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Doping profiles of n-type GaAs layers grown on Si by the conformal method

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ABSTRACT

We study doping profiles in selectively Si-doped GaAs layers grown by the conformal method. This growth technique allows to obtain GaAs/Si with optoelectronic quality. The samples are laterally grown, and selective doping with Si is carried out in such a way that doped stripes are intercalated with undoped ones. The study of the doping profiles was carried out by cathodoluminescence (CL) and micro-Raman (µR) spectroscopy. Abrupt doping profiles between doped and undoped stripes were demonstrated by monochromatic CL images. Deep level related CL bands can be observed between 1000 and 1400 nm, evidencing the complex mechanism for Si incorporation at the growth temperature (730 °C). Net doping concentrations and mobilities across the layers were determined from the analysis of the phonon-plasmon coupled modes in the µR spectra obtained with a lateral resolution better than 1 µm.

INTRODUCTION

Matching gallium arsenide to silicon, which currently shows up in special applications, that combine the low-cost robustness of silicon with the higher optoelectronic performance of the gallium arsenide, has been a technological goal for many years [1-5]. For example, this development could permit the integration of optical components like solid state lasers with the conventional electronic devices in the same chip, enabling on-chip and chip-to-chip optical interconnects; the design of new wireless devices, like radar systems that would help automobiles avoid collisions, and new semiconductor-based lighting systems. However, the obtention of defect free epilayers is subjected to some problems because of the large lattice (4%) and thermal (55%) mismatches between Si and GaAs, as well as the difficulties of growing a polar semiconductor on a non-polar one. Nowadays, important achievements were got using different deposition techniques and treatments (annealing[2], buffering layers in vertical growth[3], or passivating layers in lateral growth[4]). In spite of this, the density of crystal defects remains high enough to render unsuitable these layers for reliable optoelectronic applications. Pribat et al. [5,6] proposed an effective method to produce GaAs layers on Si substrates that consists of a lateral epitaxial growth on the sidewall of a GaAs seed stripe previously deposited on a Si substrate.

We present in this paper the study of doping profiles in selectively Si-doped GaAs layers grown by the conformal method, using optical techniques. The carried out measurements evidence the complex mechanism of Si incorporation in the GaAs layers.
EXPERIMENTAL DETAILS

The conformal GaAs layers were prepared according to the procedure previously described [5], on 2° misoriented (001) silicon substrates. First, 0.7–1.5 μm thick GaAs layers were grown by MOVPE. These sacrificial layers usually exhibit dislocation densities above $10^8$ cm$^{-2}$. Then, the GaAs layer is covered by a dielectric capping layer, in which either $<110>$ or $<110>$ oriented GaAs stripes are periodically opened (10 μm wide every 200 μm). The GaAs layer is then selectively underetched using an H$_2$SO$_4$/H$_2$O$_2$/H$_2$O solution, so as to obtain 125 μm wide GaAs seed stripes. Conformal growth is then carried out by selective hydride vapor phase epitaxy using gaseous GaCl and As$_4$ for the growth of GaAs and timely adding SiH$_4$ for the growth of doped layers intercalated with the undoped ones, see figure 1. The first layer consists of undoped GaAs whose growth is initiated on the lateral sidewalls of the GaAs seed stripes and develops laterally inside the cavity formed in between the oxidized silicon substrate and the overhanging dielectric capping layer. When this layer is about 3 μm width, silane is pushed into the reaction chamber to introduce the Si dopant in the GaAs film. This is maintained so up to growth a 3 μm wide doped stripe. Thereafter, the steps are repeated to produce up to 7 stripes at the growth temperature of 730 °C.

One has to note that the conformal growth allows for an independent control of the vertical and lateral extensions of the GaAs film, as the vertical one is settled by the thickness of the GaAs sacrificial layer. The 60° type threading dislocations initially present in the sacrificial layer cannot propagate far through the conformal GaAs growing layer as they are blocked by either the capping layer or the substrate itself. This constitutes an efficient geometrical dislocation filter as shown in figure 1. The thin SiO$_2$ layer formed from the oxidation of the Si substrate during the underetching step was not removed before the conformal growth step.

