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Optical properties of self-organised SSMBE and GSMBE Ge nanostructures grown on SiGe template layers on Si (118)

G. Brémond^(a), P. Ferrandis^(a), A. Souifi^(a), A. Ronda^(b), I. Berbezier^(b)

^(a) Laboratoire de Physique de la Matière, UMR-CNRS, INSA de Lyon, bat 502, 20 Av. Albert Einstein – F-69621 Villeurbanne CEDEX, France

^(b) Centre de Recherche sur les Mécanismes de la Croissance Cristalline, CRMC2 – UP-CNRS, Campus de Luminy, case 913, F-13288 Marseille, France

ABSTRACT

This work reports on the photoluminescence properties of self-organized fully strained Ge dots fabricated using two different growth techniques: gas source molecular beam epitaxy (GS-MBE) and solid source molecular beam epitaxy (SS-MBE). Variable temperature photoluminescence (PL) measurements were carried out on Si/(n)Ge/SiGe/Si structures (n varying from 1 to 7 monolayers) consisting in double layer structures (Ge(n)/Si_{1-x}Ge_x) deposited on (118) oriented Si substrates. The process used consists in realising in a first step a Si_{1-x}Ge_x template layer with a “self-patterned” morphology. Such patterning, based on periodic morphological modulation of the surface is used to confine and organise the Ge dots in a second deposition step. Similar series of experiments with various growth temperatures, Ge coverage levels and Si_{1-x}Ge_x concentrations (x) were done by both GS-MBE and SS-MBE. The PL from the 2D wetting layer in the case of n = 3 ML has been found to be more intense in GS-MBE thanks to the passivating role of the hydrogen atoms. The 2D to 3D growth transition is accompanied by the occurrence of a red-shifted broad PL band (L) attributed to the Ge dots. While broadened luminescence is obtained from dots directly deposited on the Si substrate, a narrower band is obtained from dots deposited on the template layer. Moreover the red-shift of the (L) band observed in the latter case is attributed to higher Ge concentration in the dots. On the other hand, there is no effect of the hydrogen on the formation of the islands which show similar optical and structural properties in both growth techniques. The main difference between GS-MBE and SS-MBE concerns a low energy shift in the PL of the SSMBE Ge dots we interpret as due to size, dispersion and Ge concentration or strain effects

INTRODUCTION

These last years, there have been a great number of studies aimed at the realisation of an optical device exploiting the strained SiGe/Si semiconductor system by realising optoelectronic integrated circuits using Si processing techniques [1]. The control of Ge/Si self-organized low dimensional nanostructures becomes very important due to the great potentiality of this semiconductor to form quantum dot nanostructures for theoretical modelling and for technological application in nanoelectronics and optoelectronics. According to this aim, we have realised several Si/Ge/SiGe/Si structures grown by both Gas Source Molecular Beam Epitaxy (GS-MBE) and Solid Source Molecular Beam Epitaxy (SS-MBE) on (100) and (118) silicon surfaces with various Ge coverage. These structures give small Ge island or dots formed with Stranski-Krastanov self-organised growth mode which offers the advantages of cheap and damage-free processing. However, self organised growth presents difficulties in controlling the lateral size and the homogeneity of the dots. Recent works have demonstrated that the stabilisation of undulated strained Si_{1-x}Ge_x layers grown on Si is clearly governed by

both stress and surface topography (mainly step density and nucleation step energy)[2]. We now successfully apply these results to achieve Ge dots with confined lateral sizes on top of such a $\text{Si}_{1-x}\text{Ge}_x$ template layer. In order to increase the step density which drives mainly the self-assembled mechanism, we use (118) oriented Si surface.

This study reports on low temperature photoluminescence (PL) measurements performed on Si/Ge/SiGe/Si nanostructures performed in order to compare the influence of the growth technique on the optical properties of the template layer and of the dots.

