EFFECTIVENESS OF AlGaAs / GaAs SUPERLATTICES IN REDUCING DISLOCATION DENSITY IN GaAs ON Si

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The effectiveness in reducing the dislocation density in a GaAs layer on a Si substrate (GaAs-on-Si) is investigated by using AlGaAs/GaAs superlattices grown by metalorganic vapor phase epitaxy (MOVPE). The degree of dislocation density reduction is compared among several types of AlGaAs/GaAs superlattices with various layer thicknesses, various numbers of layers and various AlAs content of AlGaAs layer. The thicker each layer is, the larger the number of layers, or the larger the AlAs content, the larger is the degree of dislocation density reduction. As a result, the dislocation density is reduced to 1×10^6 cm⁻² by using five periods of (20 nm Al_{0.85}Ga_{0.15}As)/(100 nm GaAs superlattice). The reduction of the dislocation density and the degree of this effect can be explained by the crystal hardening of AlGaAs and the bending of dislocations at the AlGaAs/GaAs superlattice.

1. Introduction

One of the major problems with GaAs-on-Si is the existence of a large defect density, which deteriorates the performance of GaAs devices fabricated on Si substrates, especially for minority carrier devices. Deppe et al. [1] have described the characteristics of a p-n diode Al, Ga_{1-x}As-GaAs quantum well heterostructure laser on a Si substrate. The threshold current and the diode stability are inferior to those fabricated on a GaAs substrate. Recently, Choi et al. [2] have reported that the dislocation density could be reduced to a range as low as 10⁵ cm⁻² by using InGaAs/GaAs strained layer superlattices (SLSs) followed by annealing steps. However, our comparative study on this InGaAs/GaAs SLS by means of transmission electron microscope (TEM) and molten KOH etching [3] has shown that the TEM observation tends to have an error in quantitative estimation of dislocation density, especially in the range lower than 10⁷ cm⁻² and that the dislocation density should be in the range of lower 10⁶ cm⁻² in the GaAs layer upon the InGaAs/GaAs SLS.

Furthermore, a InGaAs/GaAs SLS leads to an additional deterioration of the crystalline quality and new misfit dislocations are generated just upon the InGaAs/GaAs SLS, because this SLS is a lattice-mismatched system.

In this paper, we present for the first time the remarkable reduction of dislocation density due to the adoption of a lattice-matched AlGaAs/GaAs superlattice in which there are found no such problems as mentioned above. Furthermore, we discuss the mechanism of dislocation density reduction by this superlattice.

2. Experimental procedure

The epitaxial layers were grown in a reduced pressure MOVPE reactor. Fig. 1 shows the layer structure. The growth sequence was as follows: The growth pressure was 130 Torr. The Si(100) 4° off toward [011] direction substrates were heated up to about 900°C in the flow of H2 and AsH3 for 20 min, and were cooled down to 400°C, and a 10 nm thick GaAs layer was grown. Subsequently, the substrates were heated up to 780°C and then a 2 µm thick GaAs layer was grown. Then these layers were annealed at 900°C for 30 min in a flow of H₂ and AsH₃. On this buffer layer, the AlGaAs/GaAs superlattice was grown, and finally a 4 µm thick top GaAs layer was grown. Table 1 shows the variation of AlGaAs/ GaAs superlattice structures. Six types of superlattice were tested; that is, the thickness of the AlGaAs and GaAs layers, the number of layers

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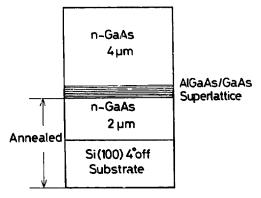


Fig. 1. Schematic of the layer structure. The AlGaAs/GaAs superlattice is used to reduce the dislocation density of the top GaAs layer.

Table 1 Variation of AlGaAs/GaAs superlattice structure

Sample	of AlGaAs		Number of superlattices	AlAs content of AlGaAs
a	10	10	20	0.6
b	16	100	5	0.6
c	20	100	5	0.6
d	70	100	5	0.6
e	70	100	10	0.6
f	20	100	5	0.85

and the AlAs content of the AlGaAs layers were changed.

In-depth profiles of etch pit density (EPD) were measured to clarify the effectiveness of Al-GaAs/GaAs superlattices in reducing the dislocation density. The selective step mirror etching was done by 5H₂SO₄-1H₂O₂-1H₂O solution at 0°C, and molten KOH etching was employed to reveal the dislocation on the epitaxial layer at each depth. Small hexagonal etcn pits were revealed clearly after etching about 300 nm deep. Ishida et al. [4] have indicated that these small etch pits correspond to the dislocations, by means of plan-view TEM observation and molten KOH etching measurement at the surface of GaAs-on-Si. In this experiment, these small etch pits were counted as dislocations. Furthermore, the cross-sectional TEM observation was used to study the role of the AlGaAs/GaAs superlattices. The samples for TEM observation were prepared by mechanical thinning followed by ion milling.