The optical and transport properties of the samples were studied by cathodoluminescence (CL) and micro-Raman (μR) spectroscopy. The CL measurements were done in a scanning electron microscope (SEM) using an Oxford mono-CL2 system and were carried out at liquid-nitrogen temperature. The Raman spectra were recorded using a DILOR spectrometer with a liquid-nitrogen-cooled charge coupled device (CCD) detector, attached to a metallographic microscope. The scattered light is collected by the microscope objective conforming a nearly backscattering geometry. The Raman spectra were taken at room temperature. The frequencies and linewidths of the longitudinal optic (LO) phonon and LO phonon-plasmon coupled (LOPC) modes were determined by fitting with an spectral accuracy of approximately 0.1 cm$^{-1}$. The spectra were calibrated using a plasma line of the laser.

![Figure 1. Schematic view of the conformal growth process showing the formation of the different doped and undoped stripes and the dislocation blocking mechanism.](image)
DISCUSSION

Raman spectra

The Raman spectra of the GaAs conformal stripes excited under non-resonant conditions with the 514.5 Å Ar⁺-laser line in the backscattering geometry shows the LO-phonon mode and the forbidden by symmetry selection rules TO mode. The appearance of the TO mode is possibly due to the misalignment from the true backscattering geometry. The n-doped stripes, shows the coupled LO phonon-plasmon modes \( L_+ \) and \( L_- \) with frequencies \( \omega_+ \) and \( \omega_- \), respectively; the uncoupled LO phonon mode from the depletion layer and the second-order phonon spectrum in some cases overlapping the relatively broad \( L_+ \) mode.

Figure 2 shows the typical spectra obtained from an undoped GaAs stripe (figure 2a) and from an n-type doped GaAs stripe (figure 2b). The structure near the LO peak is related to the second-order phonon bands \( TO + TA(X,K) \) associated with different crystal perfections [7]. In n-GaAs the position of the \( L_+ \) mode strongly depends on the charge carrier concentration and can be used for its calculation. The LO phonon peak intensity decreases with the carrier concentration due to the decrease of the depletion layer. The determination of the frequency of the LOPC mode is sometimes complicated by the strong damping of the high-energy \( L_+ \) mode and its superposition with the second-order phonon spectrum, specially the \( 2LO(\Gamma), 2TO(\Gamma) \) and \( 2TO(X,K) \) peaks. To overcome this problem and avoid confusions with possible LOPC peaks, the second-order phonon spectrum was substracted from the spectra. In this case, the carrier concentration can be calculated using the known relation for the low (\( L_- \)) and high (\( L_+ \)) frequency branches obtained by solving the system dielectric function \( \varepsilon(\omega) = 0 \) longitudinal modes for n-type doping [8]:

![Raman Shift Diagram](image)

**Figure 2.** Typical Raman spectra obtained from (a) an undoped GaAs stripe and (b) an n-type doped GaAs stripe of the conformal layer formed with 7 different intercalated stripes.
\[ \omega_1^2 = \frac{1}{2} \left( \omega_{LO}^2 + \omega_p^2 \right) \pm \left( \left( \omega_{LO}^2 + \omega_p^2 \right)^2 - 4 \omega_p^2 \omega_{TO}^2 \right)^{1/2} \]  \hspace{0.5cm} (1)

and the expression: \( \omega_p^2 = n e^2 / \varepsilon_0 m^* \) for the plasmon frequency, where \( \omega_{LO}, \omega_p, \omega_{LO}, \omega_{TO} \) and \( \omega_p \) are the frequencies of the high and low LOPC branches, LO and TO phonon modes and the plasmon respectively. Using \( m^* = 0.0632 m_0 \) and \( \varepsilon = 10.6 \) for GaAs, the following expression can be obtained for calculating the carrier concentration:

\[ n = 7.49 \times 10^{12} \omega_p^2 \left[ \text{m}^{-3} \right] \]  \hspace{0.5cm} (2)

Here \( \omega_p \) is given in cm\(^{-1}\).

The calculated carrier concentration for our Si-doped GaAs conformal stripes using Eq. 2, is shown in figure 3a. These results show relatively abrupt interfaces as was expected keeping in mind that the laser spot is not punctual. The expected increase in the carrier concentration with the SiH\(_4\) flow is also observed but the \( \mu \)R spectra calculated concentrations are larger than the expected values.

