

Growth of GaAs on Si(100) with $(\text{GaAs})_{1-x}(\text{Si}_2)_x/\text{GaAs}$ Strained-Layer Superlattice by Migration-Enhanced Epitaxy

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$(\text{GaAs})_{1-x}(\text{Si}_2)_x/\text{GaAs}$ strained-layer superlattices (SLS) have been used as buffer layers to reduce the dislocation density in GaAs on Si grown by migration-enhanced epitaxy. $(\text{GaAs})_{1-x}(\text{Si}_2)_x$ layers relax little, even at high growth temperatures ($\sim 500^\circ\text{C}$) compared with $\text{In}_x\text{Ga}_{1-x}\text{As}$, which is a constituent of conventional SLSs. Cross-sectional transmission electron microscopy investigations revealed extensive threading dislocation bending at the $(\text{GaAs})_{1-x}(\text{Si}_2)_x/\text{GaAs}$ SLSs. Etch-pit density measurements indicated average dislocation densities of $\sim 5 \times 10^5 \text{ cm}^{-2}$, more than half an order of magnitude lower than for samples with ordinary $\text{In}_x\text{Ga}_{1-x}\text{As}/\text{GaAs}$ SLSs. The $(\text{GaAs})_{1-x}(\text{Si}_2)_x/\text{GaAs}$ SLS is thus more promising for reducing the dislocation density in GaAs grown on Si at high temperatures than are conventional SLSs, such as $\text{In}_x\text{Ga}_{1-x}\text{As}/\text{GaAs}$.

1. Introduction

The heteroepitaxial growth of GaAs on Si substrates (GaAs/Si) has attracted much attention in recent years because of its potential for integrating Si- and GaAs-based device structures. In previous papers¹⁻³, we demonstrated that low-temperature (300°C) migration-enhanced epitaxy (MEE) growth can produce very low dislocation density ($\sim 7 \times 10^4 \text{ cm}^{-2}$) GaAs/Si with the aid of an $\text{In}_{1-x}\text{Ga}_x\text{As}/\text{GaAs}$ strained-layer superlattice (SLS). However, an important problem is that annealing at temperatures above 450°C increases the dislocation density. This is partially due to strain relaxation of the SLS.

Recently, pseudobinary alloys $(\text{GaAs})_{1-x}(\text{Si}_2)_x$ were successfully grown by MEE on GaAs (100) substrates in the range of $0 < x < 0.25$.⁴ We also found that the alloys are promising materials for an SLS buffer layer for overcoming the aforementioned problem.⁵

In this paper, we report preliminary results on the characteristics of those alloys and their application as an SLS buffer layer for GaAs/Si, although high quality alloys can be grown only at substrate temperatures above 500°C at this stage.

2. Experimental

A three-chamber MBE system was employed to grow the GaAs and the $(\text{GaAs})_{1-x}(\text{Si}_2)_x$ alloys. During the GaAs growth in the MEE mode, the Ga and As₄ beam shutters are opened alternately. In the $(\text{GaAs})_{1-x}(\text{Si}_2)_x$ alloy growth, conventional PBN effusion cells were used for Si beam generation. Because of the low Si beam flux and the relatively high growth temperature ($\sim 530^\circ\text{C}$) the As₄ beam shutter opening was made to coincide with the Si deposition so as to suppress the re-evaporation of As₄. The alloy composition was varied by changing the shutter opening time for the Si cell.

In a preliminary experiment, we grew the $(\text{GaAs})_{1-x}(\text{Si}_2)_x$ alloy layers on GaAs (100) substrates. The growth of these layers has been reported in detail elsewhere.⁴

