Structural and optical characteristics of GaAs films grown on Si/Ge substrates

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Abstract. A GaAs/AlAs heterostructure and a GaAs film grown on Si/Ge substrates have been fabricated and studied. A Ge buffer on a silicon substrate was fabricated using the MBE process. A3B5 films were grown by MOCVD at low pressures. Photoluminescence spectroscopy was used to define the optical quality of A3B5 films. Structural properties were investigated using the electron beam induced current method. It was established that despite a rather high density of dislocations on the epitaxial layers, the detected photoluminescence radiation of layers indicates the acceptable crystalline quality of the top GaAs layer.

1. Introduction

Silicon is the most commonly used material for semiconductor devices due to its natural abundance, lesser weight, and better thermal conductivity. Next in popularity are GaAs and other A3B5 semiconductors, which are highly valued for their optoelectronic applications and high carrier mobility. The creation and investigation of A3B5 epitaxial structures on Si is a rapidly developing trend [1-2]. This trend is related to the solution for one of the major problems in modern functional microelectronics: creating optoelectronic elements of integrated microcircuits based on silicon. As a particular example, hybrid A3B5 heterolasers compatible with the complementary metal-oxide-semiconductor technology (CMOS) on Si provide the transition from copper wires to optical interconnects in high-performance processors [3].

The problem of creating these structures lies in the difference between the crystal lattices and thermal expansion coefficients of A3B5 and Si. Because of these differences, direct epitaxial growth of GaAs on Si is accompanied by the formation of a large number of defects that reduce the quality of a structure. Therefore, the fundamental task of the A3B5/Si heterostructure growth is a search for growth regimes that ensure an improvement in the quality of layers grown, namely, a reduction in the quantity of defects and dislocations that negatively affect the operation of devices built on the basis of such structures. This requires a combination of improvements to the appropriate technology with the use of advanced techniques for the in-depth study of A3B5 layers grown on Si substrates. In this paper, we report on the growth of GaAs-on-Si heterostructures and the study of these structures using the electron beam induced current (EBIC) measurements technique. The EBIC method combines high-
resolution visualization of electrically active defects in materials or structures with measurement of the
diffusion length of minority charge carriers [4]. The latter is a parameter that characterizes the quality
of a semiconductor material and determines the main characteristics of many semiconductor devices.

2. Fabrication of A3B5/Ge/Si structures
The A3B5/Ge heterostructures were grown on a part of a 2-inch epi-ready (100)-oriented Si substrate
with 4° off-cut toward (110). During the first stage, Si substrates were prepared as Ge intermediate
layers were deposited via molecular beam epitaxy (MBE) [5]. First of all, a 50-nm Ge layer was
deposited at 275 °C. A lower temperature was used to exclude elastic-strain relaxation via the
formation of three-dimensional islands. In this case, relaxation occurs via the formation of a large
number of misfit dislocations, and the layer with a high density of threading dislocations (> 10^{10} \text{ cm}^{-2})
is formed. Then the growth temperature was increased to 600°C and a 1-μm-thick Ge layer was
grown, which improved the crystalline quality. In the end, cyclic annealing was used (850°C/2 min,
550°C/2 min, 5 repetitions) to lower the density of threading dislocations after formation of the
structure.

During the second stage, A3B5 films were grown using a MOCVD system (AIX 200RF) at 50
mbar of pressure. The Si/Ge substrate was heated up to 650 °C in H₂ atmosphere for oxide removal
before epitaxial growth of A3B5. Then a 20-nm-thick AlAs nucleation layer was grown at 650 °C.
This layer also serves as a barrier to diffusion of Ge and As through the heterojunction [6]. After that,
a pair of 100-nm GaAs:C and 20-nm AlAs layers were alternately deposited, with 5 repetitions in
total. The carrier concentration in the GaAs:C layer amounted to 1·10^{18} \text{ cm}^{-3}. Next, a 1-μm GaAs:Si
layer was grown with a carrier concentration of 2·10^{18} \text{ cm}^{-3}. Trimethylgallium Ga(CH₃)₃,
trimethylaluminum Al(CH₃)₃ and arsine AsH₃ were used as precursors.

To analyze the quality of epitaxial layers, the optical characteristics of samples were investigated
by photoluminescence (PL) spectroscopy alongside with structural investigation by EBIC. For the
EBIC measurements, the Al Schottky contact was deposited to the top of the sample, and the Ohmic
contact was applied to the back of the sample. Details of EBIC technique are described elsewhere [4].

3. Photoluminescence study
The photoluminescence measurements were carried out with a Nanometrics RPM-2000 system that
allows scanning of samples with a resolution down to 0.1 mm. The results of measurements are the PL
maps that visualize the distribution of basic PL parameters over the area of a scanned sample. The
parameters are the wavelength of the PL peak maximum, the spectral width of the PL peak (FWHM or
full width at half maximum), the intensity of the spectra maximum, etc. PL was excited by an
Nd:YAG laser with a wavelength of 532 nm and an optical power density of 386.4 W/cm².

![Figure 1. PL spectra of the GaAs/AlAs/Ge/Si sample.](image1)

![Figure 2. The wavelength peak map of the GaAs/AlAs/Ge/Si sample.](image2)
The PL spectrum with a maximum at 873.3 nm corresponding to GaAs is shown in figure 1. Figure 2 shows the wavelength peak map. PL maps demonstrate the uniformity of the grown GaAs top layer. For instance, FWHM distribution amounts to 36.5±0.3 nm. This amount is higher than the average FWHM amount for PL peaks of GaAs grown on native substrates using the same MOCVD system (about 23 nm for layers with a comparable level of doping). This is explained by the presence of non-radiative recombination centers and charged defects.

4. Structural characteristics
The primary evaluation of the surface quality was performed by etching the GaAs surface using standard selective dislocation etchants and direct counting of etch pits using an optical microscope. An example of an etched GaAs surface image taken with a LEIKAI DM 4000M microscope is shown in figure 3. Average dislocation pit density was calculated for 5 fields of view and amounted to 2·10^5 cm^-2.

A more in-depth and comprehensive study was conducted using the EBIC method. The EBIC scan of the sample is presented in figure 4. One can see a complex of visualized bulk defects, which is probably due to the complexity of the structures including a number of interfaces. In particular, the black dots in the EBIC image correspond to the electrically active threading dislocations. The dislocation density estimated from the EBIC image is about 10^8 cm^-2.

![Figure 3. Etched GaAs surface image taken with an optical microscope.](image1)

![Figure 4. The EBIC image of the investigated sample measured under the electron beam with an accelerating voltage of 35 kV.](image2)

The revealed disagreement between the optical and EBIC estimations of the dislocation density is supposedly due to different regions of data collection used for the two methods. The optical data were collected from the top GaAs:Si layer, whereas the EBIC measurements may visualize the dislocations which grow from the Si substrate through the Ge buffer layer and are blocked at numerous GaAs/AlAs interfaces. Preliminary capacitance-voltage data confirm that the EBIC signal is most likely collected from the Ge buffer layer (with a hole concentration of about 3·10^17 cm^-3) in the vicinity of the Si/Ge interface. To validate this hypothesis, some additional experiments are required. However, a relatively high photoluminescence signal (figure 1) is another indication of the good quality of the top GaAs layer.

In conclusion, we have grown and investigated a GaAs/AlAs heterostructure and a GaAs film on Si/Ge substrates. Although the measurements reveal a relatively high dislocation density from the entire heterostructures, the top layer is probably of better crystalline quality and thus can be used as an active region for GaAs-based semiconductor devices.
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