# Pregrowth treatment induced below-bandgap states in GaAs

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## Abstract

Below-bandgap states induced by pre-epitaxial growth treatments in GaAs have been investigated by photoluminescence (PL). Various electronic states giving rise to near-infrared (NIR) PL peaks are generated through processes such as annealing or buffer growth that are standard for epitaxial growth of InAlGaAs structures on (001) GaAs substrates. These states often overlap with those from InGaAs structures, not only complicating the interpretation by also altering the electronic properties of the devices. The present work provides guides for distinguishing the desired electronic states from the pregrowth treatment-induced defect states.

### 1. Introduction

During the past few decades, GaAs-based materials have played a key role in optical devices. In particular, for applications such as near-infrared (NIR) telecommunications or intermediate band solar cells, use of InAlGaAs-based structures on (001) GaAs wafers has been intensively explored. During the course, the presence of various below GaAs bandgap states induced by defects has been reported. Since such defect states often degrade the device performances, their origin and ways to avoid their formation have been investigated [1-4].

Defect states may exist intrinsically, but also may be induced by dopants or by sample treatments such as high temperature annealing. However, we find that various defect states can be generated by standard treatments used in molecular beam epitaxy (MBE) or metalorganic chemical vapor deposition (MOCVD), at temperatures that are not particularly 'high.' Many of these states lie at levels that overlap with NIR devices. While we reported that As-antisite (Ga<sub>As</sub>) defects may act as a shallow intermediate state for photon upconversion [5], most defect states degrade the device performance. Here, we performed a systematic study on the formation of defect states by pre-MBE growth treatments.

## 2. Experiments and Results

The below-bandgap states formed in GaAs wafers by pregrowth processes employed in MBE, i.e., prebaking at ca. 300°C, oxide desorption at ca. 600°C, and buffer growth at ca. 590°C, on s.i. (001) GaAs wafer supplied by Wafer Technology Ltd. (vertical gradient freeze). The treatments are all those inevitable regardless of the device structures to be grown [6]. Buffer growth was performed using solid source MBE with As<sub>4</sub> beam equivalent flux of ca  $7.8 \times 10^4$  Pa. Photoluminescence (PL) measurements were performed using Ti:sapphire laser with wavelength of  $\lambda_{ex}$  : 700 ~ 900 nm

as the excitation light at 4K. Below-bandgap excitation at  $\lambda_{ex}$  > 820 nm provided us with information about electronic states spatially lying deep inside the wafer due to long penetration depth. Two detectors, which are sensitive to signals at 1 to 1.7  $\mu$ m and 1.2 to 2.2  $\mu$ m, were used.

A typical PL spectrum using above bandgap excitation at  $\lambda_{ex} = 740$  nm observed from the as supplied s.i. GaAs substrate is shown in Fig. 1. The 818 nm peak is bulk GaAs band edge free exciton peak and the 828 nm is carbon-related. The broad peaks at ca. 1550 nm and 1910 nm are assigned to those from Ga<sub>As</sub>-antisite and EL2 defects [2,3]. These defect states cannot be ignored when GaAs wafers are used for NIR devices.



Fig. 1 Photoluminescence spectrum of as-supplied s.i. GaAs substrate excited at 740 nm measured at 4K. Sharp peaks at 818 and 828 nm correspond to the free-exciton (FE) and free-exciton to carbonacceptor (FE-A) transitions respectively.

We now look into a sample that has gone through the three processes, prebake at 300°C, oxide desorption at 600°C, and buffer growth at 590°C. The PL spectra obtained are shown in Fig. 2. The blue solid curve is obtained by above bandgap excitation (AGE)  $\lambda_{ex} = 740$  nm. The 815 nm peak is bulk GaAs band edge, and the 825 nm is carbon-related, as observed in the as-supplied wafer. The broad peak extending beyond 1.3 µm is due to from Ga<sub>As</sub>-antisite and EL2 defects as already discussed.

The red solid curve shows the PL of below bandgap excitation (BGE)  $\lambda_{ex} = 840$  nm. The excitation light penetrates deep into the sample, and so does the PL signal. A new peak is found to have arisen at around 940 nm. Previous works suggest that the peak is most likely due to Ga<sub>As</sub>-antisite [1] or  $V_{As}$ -vacancy [3]. The broad structure observed between 1000 to 1300 nm can be deconvoluted into peaks of 1000 nm and 1150 nm, which are attributed to  $V_{Ga}$ -vacancy [4] and InGaAs states [6]. The latter, InGaAs states, arises due to diffusion of backside In solder which is used to fix the substrate onto Mo block for MBE, into the bulk. For this reason, the InGaAs peak should be localized close to the back surface of the wafer. This assumption is supported from the fact that the 1150 nm peak is only observed in the BGE spectrum in which the excitation beam can penetrate deep in from the front surface. Finally, we note that the intensities of the additional peaks found in the BGE PL are much stronger than that of excitonic transition in the AGE PL for a given excitation power, highlighting their potential influence to the performance of NIR devices.



Fig. 2 Photoluminescence spectrum of 100-nm GaAs buffer sample excited at 740 nm for AGE and at 840 nm for BGE at 4K. Dashed lines are fits of the BGE data. Peaks at 940, 1000, and 1150 nm are attributed to the As-vacancy ( $V_{As}$ ) defect, Ga-vacancy ( $V_{Ga}$ ) defect, and InGaAs states, respectively.

A summary on the observed below-bandgap states are given in Table I.

| Table I Summary of observed PL peaks. |   |                          |               |  |
|---------------------------------------|---|--------------------------|---------------|--|
| λ <sub>PL</sub><br>(nm)               | E(eV)                                     | Δλ <sub>PL</sub><br>(nm) | ΔE<br>(meV)   | Identity   |
| 815                                   | 1.52                                      | 4.7                      | 8.8           | GaAs band edge   |
| 825                                   | 1.50                                      | 4.7                      | 8.6           | Carbon-related   |
| 940                                   | 1.32                                      | 31.5                     | 44.6          | Ga <sub>As</sub> -donor [1] or<br>V <sub>As</sub> -related [3] |
| 1000                                  | 1.24                                      | 269                      | 253           | V <sub>Ga</sub> -related [4]                                   |
| 1150                                  | 1.07                                      | 24.8                     | 37.6          | InGaAs states [6]  |
| 1550<br>1910                          | $\begin{array}{c} 0.80\\ 0.65\end{array}$ | 346.7<br>263.2           | 181.4<br>89.0 | Ga <sub>As</sub> antisite [2,3]<br>EL2 [2,3]                   |

These electronic states are formed unintentionally, and interfer with the device performances, and hence needs to be dealt separately from those that are designed. We will discuss how these states are generated, and show further evidence to support our model. In the meantime, to extract the maximum performance from GaAs-based NIR devices, it is necessary to explore methods to reduce or passivate these defects, if not, conversely, make use of these defects as the origin of the working NIR states [7]. Possible countermeasures, including epitaxial lift-off techniques and specialized buffer layers, may be worth exploring in future studies.

### 3. Conclusions

A systematic study on the formation of defect states by pre-MBE growth treatments has been performed by PL spectroscopy. It was observed that defects such as EL2, Ga<sub>As</sub>-antisite,  $V_{As}$ -/ $V_{Ga}$ -vacancies, and InGaAs states can be formed by pregrowth treatments, and that they should be distinguished from the desired electronic states used for NIR devices.

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