Extended Abstracts of the 1993 International Conference on Solid State Devices and Materials, Makuhari, 1993, pp. 125-127

Threading Dislocations in GaAs on Pre-Patterned Si and in Post-Patterned GaAs on Si

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A detailed correlation has been investigated among the threading dislocation density, the residual stress and the growth area for stripe and square mesas of MBE grown 3 μm-thick GaAs on pre-patterned and of post patterned 3 μm-thick GaAs on Si. The density of dislocations in each patterned area is found not to be influenced by the pattern size, although the residual stress clearly shows a decrease with a decrease in the pattern size, independent of the patterning method.

1. INTRODUCTION

A large lattice mismatch (~4 %) and a large difference in the linear thermal expansion coefficient ($\sim 4.2\times10^{-6}$ /°C) between GaAs and Si results in the formation of heteroepitaxial GaAs layers on Si having a significant interfacial strain and high density structural defects. On the other hand, it has already been established that the residual strain of GaAs on Si decreases monotonically along with a reduction in the growth area. This has been confirmed not only for GaAs on pre-patterned Si [1)], but also for GaAs on Si by post-growth patterning [2)]. Also, etch pit density has been shown to be reduced with a decrease in the grown size [3)]. However, no detailed correlation among the threading dislocation density, the residual stress and the growth area has been obtained. In the present study, we carried out detailed cross-sectional TEM (XTEM) observations for MBE grown GaAs films of stripe and square mesas of varying width in order to reveal the threading dislocation densities in each selected area.

2. EXPERIMENTS

The samples consisted of GaAs on pre-patterned Si and post-patterned GaAs on Si. The patterning was directly performed on both Si substrates (tilted 3° from [001] toward [110]) and on 3 μm-thick GaAs layers on Si by conventional lithography and a dry etching technique. The shapes of mesa areas were squares ($1\times1\ \mu m^2$-$100\times100\ \mu m^2$) and stripes (1-100 μm width and 9 mm length). The 3 μm-thick GaAs layers were grown on pre-patterned and unpatterned Si substrates by two step growth: a 40 nm-thick buffer layer was deposited at 350 °C, followed by GaAs growth at 600 °C. The residual stress was evaluated for these mesa samples by using newly constructed micro- (2 μm beam diameter) photoluminescence (PL) equipment at 7 K. The structural defects in the GaAs films were examined at 200 keV by XTEM.

3. SURFACE MORPHOLOGY

Figure 1 shows SEM photographs of the square mesa patterns of different sizes of GaAs on patterned Si (a) and of GaAs on Si by post-growth patterning (b). In both cases, the sides of the mesas were parallel to the <110> directions. The GaAs films grown on patterned Si were surrounded by facets formed along the <110> sides, although, of course, the sides of post-patterned GaAs showed clear vertical features. Figure 2 shows a magnified SEM picture of a GaAs layer grown on a 6 μm mesa, indicating that the periphery of the film along the $[1\bar{1}0]$ direction exhibits a comparatively smooth morphology in contrast to the rough surface of the [110] oriented periphery. Detailed inspections of these facts on pictures revealed that the facets comprise (111)A (along the [110] direction) and (111)B (along the $[1\bar{1}0]$ direction) planes. The formation of these <111> facets was caused by the slower growth rate in <111> than that in <100>[4)]. This facet formation resulted in new sources of twins, stacking faults and dislocations from each side of as-grown layers (Fig. 4 (a)).

4. RESIDUAL STRESS

Figure 3 shows the main peak shift of the PL spectra obtained from GaAs on pre-patterned Si of stripe and square mesas with respect to that of GaAs/GaAs as a function of mesa size. The peak shift as well as the corresponding residual stress decreased with decreasing the mesa size, especially for sizes of less than 25 μm.

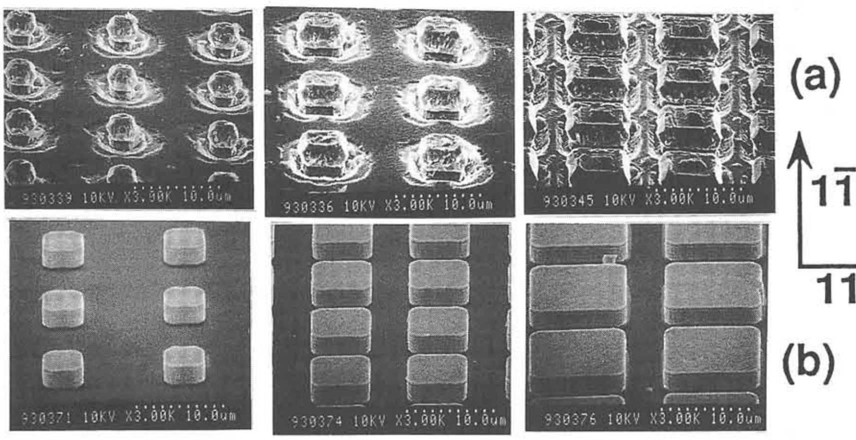

Fig. 1 SEM photographs of square mesa patternes of different sizes (L) of GaAs on pre-patterned Si (a) and of post-patterned GaAs on Si (b). L of 2, 4 and 6 μm in (a) and 4, 6 and 8 μm in (b) from left to right, respectively.