3. Results

3.1. In-depth profile of EPD

Fig. 2 shows the in-depth profiles of EPD for the samples with different thickness of AlGaAs and GaAs layers within superlattices (samples a, b, c and d). The profile for the sample without any superlattices is also shown in fig. 2. When the GaAs layers within superlattices are thin (10 nm), the dislocation density reduction is not observed (for sample 0), while when the GaAs layers are thicker (100 nm), the dislocation density reduction is clearly observed in spite of the small number of layers (for samples b, c, d and e). Furthermore, it can be seen that the effect of dislocation density reduction becomes larger, the thicker the AlGaAs layers within the superlattices. Fig. 3 shows the in-depth profiles of EPD for the samples with a different number of layers and different AIAs

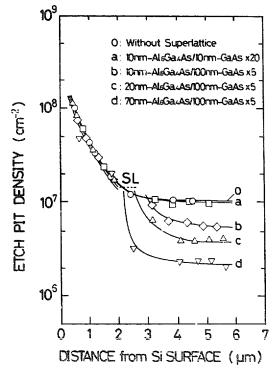


Fig. 2. In-depth profiles of etch pit density for GaAs layers on Si substrate with AlGaAs/GaAs superlattice. Each line represents the results for samples with different thickness of AlGaAs and GaAs layers. Open circles correspond to the result for a sample without any superlattices. The position of the superlattice is indicated by "SL" in the figure.

a

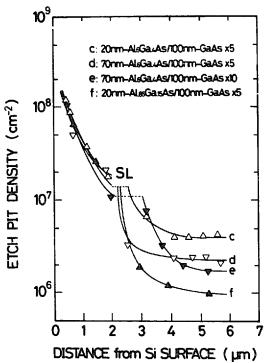


Fig. 3. In-depth profiles of etch pit density for the GaAs layers on Si substrate with AlGaAs/GaAs superlattice. Each line represents the result for samples with a different number of layers and a different AlAs content of AlGaAs layers. The position of the superlattice is indicated by "SL" in the figure.

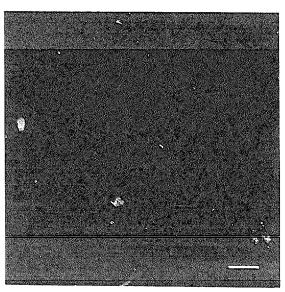
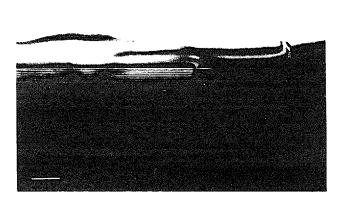
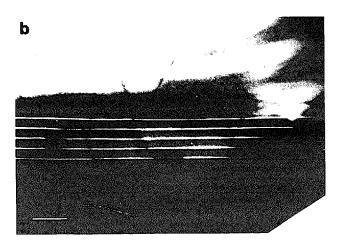


Fig. 4. Nomarski micrograph of the KOH etched surface of a GaAs layer on a Si substrate with five periods of (20 nm Al $_{0.85}$ Ga $_{0.15}$ As)/(100 nm GaAs) superlattice. Marker represents 10 μ m.





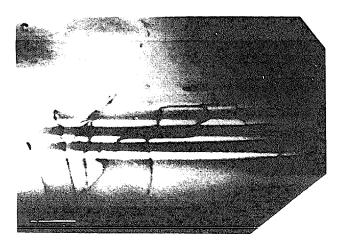


Fig. 5. Cross-sectional TEM photographs of the superlattice position for (a) sample a with twenty periods of (10 nm $Al_{0.6}Ga_{0.4}As$)/(10 nm GaAs) superlattice, for (b) sample c with five periods of (20 nm $Al_{0.6}Ga_{0.4}As$)/(100 nm GaAs) superlattice and for (c) sample d with five periods of (70 nm $Al_{0.6}Ga_{0.4}As$)/(100 nm GaAs) superlattice. Markers represent 0.5 μ m.

content of AlGaAs layers within the superlattices (samples c, d, e and f). It can be seen that the effect of dislocation density reduction becomes larger, the larger the number of layers or the larger the AlAs content of the AlGaAs layers. In figs. 2 and 3 the dislocation densities decrease drastically just upon the AlGaAs/GaAs superlattices and saturate sharply just above the superlattices for all samples, while the dislocation density decreases continuously with the thickness even after passing through the superlattice position using InGaAs/ GaAs SLS [3]. This result indicates that no new dislocation is generated in AlGaAs/GaAs superlattices. Consequently, the best dislocation density reduction is obtained by using five periods of $(20 \text{ nm Al}_{0.85}\text{Ga}_{0.15}\text{As})/(100 \text{ nm GaAs})$ superlattice. Fig. 4 shows the Nomarski micrograph of a molten KOH etched surface of the GaAs-on-Si with this superlattice. From this micrograph, the dislocation density can be estimated to be 1×10^6 cm⁻². This value is as low as ever reported [8].