EXPERIMENTAL DETAILS

The samples were grown either in a GS-MBE chamber using Si_2H_6 and GeH_4 gas precursors or in a SS-MBE chamber using an electron gun for Si deposition and a Knudsen cell for Ge deposition. The residual vacuum in the both cases was about 10^{-11} Torr. More details are in reference [2] The dynamics of the growth was continuously monitored in situ by RHEED. Growth experiments were performed at about 550°C. At this temperature, the growth is limited by H desorption in the GS-MBE growth regime and, in a first approximation, we can consider that the Si substrate is H terminated (This means that nearly all the Si dangling bonds are saturated by H). In all the samples a Si buffer layer of 100 nm thick was grown prior to the growth of the $\text{Si}_{0.7}\text{Ge}_{0.3}/\text{Ge}$ layers. The Ge coverage varied between 1 and 7 ML. The $\text{Si}_{0.7}\text{Ge}_{0.3}$ layer thickness was chosen to be lower than the critical thickness for plastic relaxation. All the wafers were first chemically cleaned ex situ, prior to being flashed in situ.

The samples analysed by photoluminescence were capped by a Si 15 nm thick layer. PL was excited by the 514 nm line of an Ar^+ laser with power densities of 0.05-50W/cm² and was detected by a high sensitivity nitrogen cooled Ge detector in a lock-in configuration.

The substrates used consisted of Si (001) and Si (118) p-type (B) doped wafers. The relative disorientation between the (001) and (118) planes is 10° towards [110]. The (118) surface is composed of 0.77 and 1.54 nm (001) terraces separated by single or double steps running parallel to [110] [3]. The formation of {118} facets has been reported during the heteroepitaxial growth of Ge/Si [4], suggesting that {118} facets are energetically stable [5].

RESULTS AND DISCUSSION

The results reported in the literature about quantum dots grown on Si (100) substrates either in GS-MBE and in SS-MBE show a 2D/3D changeover corresponding to a Ge coverage between 3 and 4 ML [6-9]. In order to investigate the influence of the substrate orientation on the 2D/3D Stranski-Krastanov growth mode [10,11] changeover with both techniques, we compare PL measurements performed on Si/nGe/ $\text{Si}_{0.7}\text{Ge}_{0.3}$ /Si (118) structures for n = 1, 3 and 7 ML respectively.

For GS-MBE and for n=1 and 3 ML, we observe, in figure 1, the luminescence arising from the silicon substrate (TO line at 1.091 eV) and a 2D SiGe luminescence which consists in a no phonon (NP) line and its transversal optical replica (TO) separated by 58 meV is observed in the two samples. The energies of these NP/TO pairs is in good accordance with the $\text{Si}_{0.7}\text{Ge}_{0.3}$ wetting layer characteristics. Indeed, the redshift observed between sample for n=1 ML and sample for n=3 ML well-corresponds to the increase of a Ge content. This phenomena is observed until n=6 ML. But for n=7 ML (Fig. 1, sample n=7ML), a broad band

