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Experimental study of structural and optical properties of integrated MOCVD GaAs/Si(001) heterostructures

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A B S T R A C T

This is the first report of the control of the structural and optical functional characteristics of integrated GaAs/Si(001) heterostructures due to the use of misoriented Si(001) substrates with protoporous sublayer. The growth of the epitaxial GaAs layer on silicon substrates without formation of the antiphase domains can be performed on substrates deviating less than 4°–6° from the singular (001) plane or without the use of a transition layer of GaAs nano-columns. Preliminary etching of the silicon substrate with protoporous Si sublayer formation facilitated the acquisition of an epitaxial GaAs film in a single-crystalline state with a considerably less residual strain factor using MOCVD, which has a positive effect on the structural quality of the film. These data are in a good agreement with the results of IR reflection spectroscopy as well as PL and UV spectroscopy. The optical properties of the integrated GaAs/Si (001) heterostructures in the IR and UV spectral regions were also determined by the residual strain value.

1. Introduction

The main barrier to further development in the optoelectronic industry, as well as solar photopower engineering, is the relatively high cost of the final product, since the main materials applied for production of high-performance devices in this area are semiconductors of the GaAs group [1,2]. Production technology of A_3B_5 compounds < components and devices are rather expensive. Moreover, A_3B_5-based devices and modules consume more power than their silicon-based analogues. Thus, the most promising approach to overcome this issue, is the integration of semiconducting compounds of the GaAs group with silicon (Si) [3]. The emergence of formation technologies allowing implementation of A_3B_5-functional elements on the surface of silicon chip will provide prerequisites for new optoelectronic devices, with a principally new architecture in comparison with the current CMOS circuits [4]. Nevertheless, integration of A_3B_5 materials with Si is challenging, mainly due to the inconsistency of the crystal lattice parameters in the A_3B_5/Si heterocouple, as a result of the diverse properties of silicon and semiconducting A_3B_5 compounds (e.g., thermal expansion coefficients, polarity of semiconductor, band structure, etc.) [1,5].

In order to solve these problems, various approaches to combine semiconducting materials of GaAs-groups and silicon chips [6] have been developed; however, they have had varying degrees of success. The growth of a polar semiconductor on a non-polar substrate resulting in the formation of antiphase domains with a great density has been achieved by the application of Si or Ge substrates deviated from a singular plane (001) by 4°–6° [5,7] or with the use of more cost-based method of growth on the transition layer of GaAs nano-stakes [8]. A rather high (~4%) difference in the parameters of the crystalline lattices for GaAs/Si system, as well as a significant difference in the coefficients of thermal expansion, facilitate formation of numerous dislocations and appearance of micro-cracks in the GaAs film during its growth [6]. This problem is solved by high-temperature treatment of A_3B_5/Si heterostructures (anneals, thermo-cycling), considerably improving the crystalline perfection of these platforms. In turn, it is unacceptable for the growth of GaAs in the windows of Si substrates with the readily available elements of the integral circuits, as well as by the way of growing of a number of transition buffer GaAs/Ge/Si layers [9,10], which is also often undesirable.

The approach concerned with the design of “conformable” substrates based on a porous layer formed directly on Si crystal is interesting, but rather challenging for the integration of A_3B_5 materials with silicon. Although certain isolated attempts of A_3B_5 growth on the porous layer

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demonstrated the possibility of such an approach for the formation of integrated A_3B_5/Si heterostructures, it did not result in the development of the proposed technology. In our opinion, this is related to the formation of a macro- and mesoporous silicon layer as a conformable substrate [11,12].

It should be noted that there is no information in scientific literature concerning the structural and optical properties of GaAs grown by the MOCVD technique on a conformable substrate - thin layer of porous Si. Therefore, the aim of this study was to investigate the impact of substrate misorientation and its preliminary etching on the structural and optical properties of the integrated MOCVD GaAs/Si(001) heterostructures.

2. Materials and methods

A series of the test samples was grown at the MOCVD epitaxy facility «EMCORE GS 3/100» in a vertical reactor with a high rotation speed of the substrate holder. The epitaxial film of each sample had an identical design as presented in Fig. 1. The plates of the following compounds were used as the substrates (see Table 1). The substrate holder temperature during the epitaxial growth was 700 °C, the pressure in the reactor was 77 Torr, and the rotation speed of the substrate holder was 1000 rpm. Gallium tri-methyl $Ga(CH_3)_3$, aluminium tri-methyl $Al(CH_3)_3$ and arsine AsH_3 were applied as the initial reactants. The samples were grown through the course of one technological process, with a GaAs growth rate of ~770 A/min.

The preliminary treatment of Si(100) substrate (sample #3) was formed by etching the original substrate for 1 min in a solution of 1 part HF, 1 part acetic acid and 40 parts nitric acid. As a result of chemical poisoning, nanoprofiled surface of silicon was formed with a significantly developed relief – protoporous silicon, i.e. porous silicon at the stage of pore formation. The thickness of the layer is commonly ~10 nm [13].

Microscopic investigations of the quality of the heterointerfaces were performed with a Libra 120 Carl Zeiss electron microscope.

