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Optical and structural properties of the GaAs heterostructures grown using AlGaAs superlattice buffer layer on compliant Si(100) substrates with the preformed porous-Si (por-Si) layer.

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Abstract. 360 nm and 700 nm thick GaAs layers were grown by MO MOCVD growth technique directly on compliant Si (100) substrate and on super-lattice (SL) AlGaAs buffer layer. The XRD study revealed better structural quality for the sample grown on SL / por-Si buffer. AFM study revealed a smoother sample surface with blocks of more regular rectangular shape and larger size as well. Photoluminescence spectra of the samples revealed an energy shift of PL maximum intensity for both samples. Sample grown on SL buffer also showed higher PL intensity corresponding to better crystalline perfection.

1. Introduction

The integration of the III-V technology with the most developed Si technology is an actual problem for the state of art science. III-V / Si heterostructures will combine the advantages of both material systems and help to create high-efficient, low cost optoelectronic and power devices. However, large lattice and thermal expansion coefficient (TEC) mismatch between Si and GaAs (~120.4% and ~4.1%, respectively) [1] leading to the generation of high density of threading dislocations (TD) and other defects during the growth procedure, which acts as nonradiative recombination centers and affect on terminal-device efficiency and reliability. The difference in thermal expansion coefficients can led to bending of heterostructures which significantly complicates its post-growth processing, and in some cases can lead to delamination of the films from substrates. As it was shown in our previous work [2] the usage of por-Si layer helps to suppress stress generation and TD propagation due to unique properties of nanoporous material. Due to the presence of nanopores, Si layer can be deformed and obtains less lattice mismatch with overlaying heterolayer. In this work we compare optical and structural properties of GaAs layers grown by MO MOCVD technique on por-Si/Si(100) (sample A) and SL/por-Si/Si(100) (sample B) templates. The presence of stresses of different signs in SL layers as well as a number of interfaces between GaAs and AlAs layers helps to suppress threading dislocations propagation by their inclination and annihilation in the compressively strained fields [3]. GaAs layer grown on AlGaAs-SL buffer demonstrated more intense PL and XRD spectra.
corresponding to better structural quality. Besides, AFM revealed smoother surface with blocks having a more pronounced rectangular shape and larger size for the layer grown on SL buffer.

2. Experiment
Porous layer of silicon, por-Si, as a “compliant” virtual substrate was formed on a single-crystalline c-Si (100) plate by its electrochemical etching in the alcohol solution of the fluoric acid according to the standard procedure [4]. Growth procedures were performed on EMCORE GS3100 MO MOCVD setup under the pressure of 77 Torr and substrate rotation speed of 1000 rpm. Trimethylgallium ((Al(CH₃)₃)) and Arsine (AsH₃), were used as source gases and hydrogen was applied as a carrier gas. Before growth, both substrates were annealed for 20 min in AsH₃ flow and substrate temperature (Tₛ) of 750 °C. After annealing the 10-nm-thick AlAs overlaid by 20-nm-think GaAs buffer layer was grown at the Tₛ=450 °C. GaAs layer with a thickness of 390 nm was grown for sample A and the SL buffer layer with a thickness of 100 nm and overlaying 700-nm-thick GaAs layer was grown for sample B at the Tₛ=550 °C.

3. Results and discussion
The AFM study of both samples (Figure 1.a and 1.b) revealed mosaic surface morphology, but for sample B the surface blocks have larger size and the shape more close to a rectangular corresponding to better crystalline quality. Well known that larger lateral sizes of the nucleation blocs led to lower generation of threading dislocations during misorientated blocs coalescence.

Figure 1. The AFM image (a, b) XRD spectra (c), and PL spectra (d) of sample A and B.
Moreover the 3D morphology of the samples surface corresponding to mosaic structure of all film, thus the TD’s can annihilate on blocs free surfaces. This fact is also confirmed by XRD study of the samples (Figure 1.c) where a more intensive (400) peak can be observed for the sample B. As well, no other peaks except (200) and (400) were observed, corresponding to monocrystalline structure of the GaAs epitaxial layer for the both samples.

The PL spectra of the samples (Figure 1.d) demonstrate bright emission at ~1.39 eV for sample A and 1.5 eV for sample B shifted from normal value for GaAs 1.42 eV to the low energy range. The nature of this redshift is under study. The higher PL intensity for sample B confirms the better structural quality of the GaAs layer grown on SL buffer.

Using high-resolution XRD (HRXRD) high-resolution X-ray diffraction on the basis of inverse q-space mapping of the samples (Figure 3) we have calculated the lattice parameters, strain and stress levels in both heterostructures. The images of XRD mapping across symmetric (004) and skew symmetric (511) reflections are listed in Figure 3. It shall be noted that in the Figure 3b (511) reflection from SL can be observed. Using these data we calculate the lattice parameters as $a_{GaAs}=5.6528 \text{Å}$, $a_{SL}=5.5791 \text{Å}$. It should be also noted that the calculated SL lattice parameter is significantly different from that one in AlGaAs binary alloy of the same composition. This difference is associated with atomic self-ordering which is typical for three-component III-V semiconductor alloys with the composition ($x \approx 0.50$) [5].

![Figure 2. XRD mapping images symmetric (004) (a) and skew-symmetric (511) (b) reflections of GaAs/SL/proto-Si(100) heterostructures.](image)

However, aAlGaAs lattice parameter calculated in our previous work [6] is different from the value calculated in this work as well as from that one theoretically obtained by S. Laref et. al. in [7]. We believe that this decrease in the lattice parameter of SL in comparison with the values that we observed in our previous works is related to features of the low-temperature growth process, which been used for heterostructure formation.

Our previous researches [8-11] revealed that the growth of GaAs and III-N based epitaxial layers on compliant substrates presented by preformed nanoporous Si layer have advantages in comparison with growth on traditional c-Si substrates: lower TD density, higher PL intensity and less stress level at the RT.

In this work, we confirmed the sufficient improving of the crystalline and optical quality of AlGaAs epitaxial layers grown on substrates with preformed nanoporous Si layer and SL-ALGaAs
buffer layer. The AFM study revealed better surface morphology, XRD analysis – better structural quality and PL spectra revealed higher intensity for sample grown on complex substrate SL-AlGaAs/por-Si/Si. The results obtained in this work confirm a positive influence of the usage of compliant Si substrates with porous Si layer and slight misorientations from (111) direction as well as usage SL-AlGaAs buffer layer.

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