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Study of morphology and composition of nanoscale AlGaN heterostructures obtained by PA MBE technique on the silicon substrates with the use of porous silicon as buffer layer

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Abstract. In this work, we study the morphology, composition and optical properties of AlGaN epilayers grown by plasma-assisted molecular beam epitaxy on the AlN buffer layer which was performed on regular Si substrate and compliant Si substrate with a preformed buffer porous silicon layer (*por*-Si) and carbonized porous layer(SiC/*por*-Si). The AlGaN layers formed on the *por*-Si buffer revealed a 15% higher intensity of photoluminescence spectra in visible range in comparison with ones formed on regular Si substrate.

Keywords: AlGaN, epitaxy, buffer layer, porous silicon

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Материалы конференции
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Исследование морфологии и состава наноразмерных гетероструктур AlGaN, полученных методом ПА МПЭ, на кремниевых подложках с использованием пористого кремния в качестве буферного слоя

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Аннотация. В работе были проведены исследования морфологии, состава и оптических свойств эпитаксиальных слоев AlGaN, выращенных методом плазменной молекулярно-лучевой эпитаксии на буферном слое AlN, сформированном на обычной подложке монокристаллического c-Si и податливых подложках c-SiC предварительно сформированными на них буферными слоями пористого кремния (*por*-Si) и карбидизированным пористым слоем (SiC/*por*-Si). Слои AlGaN, сформированные на буфере *por*-Si, показали на 15% более высокую интенсивность спектров фотолюминесценции в видимом диапазоне, по сравнению со слоями, сформированными на обычной подложке Si.

Ключевые слова: AlGaN, эпитаксия, буферный слой, пористый кремний

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Introduction

Heterostructures on the basis of (Al, Ga) N system attract great interest since they are currently used as for the fabrication of radiation-hardened high temperature high mobility transistors, as for the application of optoelectronic devices. Basic techniques for the growth of heterostructure devices are known to be vapor-phase epitaxy from metal-organic compounds (MOS VPE) and molecular beam epitaxy (MBE). Combination of AIIIN materials with silicon devices for signal processing opens new ways for appearance of the new functional units that could merge high-quality optoelectronic characteristics of AIIIN and the developed more profit-proved technologies on the basis of Si substrates. Moreover, the use of silicon substrates for the growth of III-N heterostructures is useful from the practical point of view due their commercial availability and maturity of Si-technologies.

However, the formation of III-N/Si heterostructures is yet impeded due to the differences in the thermal expansion coefficient and lattice parameters that results in the generation of the threading dislocations with high density, delaminating and cracking of heterostructures, thus impairing the instrument characteristics of the terminal devices. One of the perspective technological processes providing possibility of obtaining high functional properties in the fabricated hybrid heterostructures can be based on the usage of the compliant structured silicon substrate composed of porous silicon [1–3].

The aim of our work was to determine the effect of incorporation of the transition layer, nanoporous silicon *por*-Si, into technological process of $Al_xGa_{1-x}N$/AlN/*por*-Si/Si(111) heterostructure growth as well as carbonized porous silicon on the structural-morphological characteristics and atomic composition of the surface layers applying microscopy and X-ray photoelectron spectroscopy technique.

Materials and Methods

In order to grow $Al_xGa_{1-x}N$/AlN heterostructures, silicon substrates Si (111) were used with different kinds of surface modification: standard smooth substrates of *c*Si, Si (111) substrates with the layer of porSi/*c*Si formed on the substrate surface, as well as SiC/*por*Si/cSi substrates. The layers of porous silicon (~50 nm) were obtained by electrochemical etching of single-crystalline silicon wafers of KDB type with (111) orientation in fluorine acid solution, similar to that one described in [4, 5] and SiC layer was formed with the use of the atom replacement technique [6].

AlGaN epitaxial layers on the substrates of three types (*c*-Si, *por*-Si and SiC/*por*-Si/*c*-Si) were grown in a common growth process by molecular beam epitaxy with the addition of plasma-activated nitrogen (PA MBE) in the Veeco Gen 200 facility.