For the study of GaAs/Si growth, we used 3-inch Si (100) substrates with off-orientations of 2° toward the [011] direction. The details of the MEE growth and of the substrate preparation have been described elsewhere.^{1,2} A standard two-step growth procedure was employed for these samples. The layer structure is shown in Fig. 1. We inserted 3 SLS packets of 5-periods of $(\text{GaAs})_{1-x}(\text{Si}_2)_x/\text{GaAs}$, with $x=0.2$, where the $(\text{GaAs})_{0.8}(\text{Si}_2)_{0.2}$ layer is 20nm thick and the GaAs is about 17nm. Before growth, the Si substrate was heated at 1000°C for 15 min to remove the surface oxide layer and to form a single-domain surface structure. After the substrate was cooled to 300°C , a 100-nm-thick GaAs layer was grown by MEE to serve as a initial nucleating buffer layer. This was followed by a 15 min annealing at 580°C . Then, the GaAs layers and three SLS packets of 5-period $(\text{GaAs})_{0.8}(\text{Si}_2)_{0.2}/\text{GaAs}$ were grown at 520°C by MEE (Fig. 1). The top GaAs layer of $3.0 \mu\text{m}$ was grown by either MBE (at 580°C) or MEE (at 530°C). The total film thickness was about $4 \mu\text{m}$ for all GaAs/Si samples. For comparison, GaAs/Si samples with conventional $\text{In}_x\text{Ga}_{1-x}\text{As}/\text{GaAs}$ SLSs were also prepared. Here, it should be noted that the present SLS parameters, such as the Si percentage, thickness and period, have not been optimized.

For these samples, the x-ray diffraction was measured with a high-resolution double-crystal x-ray diffractometer. Some of the samples were also examined by transmission electron microscope (TEM) and etch-pit density (EPD) observations. The EPD was determined by Nomarski optical microscopy for samples etched in molten KOH for 4 min at 350°C .

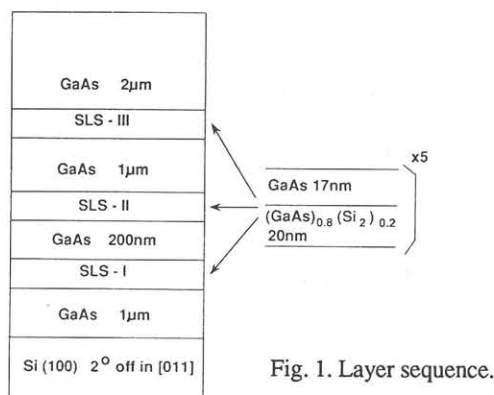


Fig. 1. Layer sequence.

3. Results and Discussion

First, we report preliminary results on the characteristics the $(\text{GaAs})_{1-x}(\text{Si}_2)_x$ alloys. Structural analysis of the $(\text{GaAs})_{1-x}(\text{Si}_2)_x$ layers indicated a single-crystal zincblende structure with no evidence of phase separation. The lattice constant of the alloys decreased nearly linearly with increasing Si content, in good agreement with Vegard's rule (Fig. 2). In conventional SLSs, the typical mismatch between the constituent materials is about 0.5 to 1%. The mismatch of the $(\text{GaAs})_{1-x}(\text{Si}_2)_x$ alloy to GaAs is about 0.8% for x of

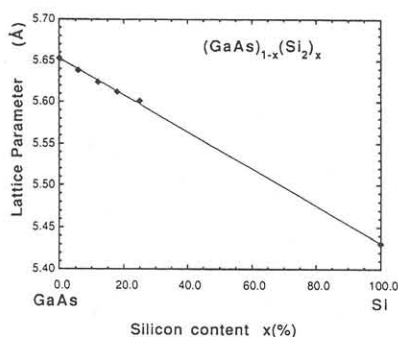


Fig. 2. Measured variation in lattice constant for $(\text{GaAs})_{1-x}(\text{Si}_2)_x$ alloys as a function of x .

about 0.2. Double-crystal X-ray diffraction rocking curve measurements and cross-sectional TEM microscopy studies on a 10-period $(\text{GaAs})_{0.8}(\text{Si}_2)_{0.2}/\text{GaAs}$ SLS grown on a GaAs substrate⁴ indicate sharp and abrupt interfaces of high crystalline quality. The $(\text{GaAs})_{1-x}(\text{Si}_2)_x/\text{GaAs}$ SLS, therefore, can be used as buffer layers to reduce the threading dislocation density in GaAs/Si.

