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Control of GaAs on Si Interface Using Atomic Layer Epitaxy

Kuninori KITAHARA, Nobuyuki OHTSUKA, Osamu UEDA, and Masashi OZEKI

Fujitsu Laboratories Ltd., 10-1 Morinosato-Wakamiya Atsugi 243-01, Japan

Control of GaAs on Si interface was made by atomic layer epitaxy (ALE) suppling source gases as a pulsed jet. The species of prelayers (As, Ga, and Al) and buffer layers (GaAs and AlAs) were varied for examine the initial stages of ALE. The crystalline quality of the GaAs active layers grown on them were also examined. An in-situ reflection high-energy electron diffraction developed for the vapour-phase epitaxy and other techniques were used for measurements. The best results were obtained with an AlAs buffer layer on As prelayer grown at 850°C.

1. Introduction

The growth of GaAs on Si has applications to monolithic ICs and integrated optoelectronics. However, mismatches of lattice constant, polar-nonpolar, surface free energy, and thermal expansion can all generate a high dislocation density and cause island growth at the initial stage. Although these problems are reduced by two-step growth,[1] better crystalline quality is required.

Recently, atomic-layer epitaxy (ALE) using apparatuses for molecular-beam epitaxy (MBE) or vapour-phase epitaxy (VPE) has been used to grow GaAs on Si.[2-5] We have reported the ALE of GaAs on Si by pulsed-jet epitaxy (PJE)[2,3] a VPE technique. Single crystal GaAs could be grown directly on Si substrates. The coverage of initial growth on Si was remarkably improved by initiating the growth from AlAs instead of GaAs.

PJE can control the heterointerface because it is self-limiting at a period of an atomic layer.[6] However, as other VPE techniques, it is not easy to find the optimum conditions for initial growth because of the lack of in-situ observation techniques such as reflection high-energy electron diffraction (RHEED) in MBE. Although GaAs growth can be analyzed by other observations after it is removed from the reactor, AlAs cannot be directly examined because exposure to air severely degrades the surface.

In this paper, we controlled the heterointerface by varying the prelayer atoms (As, Ga, and Al) and the buffer layers grown on them (GaAs and AlAs). Coverage was estimated with Auger electron spectroscopy (AES). AlAs layers were covered with GaAs. We developed new system combining RHEED and a VPE reactor to eliminate uncertainty involved in these measurements. The lattice structure at the heterointerface was observed with a transmission electron microscopy (TEM). We used X-ray diffraction and mesa etching to examine the effects of the heterointerface control on the quality of GaAs active layers.

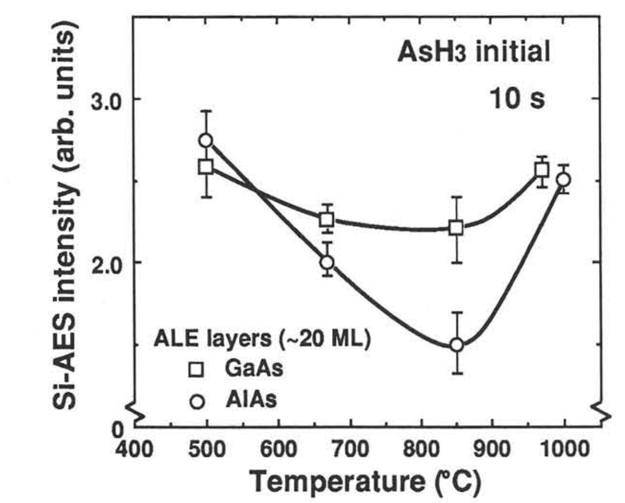

Fig. 1 Relationship between the Si-AES intensity and the temperature of the As-prelayer deposition.

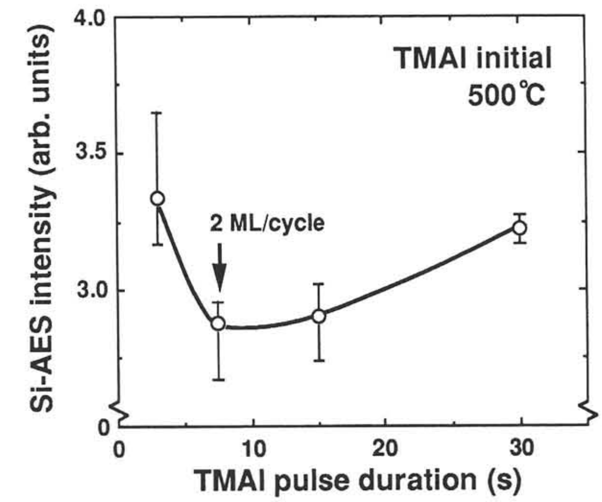

Fig. 2 Relationship between the Si-AES intensity and pulse duration of the TMAl in prior to the ALE-AlAs growth.