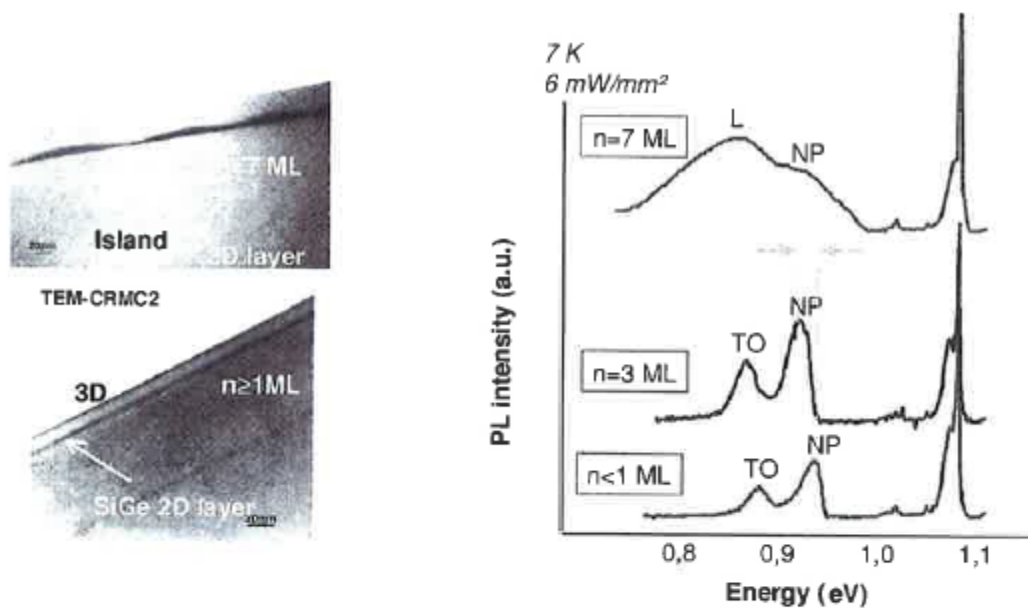


Figure 1. Low temperature photoluminescence spectra for GSMBE Si/nGe/Si_{0.7}Ge_{0.3}/Si on (118) Si structure with n = 1, 3 and 7 monolayer of Ge and associated transmission electronic microscopy images for n= 1ML and 7 ML.

labelled L and located around 870 meV is observed. This band is correlated to the Ge island formation as shown by the morphological TEM characterisation in figure 1 [12] so that the 2D/3D transition occurs at n ~ 7 ML. On the other hand, the 2D TO line luminescence disappears when the NP line persists. We can give two explanations corresponding to this behaviour : the TO line could be masked by the L broad band or maybe strongly reduced because of the band gap transformation du to strain-induced localisation [6,7]. This 2D/3D transition at a thickness close to 7 ML instead of the standard 3-4 ML can be

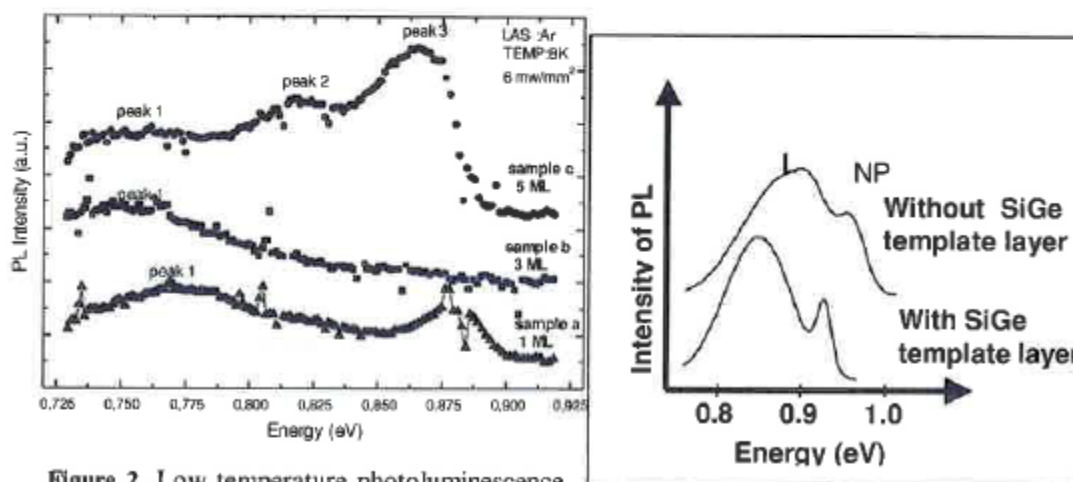


Figure 2. Low temperature photoluminescence spectra for SSMBE Si/nGe/Si_{0.7}Ge_{0.3}/Si on (118) Si structure with n = 1, 3 and 5 monolayers of Ge. Peak 1 is defect related and peaks 2 and 3 are Ge islands related (see text).

place on the edge step of the (118) silicon wafer surface and saturate the dangling bond of silicon atoms. The surface of the silicon will be terminated by H bonds. In contrast SS MBE

Figure 3. Influence of the SiGe template layer on the PL spectrum for n= 7ML on Si (118).

explained by the presence of the Hydrogen atoms at the surface which have a crucial role in modifying the structure of the surface acting as a surfactant. The ad-atoms of Hydrogen take on (118) shows that the 2D/3D transition starts close to 5 ML (Fig.2 for sample c with $n=5\text{ML}$).