Figure 3 shows the variation of misfit strain and lattice mismatch for 500 nm of $\text{In}_x\text{Ga}_{1-x}\text{As}$ and $(\text{GaAs})_{1-x}(\text{Si}_2)_x$ grown on GaAs (100) substrates at 500°C. The lattice mismatch was calculated from x as determined by SIMS measurements, while the misfit strain was obtained from x-ray diffraction measurements. With increasing Si or In content, x , the misfit strain increases in proportion to the lattice mismatch, as shown by the dashed line in Fig. 3, if the misfit is accommodated not by misfit dislocation generation but only by elastic deformation. Therefore, if the strain is relaxed by generation of misfit dislocations, the strain should be lower than that shown by the dashed line in the figure. The figure shows that the $(\text{GaAs})_{1-x}(\text{Si}_2)_x$ alloys are not relaxed in the range of $0 < x < 0.25$, probably because of the relatively strong Si-

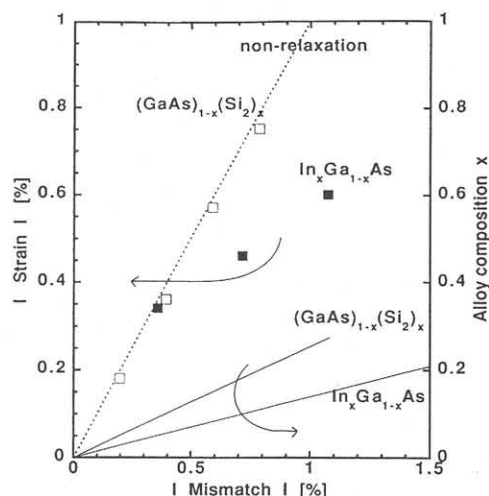


Fig. 3. Residual strain of $(\text{GaAs})_{1-x}(\text{Si}_2)_x$ and $\text{In}_x\text{Ga}_{1-x}\text{As}$ alloys as a function of lattice mismatch.

Si covalent bond. On the other hand, strain relaxation seems to occur in case of $\text{In}_x\text{Ga}_{1-x}\text{As}$, where the misfit is larger than 0.1%. As pointed out in our previous reports,²⁾ low-temperature ($\sim 300^\circ\text{C}$) grown $\text{In}_x\text{Ga}_{1-x}\text{As}/\text{GaAs}$ SLSs are hardly relaxed in the range of $0 < x < 0.3$, but high-temperature ($\sim 580^\circ\text{C}$) grown $\text{In}_x\text{Ga}_{1-x}\text{As}/\text{GaAs}$ SLSs easily relax when $x > \sim 0.1$. The present results, therefore, indicate that the $(\text{GaAs})_{1-x}(\text{Si}_2)_x/\text{SLS}$ is more promising than conventional SLSs such as $\text{In}_x\text{Ga}_{1-x}\text{As}/\text{GaAs}$, as the $(\text{GaAs})_{1-x}(\text{Si}_2)_x$ hardly relaxes, even at high growth temperatures.

It has also been suggested that a very effective way of decreasing the dislocation density is to use SLSs in which the constituent materials not only differ in strain but also have a substantial difference in elastic stiffness constants.⁶⁾ In this way it may be possible to deflect threading dislocations by using both strain and the elastic shear moduli of the individual layers. In such a situation, even when the strain in the layer is decreased and becomes less effective, the repulsion of the dislocations arising from the shear modulus mismatch remains unaffected. This is another reason for use of the alloy. The strong Si-Si covalent bond is expected to make the elastic stiffness constant (or shear modulus) of $(\text{GaAs})_{1-x}(\text{Si}_2)_x$ be higher than for any III-V compound. We adopted the $(\text{GaAs})_{1-x}(\text{Si}_2)_x/\text{GaAs}$ SLS for the buffer layers to reduce the threading dislocation density in GaAs on Si. Next, the results of applying the SLS will be discussed.