Fig. 2 Magnified SEM image of a GaAs layer on a pre-patterned 6 μm mesa.

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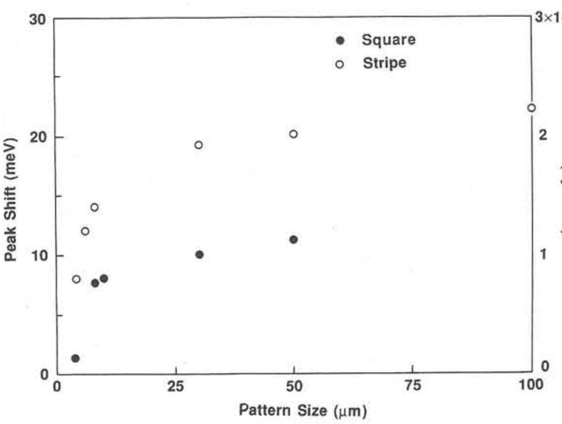

Fig. 3 Shift of PL peaks and the residual stress in GaAs on pre-patterned Si as a function of mesa size.

Also, we note that the stress of a square mesa was roughly half that of a stripe, independent of the size. This tensile stress was seen to be reduced to below 1×10^9 dyn/cm^2 when the pattern size was reduced to ~10 μm. Nearly the same results were obtained for samples of post-patterned GaAs.

5. THREADING DISLOCATIONS

The threading dislocation density did not show any clear mesa size dependence. Figure 4 compares the threading dislocation morphologies observed for GaAs on patterned Si (a) and for post-patterned GaAs on Si (b) before and after annealing at 900 °C for 10 s. In the post patterned GaAs on Si, four 1 nm thick Si layers are inserted at different depths as shown in the figure in order to prevent any upward movement of the dislocations [5]. We recognize that dislocation densities in the as-grown state were not influenced by the pattern size for both samples. Moreover, the complicated boundaries are formed near the periphery regions in GaAs grown on pre-patterned Si, which probably originated due to the <111> facet formation. This effect is severely observed for layers of pattern sizes below 2 μm. In separate dislocation contrast experiments, most of the threading dislocations were identified to be of the 60° type, independent of the patterning size and method, which was the same result as that observed in the usually grown GaAs films on unpatterned Si substrates [5].

After 900 °C-10 s annealing, although the defect density decreased due to the activation of dislocation slip systems, its reduction phenomenon does not seem to have any correlation with the variation in the growth area. Rather, the density of residual dislocations seems to be lower in samples of a 8 μm size than that in those below 4 μm. This is considered to be due to the fact that a weaker residual stress in samples of smaller sizes has a weaker influence on the movement of dislocations during annealing. On the other hand, we note that clear boundaries are formed in GaAs layers on pre-patterned Si of smaller sizes than 4 μm. One example of orientations for each grain in a GaAs layer on a pre-patterned 2 μm mesa is shown in Fig. 5, which was determined on the basis of diffraction patterns obtained from individual grains. The mechanism of the formation of these grains is not yet clear at the present, although its formation will have a strong correlation with the <111> facets. It is interesting that the defect density is lower in the grains than in the other regions just grown on substrates (see Fig. 4 (a) after annealing).