Hydrogen atoms can also passivate the surface and limit the segregation of the defect from the substrate into the silicon germanium template layer. In consequence, we notice a 2D PL signal more important on the (118) Si surface with GS-MBE as compared to SS-MBE (compare Fig. 1 and Fig. 2) which reveals a strong process for non-radiative recombination in the case of SSMBE samples.

Figure 3 show the positive influence to deposit Ge monolayers on a SiGe template layer rather than directly on the Si substrate or buffer layer. A narrower band is obtained from dots deposited on the template layer while a broadened luminescence is obtained from dots directly deposited on Si substrate. Moreover the red-shift of the (L) band observed in the case of growth on SiGe template layer is attributed to a higher Ge concentration in the dots.

In order to study the influence of the growth and to determine the fundamental mechanism of the carrier recombination in the dots grown on Si (118) vicinal surfaces, we have performed PL measurements at 6 K with variable excitation densities. Fig. 4 and 5 present the behaviour of samples with 7 ML and 5 ML of Ge on $\text{Si}_{0.7}\text{Ge}_{0.3}/\text{Si}(118)$ grown respectively by GS-MBE and SS-MBE when the excitation power increases. We observe an important shift (27 meV) of the signal toward the higher energies in both cases. This indicates a strong dependence to the excitation power. This behaviour is not conventional in SiGe/Si type-I systems, but it can be explained by a type-II band line up. In a type-II interface, a two-dimensional electron gas (2 DEG) is formed in the conduction band and when the excitation power increases, the 2 DEG fills with the photogenerated carriers. This filling induces an energetic increase of the transition, and hence we observe a blueshift. This power densities study shows us that for 7 ML of Ge deposited on the silicon germanium template layer, we have a type-II transition provided at the interface of the dots and the template layer. This excitation power density of the PL shows that peak 1 is not excitonic behaviour related but defect behaviour related. Peaks 2 and 3 are related to excitonic behaviour.

In order to compare the shape and the size of the dots, an AFM characterisation shows that the wire shaped islands with reduced lateral size formed on Si (118) have approximately

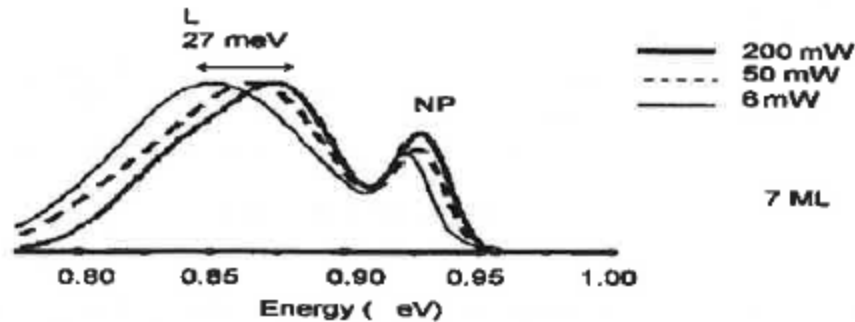


Figure 4. Study of the excitation power dependence on photoluminescence spectra of GSMBE $\text{Si}/n\text{Ge}/\text{Si}_{0.7}\text{Ge}_{0.3}/\text{Si}(118)$ structure with $n = 7$ monolayers of Ge.