3.2. Cross-sectional TEM observation

Figs. 5a, 5b and 5c show cross-sectional TEM photographs near the superlattice for the samples with different thickness of AlGaAs and GaAs layers within superlattices (samples a, c and d). When the GaAs and AlGaAs layers are thin, most of the dislocations are threaded through the superlattices (fig. 5a, for sample a). On the contrary, as the GaAs and AlGaAs layers are thicker, the dislocation bending along the superlattice interfaces is larger (figs. 5b and 5c, for samples c and d). Consequently, most of the dislocations are blocked in the superlattices and do not thread to the top GaAs layer. Furthermore, no new dislocation can be observed in the superlattices. These results coincide qualitatively with the results obtained from the in-depth profiles of EPD as mentioned in section 3.1.

4. Discussion (mechanism of dislocation density reduction)

Bedair et al. [5] have shown that the effectiveness of an InGaAs/GaAs SLS in dislocation

bending is due to the strain in the SLS. The SLS is constructed of layers with different lattice constant, so that each layer is alternately subjected to compressive or tensile stress. Table 2 shows the lattice mismatch and the critical thickness of various superlattices calculated by Matthews's equation [6]. On the contrary, our results indicate that dislocation bending occurs even for an Al_{0.6}Ga_{0.4} As/GaAs superlattice which is almost latticematched (lattice mismatch is 7.6×10^{-4}). The dislocation bending occurs in the layer within the AlGaAs/GaAs superlattice at a thickness below the critical thickness (about 1.1 µm) for generating misfit dislocations calculated by Matthews' equation. Consequently, the effectiveness of an AlGa-As/GaAs superlattice in the dislocation density reduction cannot be explained by this strain theory, because the built-in strain of the AlGaAs/GaAs superlattices is insufficient to suppress the propagation of dislocations.

Then, we newly propose the mechanism of dislocation density reduction. The epitaxial layers in Si are totally subjected to tensile stress caused by the difference of thermal expansion coefficient between GaAs (or AlGaAs) and Si. Furthermore, the AlGaAs layers, within a superlattice are locally subjected to the compressive stress caused by the difference of thermal expansion coefficient between AlGaAs and GaAs. On the other hand, it has been found that the dislocations hardly thread in the GaAs layer by adding only a little Al, that is to say, the critical stress of AlGaAs for dislocation threading is extremely larger than that of GaAs [7]. Since the tensile stress in the GaAs layer is considered to be higher than the critical stress, the dislocation can thread in the GaAs layer. The

Table 2
Lattice mismatch and critical thickness of various superlattices calculated by Matthews's equation

Sample	Lattice mismatch	Critical thickness (µm)
In _{0.06} Ga _{0.94} As/GaAs	4.3×10^{-3}	0.14
In _{0.12} Ga _{0.88} As/GaAs	8.6×10^{-3}	0.06
Al _{0.60} Ga _{0.40} As/GaAs	7.6×10^{-4}	1.05
$Al_{0.85}Ga_{0.15}As/GaAs$	1.1×10^{-3}	0.69

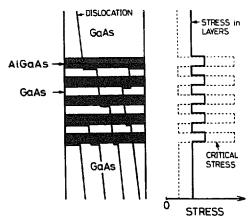


Fig. 6. Mechanism of dislocation density reduction by Al-GaAs/GaAs superlattice. The dislocation density reduction occurs due to the crystal hardening and the bending of dislocation at the superlattice.

dislocation threading becomes larger, the thinner the GaAs layer, because the subjected tensile stress is larger. However, since the locally subjected compressive stress in an AlGaAs layer within the superlattice is considered not to be larger than the critical stress, the dislocation might be blocked at the superlattice and bent along the interface plane. This means that the reduction of dislocation density is not due to the misfit strain but the crystal hardening of AlGaAs and the bending of dislocation at the superlattice. Fig. 6 shows the mechanism of dislocation density reduction by an Al-GaAs/GaAs superlattice. The degree of dislocation density reduction can be explained by the degree of crystal hardening and opportunity for trapping the dislocations. Consequently, the larger the AlAs content of the AlGaAs layer, the thicker the AlGaAs, or the larger the number of layers, the larger becomes the degree of dislocation density reduction.

5. Conclusion

The enectiveness of an AlGaAs/GaAs superlattice in reducing the dislocation density in GaAs-on-Si has been investigated by means of in-depth profile measurements of dislocation density using molten KOH etching and cross-sectional TEM observation. The degree of dislocation density reduction becomes larger, the thicker the AlGaAs layer thickness within the superlattices, the larger the number of layers, or the larger the AlAs content of AlGaAs layers. Consequently, the dislocation density is reduced to 1×10^6 cm⁻² which is as low as ever reported [8]. Furthermore, this superlattice does not bring about the deterioration of crystalline quality and no new dislocation is generated in the superlattice. The dislocation density reduction and its degree are explained by the crystal hardening of AlGaAs and the bending of dislocations at the AlGaAs/GaAs superlattice.

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