Figure 4 shows a typical cross-sectional TEM micrograph near SLS-I and SLS-II in a GaAs/Si sample with three packets of $(\text{GaAs})_{0.8}(\text{Si}_2)_{0.2}/\text{GaAs}$ SLS layers grown by MEE at a temperature about 520°C . The threading dislocation density was very high at the GaAs and Si interface, and the SLS-I indeed blocked or deflected a large number of dislocations. It is clear from the picture that SLS-II, placed about $0.2 \mu\text{m}$ above SLS-I, deflected a major part of the remaining threading dislocations. A linear dislocation density count revealed that there is at least a factor of 100 difference in the dislocation densities for the areas below and above SLS-II. SLS-III, which is placed about $1.0 \mu\text{m}$ above SLS-II and is out of sight in this picture, prevented almost all of

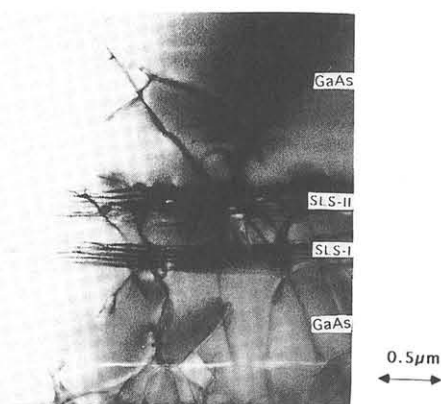


Fig. 4. Cross-sectional transmission electron micrograph of GaAs on Si grown with 3 packets of $(\text{GaAs})_{1-x}(\text{Si}_2)_x/\text{GaAs}$ SLS buffer layers. Each of the SLSs consists 5 periods of 20nm- $(\text{GaAs})_{0.8}(\text{Si}_2)_{0.2}$ and 17nm-GaAs.

the threading dislocations from propagating to the surface, and the top 2.0 μm of GaAs is dislocation free in the areas investigated by TEM. The majority of these bent dislocations were found to run along the $(\text{GaAs})_{1-x}(\text{Si}_2)_x/\text{GaAs}$ interface for hundreds of microns.

Plan-view TEM studies indicated dislocation densities of less than $5 \times 10^5 \text{cm}^{-2}$ near the surface. However, it becomes more difficult to determine the threading dislocation density as the density decreases, since TEM information, which only covers a small area, does not guarantee the uniformity of dislocation distribution for a wide range of TEM specimens. The EPD has been shown to be on the same order as the dislocation density observed by TEM, with no significant difference between them. Therefore, we also measured EPD for the samples and regard it as the threading dislocation density in this paper.

The EPD for each sample was estimated by observing three randomly chosen $100 \times 100 \mu\text{m}$ squares on each 3-inch wafer. Etched surfaces of typical samples with a $(\text{GaAs})_{1-x}(\text{Si}_2)_x/\text{GaAs}$ SLSs are shown in Fig. 5. The two surfaces in the figure represent the minimum and the maximum EPDs, $3.33 \times 10^5 \text{cm}^{-2}$ and $8.84 \times 10^5 \text{cm}^{-2}$. The average EPD was $5.63 \times 10^5 \text{cm}^{-2}$. For comparison, the EPDs of samples with conventional $\text{In}_x\text{Ga}_{1-x}\text{As}/\text{GaAs}$ SLSs were measured.

There are at least two ways to control the built-in strain in SLS. One is to vary the In content, and another is to change the GaAs and/or InGaAs thickness. In this study, the former method was adopted so as to allow direct comparison with $(\text{GaAs})_{0.8}(\text{Si}_2)_{0.2}/\text{GaAs}$ SLS of identical layer structure. The calculated In content, x , was about 0.1, which gives the same lattice mismatch as that of the $(\text{GaAs})_{0.8}(\text{Si}_2)_{0.2}$ alloy to GaAs. The respective minimum and maximum EPDs were $1.69 \times 10^6 \text{cm}^{-2}$ and $8.42 \times 10^5 \text{cm}^{-2}$ (Fig. 6). The average EPD was $1.30 \times 10^6 \text{cm}^{-2}$, clearly demonstrating that EPD for samples with the $(\text{GaAs})_{1-x}(\text{Si}_2)_x/\text{GaAs}$ SLSs is more than half an order of magnitude lower than that of samples with typical $\text{In}_x\text{Ga}_{1-x}\text{As}/\text{GaAs}$ SLSs.