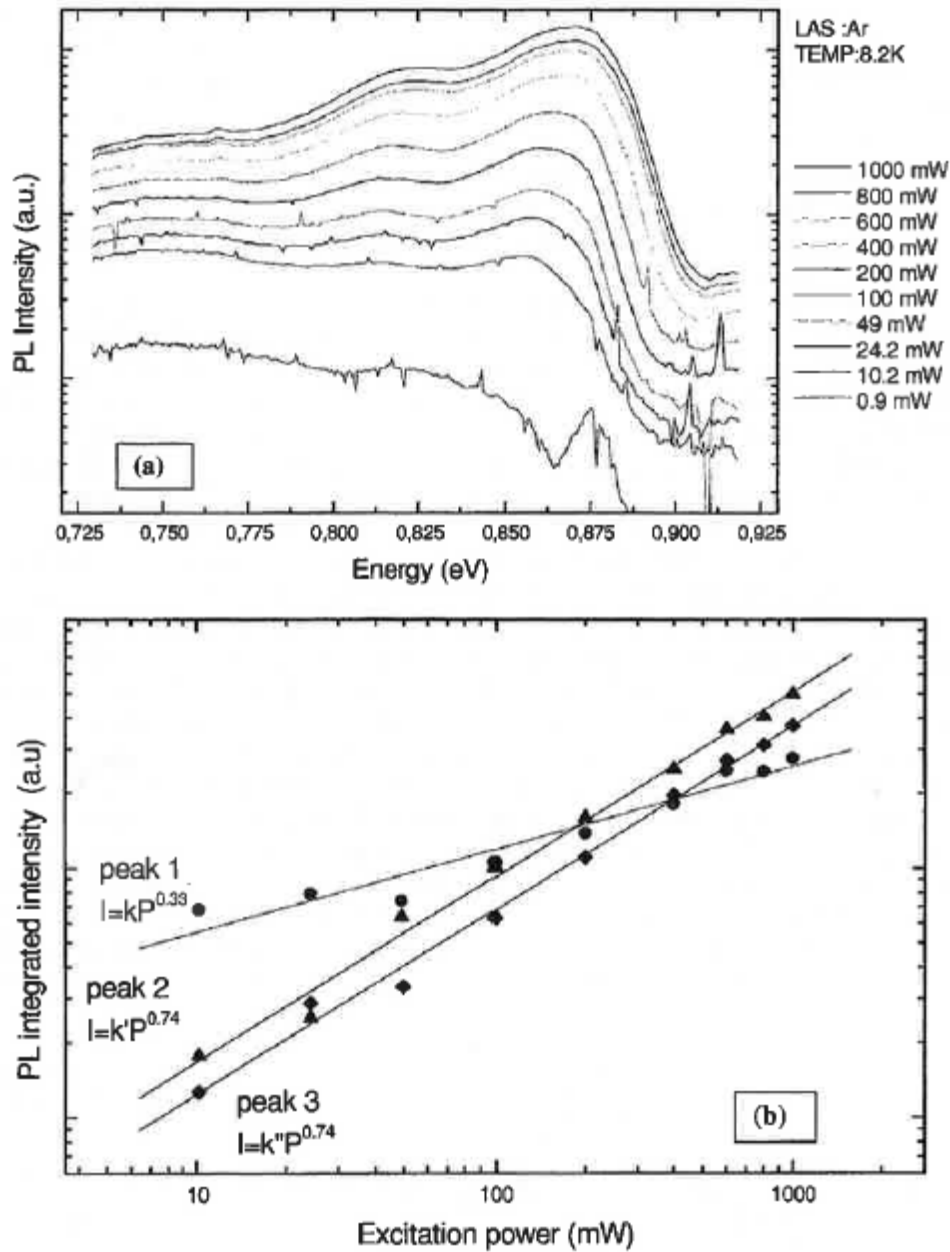


Figure 5. Study of the excitation power dependence on photoluminescence spectra of SSMBE Si/nGe/Si_{0.7}Ge_{0.3}/Si (118) structure with n = 5 monolayers of Ge (a) and PL integrated intensity versus excitation power (b).

the same size with the two growth techniques, in the range of 20 nm width, 100 nm long and 3 nm height.

The only difference of the optical properties noticed between the two growth techniques in the case of 7 ML of Ge deposited on SiGe is the higher energy of the band L in the case of GS-MBE. This could be due to a more important value of the residual elastic strain in the Ge dot in the case of SSMBE growth.

CONCLUSION

We have carried out a systematic and a complete PL study in order to investigate and compare the optical properties of Si/(n)Ge/SiGe/Si structures for $n = 1, 3, 5$ and 7 ML, grown by GS-MBE and by SS-MBE on (118) undulated surfaces. The PL of the 2D SiGe wetting layer is observed to be more intense in GS-MBE due to the crucial passivating role of the hydrogen atoms at the surface of the sample.

On the other hand, we notice that the hydrogen atoms have no effect on the formation of the islands, and we obtain the same optical and structural properties in both growth techniques which means that the role of the hydrogen atoms on the surface of the sample is restricted to ameliorate the optical quality and so the electronic quality of the wetting layer formed above the silicon buffer.

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