$Al_xGa_{1-x}N$/AlN/Si(111) heterostructures (HS) without transition layer and also with transition layer of *por*-Si were grown at on and the same time. Just before the growth process of heterostructure the substrates were annealed and nitridized for 30 minutes at the substrate temperature of $T \sim 670$ °C in the growth chamber of the facility. The growth processes of formation for all of the HS layers were realized in metal-enriched conditions. The growth rate was controlled and limited by nitrogen flow and it was equal to $F_N \sim 0.05$ μm/hour. In order to prevent etching of silicon substrate with liquid Ga accompanied with formation of Ga-Si eutectic buffer layer of AlN was formed

on the surface of the substrates. Epitaxial synthesis of heterostructures started from the formation of nucleus AlN layers at T ~ 800 °C, F_{Al} ~ 0.02 μm/hour grown for 60 minutes on the surface of substrates. After that, temperature of the substrates was reduced up to the value of T ~ 700 °C for the growth of the main $Al_xGa_{1-x}N$ layer implemented for four hours at the constant layers of F_{Al} ~ 0.01 μm/hour, F_{Ga} ~ 0.4 μm/hour and F_N ~ 0.04–0.05 μm/hour. The morphology of the grown heterostructures was examined with a JEOL JSM 6380LV scanning electron microscope (SEM).

The samples were studied by X-ray photoelectron spectroscopy (XPS) on a SPECS spectrometer. The spectra were excited with Mg Kα-irradiation (E = 1253.6 eV). The depth of the XPS analysis of the sample surface is 1–2 nm. When processing the measurement results, Shirley algorithms were used to determine the background line and subtract the background values. To determine the binding energy of the heterostructure elements, we used the C1s line of natural hydrocarbon impurities of the sample surface not subjected to special cleaning as a reference line, the binding energy E_b[C1s] = 285 eV. The core levels of the elements and their chemical state were determined using the X-ray photoelectron spectra database of the US National Institute of Standards [7].

The luminescence spectra of the samples were obtained with the unit measuring photoluminescence and optical reflection spectra Accent RPM Sigma. The studies were made at room temperature under laser excitation having a wavelength of 266 nm and a power density of W = 5W/cm^2.

Results and Discussion

Certain inhomogeneities of the structure with sub-micrometer sizes can be seen on the surface of the samples which are attributed to the columnar structure of the films, observed in SEM images of the sample chips. Similar columnar structure of the films we have also observed in $In_xGa_{1-x}N$/Si(111) heterostructures [8]. Total thickness of the grown heterostructures was of ~100–120 nm. Comparison of heterostructures morphology demonstrated that the growth on porous layer provided less scattering in the sizes of inhomogeneities on the surface. It means that the structure of the film is more homogeneous as compared with heterostructure grown without the buffer layer. At the same time even more homogeneous fine-grained structure is observed for the structure grown on the carbonized porous layer. Mean lateral sizes of inhomogeneities/globules for heterostructures grown on the crystalline silicon were of about 130 nm, while those ones on porous silicon were of about ~100 nm, and on the carbonized porous buffer layer they were of ~60 nm.

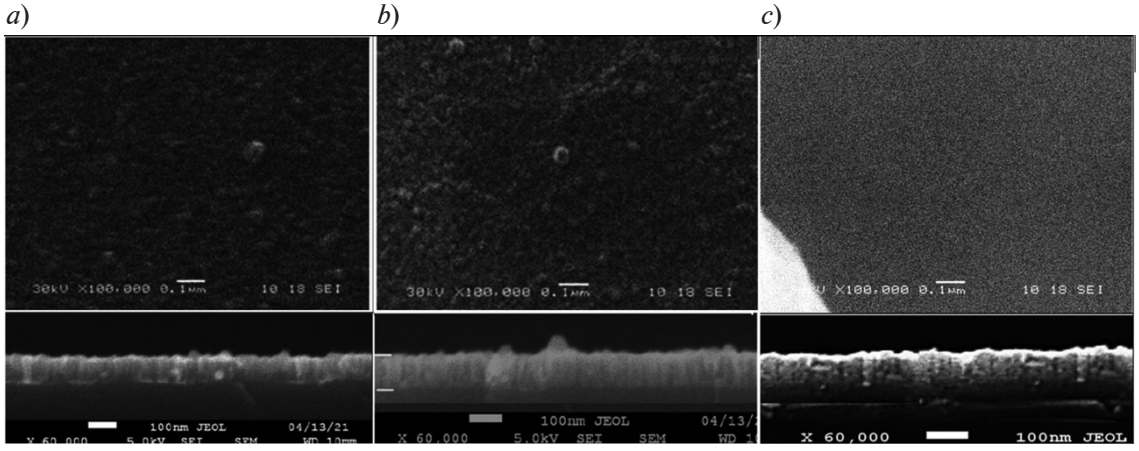

Fig. 1. SEM images of $Al_xGa_{1-x}N$/AlN/Si (*a*), $Al_xGa_{1-x}N$/AlN/*por*-Si/Si (*b*) and $Al_xGa_{1-x}N$/AlN/SiC/*por*-Si/*c*-Si (*c*) heterostructures surfaces and cross-sections respectively

Fig. 2 represents XPS spectra of the core levels of Al 2*p*, Ga 2*p* and N1s for heterostructures obtained directly on single-crystalline silicon c-Si(111) (Fig. 2,*a*), with porous sublayer (Fig. 2,*b*) and with carbonized sublayer (Fig. 2,*c*).