The free carrier mobility is obtained from the damping constant \( \Gamma_p \) of the high-energy branch (L\(_+\)) of the LOPC mode using the expression \( \mu_p = e / m^* \Gamma_p \), where \( e \) is the electron charge and \( m^* \) the electron effective mass. For n-type GaAs this expression can be reduced to:

\[ \mu_p = 1.48 \times 10^5 \left( \frac{1}{\Gamma_p} \right) \left[ \frac{\text{cm}^2}{\text{Vs}} \right] \]  \hspace{0.5cm} (3)

Here \( \Gamma_p \) is in cm\(^{-1}\). The calculated data are represented in figure 3b and the average values of carrier concentration and mobility for the three doped stripes are summarized in table I. As can be observed from the \( \mu \)R spectra of the doped stripes, the high-energy branch (L\(_+\)) of the LOPC mode is highly damped, making difficult a precise calculation of the free carrier mobility. It strongly depends on the \( \mu \)R spectra base line.

**Cathodoluminescence measurements**

Figure 4 shows CL images taken at (a) 830 nm and (b) 1150 nm respectively. The band-to-band (830) emissions from the undoped GaAs conformal stripes are clearly observed in figure
Table I. Calculated values of the carrier concentration and mobility for the three different doped stripes in the conformal layer.

<table>
<thead>
<tr>
<th>Stripe (see Fig. 5a)</th>
<th>SiH₄ flow (cm²/min)</th>
<th>( \bar{n} ) (x 10¹⁸ cm⁻³) (by silane flow)</th>
<th>( \bar{n} ) (x 10¹⁸ cm⁻³) (by Eq. 2)</th>
<th>( \mu ) (cm² V⁻¹ s⁻¹) (by Eq. 3)</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>2</td>
<td>0.8 ± 0.2</td>
<td>3.7 ± 0.2</td>
<td>2002 ± 652</td>
</tr>
<tr>
<td>4</td>
<td>4</td>
<td>2</td>
<td>4.7 ± 0.3</td>
<td>1451 ± 484</td>
</tr>
<tr>
<td>6</td>
<td>6</td>
<td>4</td>
<td>5.0 ± 0.2</td>
<td>1176 ± 422</td>
</tr>
</tbody>
</table>

Figure 4a, while the impurity related transitions (1150 nm) are observed in figure 4b. Figure 5a shows the CL intensity profiles obtained across the conformal sample in the position shown by the white line in the inset CL image. The intercalated undoped and Si-doped stripes are clearly observed and both the CL image and the CL intensity profiles show the abruptness of the interstripes interfaces. The slight superposition in the intensity profiles is due to the size of the incident electron beam. Figure 5b shows the CL spectra of the different doped and undoped stripes numbered in the inset image of figure 5a. The spectra of the undoped stripes 3, 5 and 7 have a 10x magnification for better observation. The broad peak observed at about 1150 nm is related to Si complexes formed as a result of doping at temperatures below 750°C. This broad emission band corresponds mainly to the so called self-activated (SA) luminescence band. The SA center responsible for this luminescence is said to be due to a deep acceptor (VGa) with a bound donor (SiGa) [9], and the emission is related to the internal transitions of electrons between the excited and ground states of the SiGa – VGa complex [10].

CONCLUSIONS

The transport and optical properties of selectively doped GaAs conformal stripes grown by selective hydride vapor phase epitaxy, have been studied. The free carrier concentration and mobility were determined from the high-energy branch \( L⁺ \) of the LOPC mode. Abrupt interfaces between doped and undoped stripes were revealed by CL images and intensity profiles taken at 80K. The CL spectra of the Si-doped GaAs stripes are dominated by the self-activated luminescence band produced by Si-complexes normally formed in Si-doped GaAs layers grown below 750 °C.

Figure 4. 80K monochromatic CL spectra taken on the GaAs conformal layer at two different wavelengths : a) 830 nm and b) 1150 nm. The bright stripes in (a) correspond to band-to-band transitions in the undoped stripes, while the bright stripes in (b) to the Si complex transitions in the doped stripes. Abrupt interfaces are clearly observed in both images.
Figure 5. (a) CL intensity profiles taken across the GaAs conformal layer. (b) CL spectra from the different stripes numbered in the inset CL image of (a). The spectra were taken at 80 K.

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REFERENCES