2. Experiment

Growth conditions have been detailed elsewhere.[3] In brief, substrates were (100) Si tilted 2-3° toward [011]. Thermal cleaning of the substrate was done at 1000°C for 20 min in a H_2 flow. Source gases were arsine (AsH_3), trimethyl gallium (TMGa) and trimethyl aluminium (TMAl). After prelayers were deposited under various conditions, GaAs and AlAs were grown by ALE at 500°C and a reactor pressure of 20 torr. The gas sequence of the ALE cycle was 5 s of TMGa or 7.5 s of TMAl→3 s of H_2 purge→10 s of AsH_3→3 s of H_2 purge. This cycle grew 1 monolayer (ML) of GaAs or 2 ML of AlAs on a GaAs substrate.[6] 3-μm-thick GaAs active layers were grown on ALE-buffer layers by metalorganic-vapour-phase epitaxy (MOVPE) at 1 μm/hour faster than ALE. MOVPE was done at a substrate temperature of 600°C and 50 torr.

ALE in the new reactor was done under the same conditions described above, except thermal annealing of Si was done at 830°C for 10 min and under 12 torr. Immediately after the interruption of gas supply, the reactor was evacuated and RHEED observation was made.

3. Observation of initial stage

We studied how prelayer deposition conditions affect coverage. Relative coverage of layers grown on Si was estimated from the Si AES intensity. In Fig. 1, the AES intensity of the Si-*KLL* transition is plotted as a function of the temperature of the initial AsH_3 supply. Samples with 20 or 21 ML were used for the measurement. The AlAs was covered with 10 ML of GaAs as a cap layers. For both GaAs and AlAs, AES intensity was at least at 850°C, indicating the largest coverage at this temperature. Coverage of AlAs on Si is better than that of GaAs, as we reported before.[2]

Figure 2 is the relationship between the Si AES intensity and the pulse duration of initial TMAl. The Si AES intensity was minimum at a pulse of 7.5 s, the same as the pulse duration for TMAl in ALE AlAs growth at 2 ML/cycle. A lack or excess of Al atoms on the Si substrate decreases the coverage of the ALE-AlAs layer grown on the prelayer.

RHEED observation of the initial stage was done at 500°C, the ALE growth temperature. Desorption of oxide from the Si surface was confirmed by appearance of the 2×2 surface reconstruction image. Figure 3 shows RHEED images with a [011] azimuth at the three steps; prelayer deposition, the first cycle of ALE, and the second cycle of ALE. By suppling TMGa or TMAl to deposit the prelayer, RHEED intensity decreased and the surface reconstruction image became unclear, but there were no spots corresponding to island growth. Depositing As prelayer at 500°C resulted in appearance of weak spots. Clear spots were not observed for As prelayer deposited at 850°C. After 1 cycle of ALE, intensive spots began to appear for GaAs but not for AlAs. Of AlAs grown on prelayers of As at 500°C, As at 830°C and Al at 500°C, the last had the most streaky image. The difference due to As supply temperature is consistent with the results of AES shown in Figs. 1 and 2 and is interpreted with the dependence of As-Si bonding strength on temperature.[7]

4. Characteristics of overlayers

By controlling the species of prelayer atoms, the domain alignment of overlayers can be determined. To study domain alignment, we grew GaAs MOVPE layers on two kinds of ALE AlAs (100 ML). The prelayer was either As deposited at 850°C or Al deposited at 500°C. We decided the domain orientation with facets appeared after the mesa etching through striped masks. Photographs in Fig. 4 indicate that the domain orientation of the As-initiated sample is orthogonal to that of the Al-initiated sample.

The crystalline quality of 3-µm-thick MOVPE layers grown on three different ALE layers was examined in term of the full width at half maximum (FWHM) of the X-ray rocking curves (Table 1). The largest FWHM was obtained with the GaAs buffer layer (Ga initial). With the AlAs buffer, the FWHM for the As initiated sample was 273 arcsec, much smaller than 415 arcsec of the