We believe the observed highly effective dislocation blocking is due to a combined effect of built-in strain in the SLSs and the relatively high elastic stiffness constant

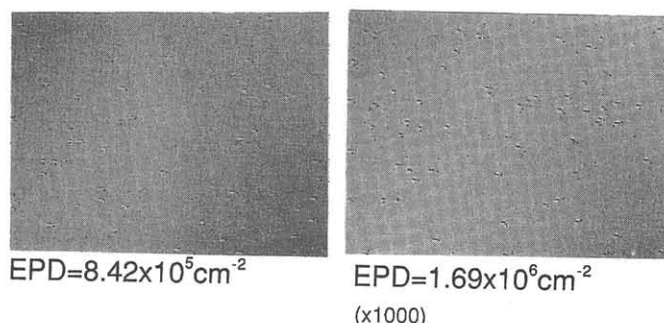


Fig. 5. Typical etched surfaces of the sample with $(\text{GaAs})_{0.8}(\text{Si}_2)_{0.2}/\text{GaAs}$ SLSs.

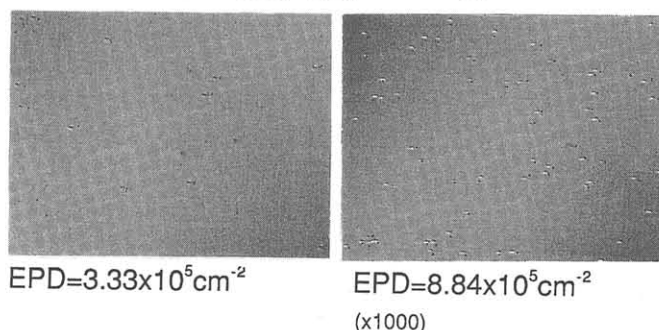


Fig. 6. Typical etched surfaces of the sample with $\text{In}_{0.1}\text{Ga}_{0.9}\text{As}/\text{GaAs}$ SLSs.

of $(\text{GaAs})_{1-x}(\text{Si}_2)_x$ alloys, because the strong Si-Si covalent bonding makes the shear modulus of Si higher than that of any III-V compounds. The use of the $(\text{GaAs})_{1-x}(\text{Si}_2)_x/\text{GaAs}$ SLS will open the way for suppressing strain relaxation even for low-temperature grown GaAs/Si heated after growth, although optimization for low-temperature growth of $(\text{GaAs})_{1-x}(\text{Si}_2)_x$ is still needed.

4. Summary

A new SLS system of $(\text{GaAs})_{1-x}(\text{Si}_2)_x/\text{GaAs}$ was used as buffer layers to reduce the threading dislocation density in GaAs on Si grown by MEE. $(\text{GaAs})_{1-x}(\text{Si}_2)_x$ layers grown on GaAs substrate hardly relax, even at high growth temperatures ($\sim 500^\circ\text{C}$) compared with $\text{In}_x\text{Ga}_{1-x}\text{As}$, which is a constituent of the conventional SLS. Cross-sectional TEM investigations revealed extensive threading dislocation bending at $(\text{GaAs})_{1-x}(\text{Si}_2)_x/\text{GaAs}$ SLSs. EPD measurements indicated average dislocation densities of $5 \times 10^5 \text{cm}^{-2}$, more than half an order of magnitude lower than that of samples with ordinary $\text{In}_x\text{Ga}_{1-x}\text{As}/\text{GaAs}$ SLSs. The $(\text{GaAs})_{1-x}(\text{Si}_2)_x/\text{GaAs}$ SLS holds greater promise for reducing the dislocation density in GaAs on Si than conventional SLSs, such as $\text{In}_x\text{Ga}_{1-x}\text{As}/\text{GaAs}$, at high growth temperatures.

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