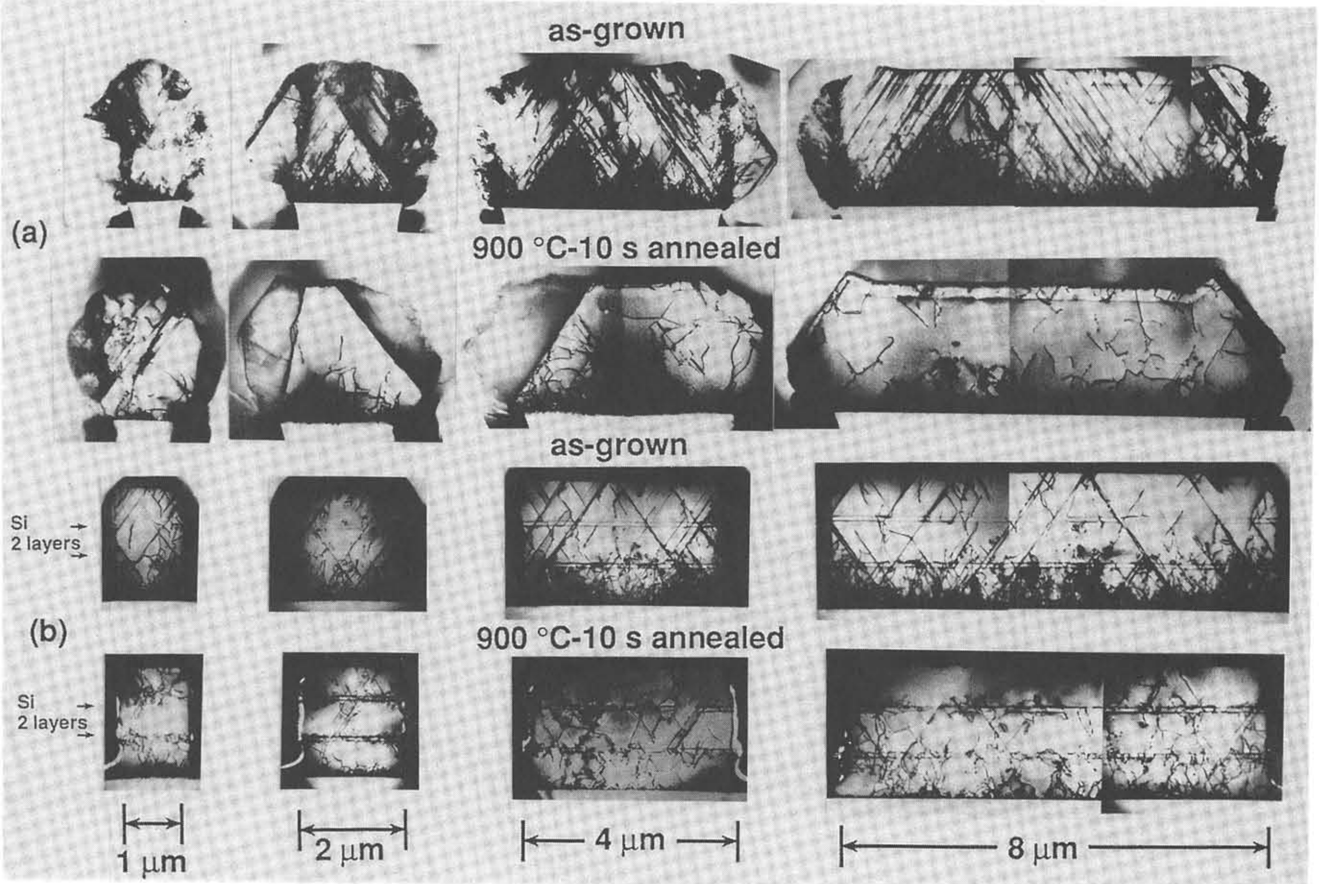

Fig. 4 XTEM micrographs showing threading dislocation morphologies in GaAs on pre-patterned Si (a) and in post-patterned GaAs on Si (b) for various mesa sizes before and after 900 °C-10 s annealing observed from the [110] direction.

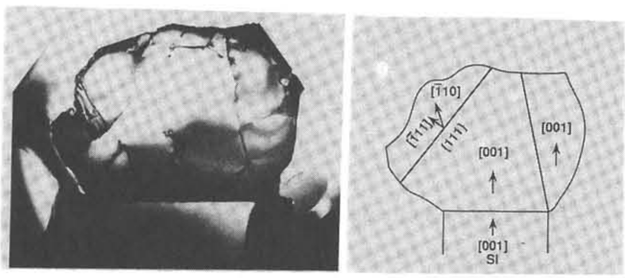

Fig. 5 XTEM micrograph showing grain formation in a GaAs layer on a pre-patterned 2 μm mesa after 900 °C-10 s annealing and its schematic drawing.

6. CONCLUSION

The results obtained in the present study clearly demonstrated a decrease in the residual stress in grown films along with a decrease in the pattern size, particularly for sizes of less than 25 μm, independent of the patterning method. However, the density of the threading dislocations remaining in each patterned area was found not to be influenced by the pattern size. In other words, the number of remaining dislocations was not decreased with the decreased pattern size. This strongly suggests that the threading dislocation generation in GaAs on Si in the present experiments is mainly governed by a lattice mismatch-induced stress, not by a thermal-expansion mismatch-induced stress.

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