X-ray phase analysis of the obtained samples was performed by X-ray diffraction using a DRON 4-07 diffractometer with a cobalt tube $CoK\alpha = 1.790$ Å.

The structural quality of the samples and determination of the lattice parameters in the alloys were performed by X-ray diffraction with a Seifert 3003 HR diffractometer involving a four-circled goniometer and monochromatized copper radiation with a $CuK\alpha_1$wavelength $= 1.5405$ Å.

The photoluminescence spectra of heterostructures were obtained at room temperature from the surface of the samples according to the standard technique using a TRIAX550 monochromator and CCD detector cooled with liquid nitrogen under excitation with argon laser (wavelength = 514.5 nm). A 10× objective was applied to provide focusing of the beam.

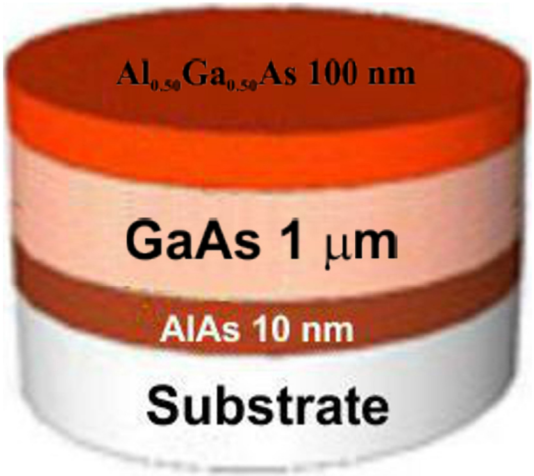

Fig. 1. Design of the epitaxial heterostructures for the studied samples.

Table 1
Characteristics of the substrates used for the growth of the heterostructures.

Sample	Type of substrate	Characteristics
#2	GaAs(001)	Semi-insulator
#3	Si(001)	Misorientation by ~3° relative to [011] + etching
#4	Si(001)	Misorientation by ~3° relative to [011]
#5	Si(001)	Misorientation by ~7.5° relative to [011]

The optical properties of the samples were studied in the range of 190–900 nm, by means of UV-spectroscopy using a LAMBDA 650 unit (Perkin Elmer) provided with the URA universal attachment allowing one to obtain reflection spectra within the range of incidence angles from 8 to 80°. The block-diagram of the attachment enabled the acquisition of absolute reflection and reflection spectra were obtained at the incidence angle of 67°.

IR-reflection spectra of heterostructures were obtained with the use of an IR-Fourier spectrometer Vertex-70 Bruker.

3. Experimental results and discussion

3.1. *Structural investigations*

Fig. 2 shows the survey diffraction patterns of the studied samples. From the data, only diffraction reflections of (002) and (004) were observed in the diffraction pattern of sample #2, which are characteristic of single-crystalline GaAs(001). The diffraction patterns of samples #3 and #5 are identical, thus only the survey diffraction pattern for sample #3 is presented. Besides the reflections (002) and (004) from GaAs layer, reflection of (004) from the Si(001) substrate can be also observed in the diffraction pattern. The presence of only reflections (002) and (004) in the diffraction pattern demonstrated a single-crystalline growth of a GaAs layer. Regarding the diffraction in sample #4, the epitaxially grown film demonstrated a polycrystalline structure, since in the diffraction pattern there were reflections not characteristic of a single-crystalline film growing in a (001) direction. It should also be noted that based on the X-ray diffraction structural analysis, a texture can be clearly observed in the (111) direction for the film of sample # 4.

Since samples #3 and #4 have the same substrate, Si (001), misoriented by ~3° relative to [011], they only differ by the fact that the Si substrate for sample #3 was preliminarily etched prior to epitaxy (meaning formation of the transition porous layer). The obtained results suggest that preliminary etching of Si (001) substrate with protoporous Si sublayer formation favoured single-crystalline growth of the epitaxial A_3B_5 film on silicon substrate. Single-crystalline growth of GaAs on Si(100) substrates becomes possible even at the lower misorientation of the substrate, which it is usually utilised in production of integrated GaAs/Si heterostructures [5]. At the same time, the use of the substrate misoriented by ~7.5° relative to [011] does not result in the appearance of polycrystallinity in the epitaxial film without preliminary etching of the substrate.

The structural quality of heterostructures grown on GaAs and Si substrates with a different degree of misorientation was estimated using high-resolution X-ray diffraction. This study was performed with the use of reciprocal q-space maps for the investigated samples, since these maps facilitated the acquisition of direct information on mismatching of the crystal lattice parameters for the epitaxial film and substrate, misorientation or relaxation of a layer, dislocation density in the layer, and its mosaic structure or curvature. For example, distribution maps of diffracted radiation intensity in q-space around symmetric lattice site (004) and the asymmetric site are presented in Fig. 3 for a series of samples (#2, #3, #5) with a single-crystalline epitaxial layer.

Analysis of symmetric and asymmetric scans of reciprocal space demonstrated that only one site was present in the maps of sample #2 corresponding to the reflection from GaAs, thus indicating the coherent