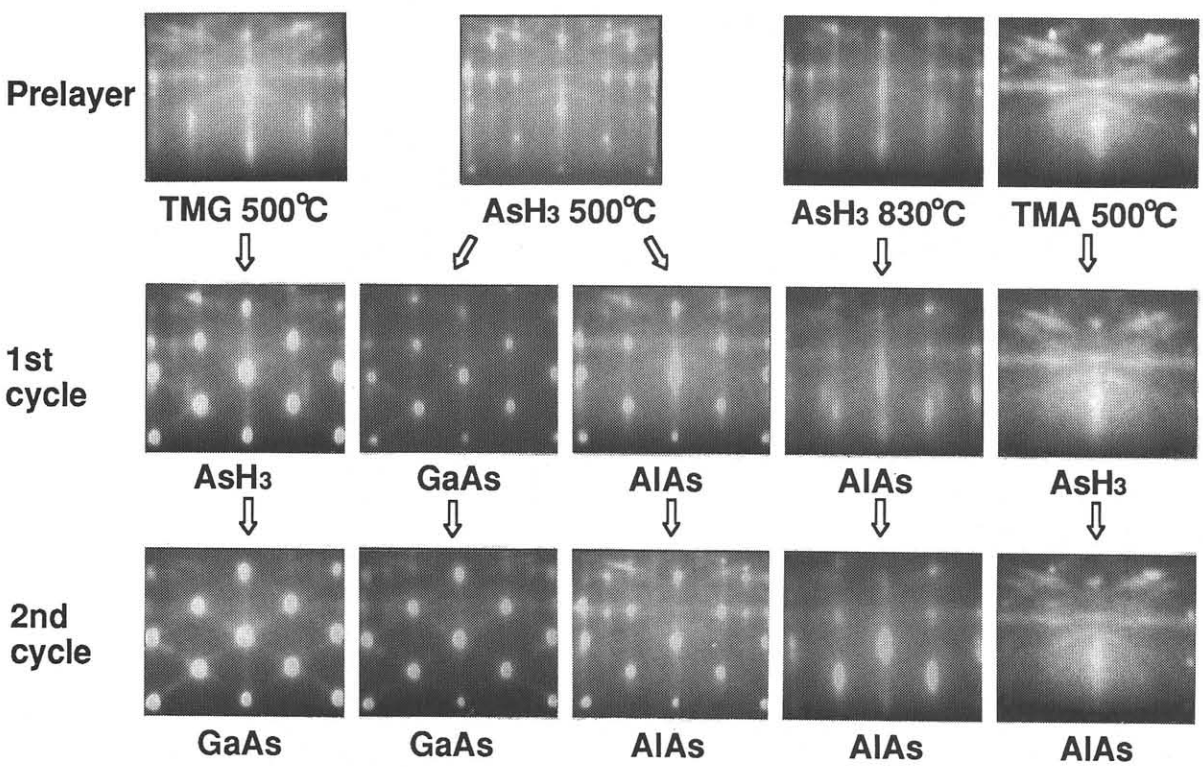

Fig. 3 RHEED images of GaAs and AlAs at the initial stage of growth.

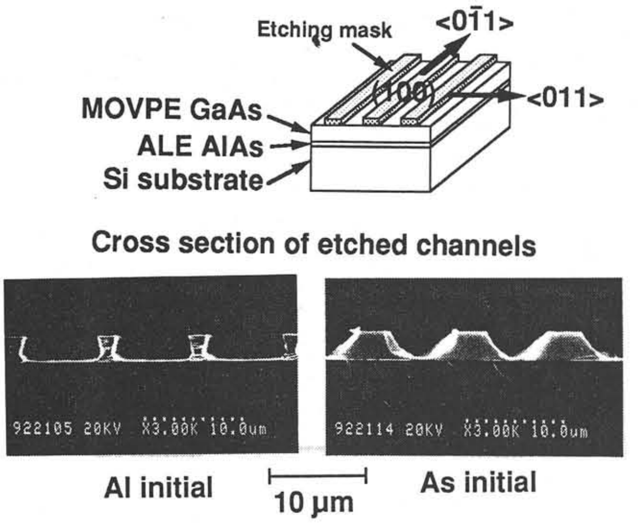

Fig. 4 Domain orientations of MOVPE GaAs layers grown on ALE AlAs. The base layer was Al deposited at 500°C or As deposited at 850°C. The observation was made along the same axis.

Al-initiated sample. After post-annealing at 850°C for 20 min with SiO_2 passivation, FWHM decreased to 176 arcsec in the Al-initiated samples and 153 arcsec in the As-initiated samples. This indicates that the mosaic structure enlarging the FWHM was eliminated by initiating the ALE AlAs from the As deposition and the post annealing.

5. Summary

ALE and AlAs buffer layers were used to control GaAs on Si interface. In addition to conventioal measurements, the new equipment combining RHEED and a VPE reactor was used to analyze the initial stage of growth. Coverage on Si depends on not only the species of the buffer layers but also the prelayers. The best coverage was obtained with an AlAs buffer layer on an As prelayer deposited at 850°C. The smallest X-ray FWHM was obtained by growing the GaAs active layer on this buffer layer. The initial stage of GaAs growth was three dimensional and that of AlAs growth was two dimensional, which is consistent with AES results. The difference of prelayer (As and Al) also caused the change of the domain alignment of GaAs overlayers grown on AlAs buffer layers indicating that the species of the prelayer atoms were controlled.

Table 1 Rocking curve FWHM of 3 µm thick MOVPE GaAs grown on ALE buffer layers.

Buffer layers	FWHM (arcsec) As-grown	FWHM (arcsec) Annealed
ALE GaAs (Ga initial)	553	249
ALE AlAs (Al initial)	415	176
ALE AlAs (As initial)	273	153

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