of Ge(Si)/Si island growth ($T_g=550$–600 °C).[13,14] The discussion of possible reasons for the observed increase of growth temperature at which the Ge(Si)/$Si_{1-x}Ge_x$ islands morphology is changed is beyond the focus of this work and can be found elsewhere.[15]

It should be noted that the lateral ordering of the Ge(Si)/$Si_{1-x}Ge_x$ islands, obtained earlier in the case of islands growth on a relaxed SiGe buffer,[16,17] was not observed in our growth experiments (Fig. 2). The absence of the islands lateral ordering in our case is related to the absence of a cross-hatch pattern on the surface of used SiGe buffer layers subjected to CMP.

The average composition of the Ge(Si)/$Si_{1-x}Ge_x$ dome islands was obtained by x-ray analysis using approximation of the uniform strained layer.[18] This approximation gives a rather small (~10%) error in the Ge content for uncapped dome islands.[19] We found out that the average Ge content in the Ge(Si)/$Si_{1-x}Ge_x$ dome islands is by 15–20% higher than that in the Ge(Si)/Si islands grown at the same temperature, and equals 80% for Ge(Si)/$Si_{1-x}Ge_x$ dome islands grown at 630 °C. The increase of Ge content in Ge(Si)/$Si_{1-x}Ge_x$ islands is caused by a smaller mismatch between the substrate (relaxed $Si_{0.75}Ge_{0.25}$ buffer layer) and the islands, which leads to reduction of the strain-driven diffusion of Si atoms to islands.

In Fig. 3(a) the PL spectra from the structures with Ge(Si)/Si dome islands ($d_{Ge}=8$ ML) are shown versus those from the structures with Ge(Si)/$Si_{1-x}Ge_x$ dome islands ($d_{Ge}=11$ ML) embedded in the middle of a 4-nm-thick ϵ-Si layer. Both structures were grown at 650 °C. It should be noted that the low sensitive InSb detector having a cutoff energy smaller than that one of high sensitive Ge detector was used for registration of PL spectra in order to avoid modification of the PL spectra caused by the spectral characteristics of the detector. There is a wide PL peak in the spectra of the structure with Ge(Si)/Si islands, which is associated with the real-space indirect optical transition between the holes confined in Ge-rich islands and the electrons located in Si on the heterojunction with the island[7] [Fig. 1(a)]. In the PL spectra of structures with Ge(Si)/$Si_{1-x}Ge_x$ islands, besides the dislocation-related PL peak in the region of 0.8–0.9 eV, there is an additional PL peak at 0.68 eV [Fig. 3(a)]. This PL peak was present only in the structures with islands embedded in the ϵ-Si layer but was not observed in the PL spectra from other Ge/Si heterostructures (strain-compensated superlattices, unstrained SiGe layers) grown on relaxed SiGe buffer layers. This fact suggests a relation between the observed PL peak and the optical recombination in islands. The intensity of the PL signal from Ge(Si)/$Si_{1-x}Ge_x$ island embedded in ϵ-Si layer is several times higher than that from Ge(Si)/Si(001) islands [Fig. 3(a)], which is associated with efficient confinement of electrons in the ϵ-Si layer on the heterojunction with islands [Fig. 1(b)]. The width of the PL peak from Ge(Si)/$Si_{1-x}Ge_x$ islands is smaller than that from Ge(Si)/Si islands because of a smaller spread of depths of the potential well for electrons on the heterojunction with island due to their effective confinement in the ϵ-Si layer (Fig. 1). The PL peak from Ge(Si)/$Si_{1-x}Ge_x$ islands is redshifted relative to the Ge(Si)/Si islands' PL peak position. We suggest that this shift is caused by a decrease in the energy of the indirect optical transition due to formation of a deep potential well for the electrons in the ϵ-Si layer [Fig. 1(b)]. Another possible reason for the shift of the PL peak from the Ge(Si)/$Si_{1-x}Ge_x$ islands is the experi-

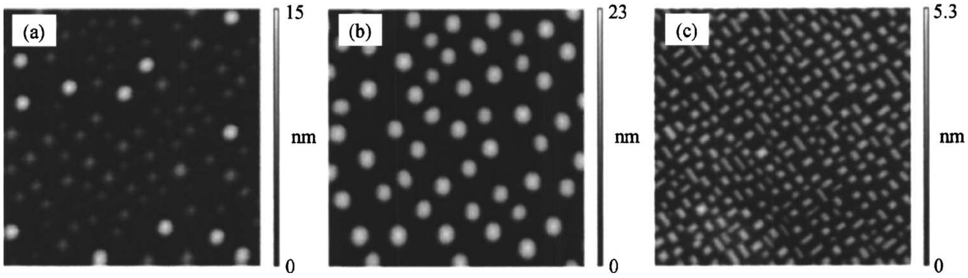

FIG. 2. The 1×1 μm^2 AFM surface images of structures with Ge(Si)/$Si_{1-x}Ge_x$ islands grown at (a) 630 °C ($d_{Ge}=8$ ML), (b) 650 °C ($d_{Ge}=11$ ML) and (c) 600 °C ($d_{Ge}=8$ ML).