Analysis of XPS spectra shows that on the surface of the samples for all heterostructures Al and Ga atoms form chemical bonds with nitrogen and they display practically the same binding energies (just as the half-widths) of the core-level spectra for all of the elements in $Al_xGa_{1-x}N$ alloy close to the values of the binding energies of aluminum and gallium in pure nitrides [7].

Besides, a contribution of low-intensity component characteristic for the oxidized aluminium Al_2O_3 (E_b = 75.5 eV) formed on the surface of the samples under their contact with the oxygen air can be seen in Al 2p core level spectra. Note, that Al_2O_3 contribution is most clearly seen for heterostructures grown on the carbonized porous layer while it is least noticeable in heterostructures grown on *c*-Si. Similar component is not observed for Ga 2*p*3/2 spectrum, however, Auger-line of nitrogen N KLL is superimposed on the low-energy part of gallium spectra thus masking gallium oxide contribution. N1s spectra of nitrogen correspond to the binding energies of Al and Ga nitrides [7].

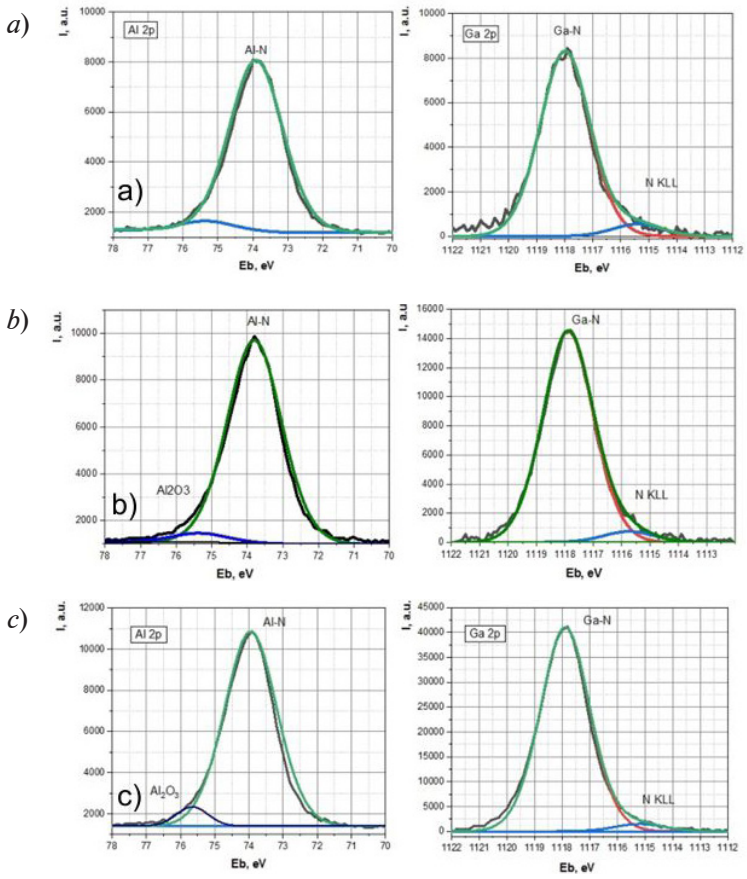

Fig. 2. XPS spectra of the core Al2*p* and Ga3*d* levels in heterostructures with different types of the substrates (a) *c*-Si, (*b*) *por*-Si/*c*-Si and (*c*) SiC/*por*-Si/*c*-Si)

Similar to the results of [8] aluminum content in the film can be calculated basin on the relationship (1):

$$x_{\mathrm{Al}} = \frac{I_{\mathrm{Al2p3}}/F_{\mathrm{Al2p3}}}{\left(I_{\mathrm{Al2p3}}/F_{\mathrm{Al2p3}} + I_{\mathrm{Ca2p3}}/F_{\mathrm{Ca2p3}}\right)}, \quad (1)$$

where I is integrated intensity of photoelectron peaks for the corresponding lines in the spectrum and F is a sensitivity factor ($F_{\mathrm{Ga}2p3}$ = 2.75 and $F_{\mathrm{Al}2p3}$ = 0.54).

The values of Al atoms concentration in the alloys determined on the basis of relationship (1) were of x_{a_cryst} = 0.49, x_{a_por} = 0.54, and x_{sic} = 0.42 for the samples grown on single-crystalline silicon, namely, $Al_xGa_{1-x}N$/AlN/Si(111), and also with the use of porous buffer layer $Al_xGa_{1-x}N$/AlN/Si/*por*-Si/Si(111) and $Al_xGa_{1-x}N$/AlN/SiC/*por*-Si/*c*-Si, respectively. The obtained values are in a good agreement with the expected technological value of $x \sim 0.50$ specified previously for the process of synthesis. The difference in x values of heterostructures can be due their structural-morphological distinctions and the attributed aluminium oxidation under sample storage in the atmosphere. Note, that most fine-grained surface of the samples grown on carbonized porous silicon just involves the greater amount of the oxidized aluminium.

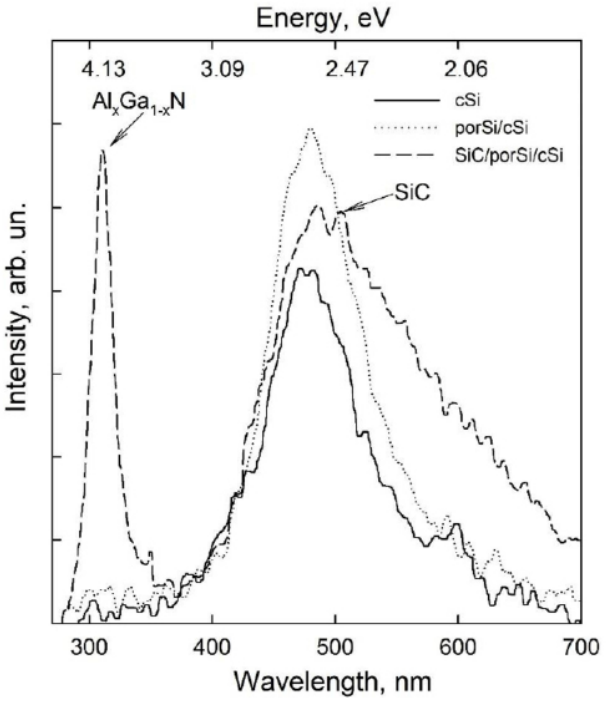

Fig. 3. PL spectra at T ~ 300 °C from Al*x*Ga1−*x*N/AlN heterostructures, grown on cSi, porSi/cSi and SiC/porSi/cSi substrates

Photoluminescence spectra of the epitaxial Al*x*Ga1−*x*N/AlN heterostructures for all types of the samples are presented in Fig. 3. One can see that the luminescence spectra of the samples in the range of 300−900 nm depend on the type of a substrate used for film growth.

These spectra show the presence of ultraviolet spectral band only for heterostructure grown on SiC/porSi/cSi substrate with the maximum energy of E_g = 3.99 eV (near 310 nm), which can be attributed to the transitions of band-to-band type in Al*x*Ga1−*x*N alloy. Moreover, in all of the spectra, additional broad yellow spectral band can be observed. It is attributed to the spurious defect that appeared due to the impurities incorporated in the process of growth [9]. For all of the structures grown on porous silicon, PL band is the most intensive one and it is by ~ 15% higher than for heterostructures with buffer layer formed with carbonized porous silicon and is by 25−30% higher than for those ones grown on crystalline silicon. One should note that in the experimental spectrum of the film obtained on the hybrid SiC/*por*Si/cSi substrate, the peak is present near 2.34 eV. This maximum can be attributed to 3*C*-SiC sublayer, with the energy value of the band-gap approximately equal to E_g ~ 2.24−2.39 eV [10].

Conclusion

In the work original $Al_xGa_{1-x}N$/AlN/*por*-Si/Si(111) heterostructures were fabricated by molecular-beam epitaxy technique using buffer layer of porous silicon *por*-Si and carbonized porous silicon.

Formation of $Al_xGa_{1-x}N$/AlN heterostructures with the use of porous silicon layers was shown to facilitate more homogeneous distribution of the alloy nanocolumns over their sizes and orientation in the base direction as compared with similar alloy grown at the same time in single-crystalline silicon without porous layer implying that the growth process was performed in the same technological conditions. It was found that variations of Al content over the samples surface can be attributed to the different intensity of the oxidation processes of the surface due to the differences in heterostructures morphology.

Applying the scanning electron microscopy, photoelectron and photoluminescence spectroscopy it was shown that thin AlGaN/AlN heterostructures formed on the *por*-Si substrate were characterized up to 15−25% more intensive photoluminescence in a visible range as compared with those ones formed on the carbonized porous buffer layer and regular Si substrate.

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