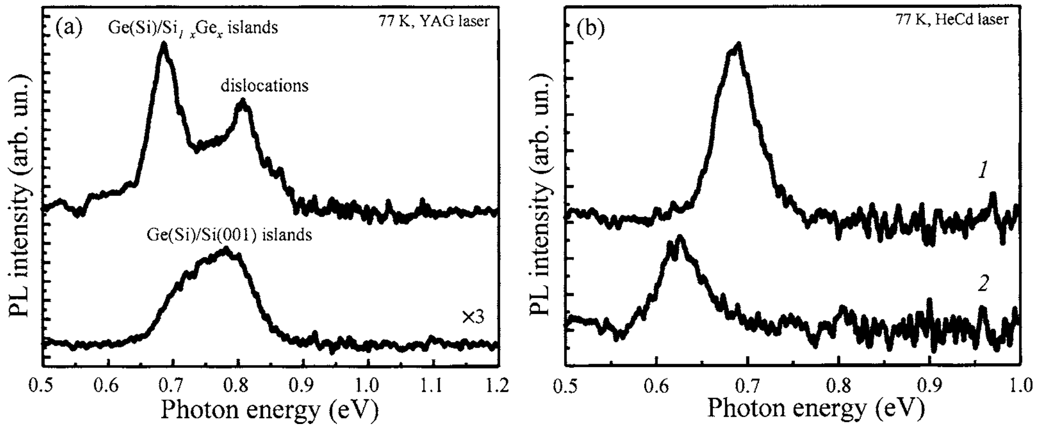

FIG. 3. (a) PL spectra of structures with Ge(Si)/Si (d_{Ge}=8 ML) and Ge(Si)/Si$_{1-x}$Ge$_x$ islands (d_{Ge}=11 ML). (b) PL spectra of Ge(Si)/Si$_{1-x}$Ge$_x$ self-assembled islands (d_{Ge}=11 ML) embedded in the middle of 4 nm (spectra 1) and 6 nm (spectra 2) thick ϵ-Si layers. All structures were grown at 650 °C.

mentally observed difference in the composition of Ge(Si)/Si$_{1-x}$Ge$_x$ and Ge(Si)/Si islands.

Because of a small ($\alpha \sim 10^4$ cm^{-1}) light absorption coefficient in silicon on the wavelength of a YAG laser radiation (λ=532 nm),[20] the PL spectra excited by YAG laser exhibit, besides the PL from the Ge(Si)/Si$_{1-x}$Ge$_x$ islands, an intensive dislocation-related PL from relaxed SiGe buffer layer [Fig. 3(a)]. The radiation of a HeCd laser (λ=325 nm) is absorbed in silicon about 100 times more effectively than the radiation of an YAG laser,[20] which allows exciting of the charge carriers only in the thin surface layer. As a result, only PL peaks associated with the optical recombination in the Ge(Si)/Si$_{1-x}$Ge$_x$ islands are present in the PL spectra excited by HeCd laser [Fig. 3(b)]. Figure 3(b) shows comparison of the PL spectra from two structures with Ge(Si)/Si$_{1-x}$Ge$_x$ islands that differ only in the thickness of the ϵ-Si layer (d_{Si}). It is seen that the islands-related PL peak is redshifted with an increase in the ϵ-Si layer thickness [Fig. 3(b)]. This redshift is associated with a change of the electron energy level in the thin ϵ-Si layer due to quantum confinement [Fig. 1(b)]. Other possible reasons, like the dependence of the composition and elastic strain of islands on d_{Si}, cannot explain the observed redshift of islands-related PL peak. The increase of d_{Si} due to Si–Ge interdiffusion should lead to the decrease of the Ge content in islands, and, as a result, to the blueshift of islands-related PL peak. The change of elastic strain around islands with the increase of d_{Si} should also cause the blueshift of islands-related PL peak due to the decrease of potential well depth for electron in the ϵ-Si layer. Thereby, the observed redshift of islands-related PL peak position with the thickness increase of the ϵ-Si layer [Fig. 3(b)] unambiguously shows that the expected model of indirect optical transition in the islands is realized [Fig. 1(b)] and the energy of optical transition in studied structures can be easily controlled by changing d_{Si}. It is necessary to note that in the PL spectra excited by HeCd laser the intensity of the Ge(Si)/Si$_{1-x}$Ge$_x$ islands, PL peak was by more than an order higher than the intensity of the Ge(Si)/Si islands' PL signal. The PL signal from Ge(Si)/Si$_{1-x}$Ge$_x$ islands in spectra excited by a low power HeCd laser ($P \sim 2$ mW) and registered by a low sensitive InSb detector was observed up to 140 K.

In summary, we used embedding of Ge(Si) self-assembled islands in a tensile-strained Si layer grown on relaxed Ge(Si)/Si(001) buffer layers in order to enhance the intensity of the PL signal from the islands. We demonstrated an increase in the intensity and a decrease in the width of the PL signal from a Ge(Si) island embedded in ϵ-Si layer as compared to the PL signal from Ge(Si)/Si(001) islands, which is associated with efficient confinement of electrons in the ϵ-Si layer on the heterojunction with islands. The redshift of the PL peak position from Ge(Si)/Si$_{1-x}$Ge$_x$ islands with an increase in thickness of the ϵ-Si layer confirms the validity of the model for real-space indirect optical transition between the electrons confined in ϵ-Si layer and holes localized in Ge-rich islands.

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