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Micro-Raman study on GaAs layers directly grown on (100) Si by molecular beam epitaxy

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Micro-Raman spectroscopy is applied to evaluate change of the crystal quality in molecular beam epitaxial GaAs layers on Si after rapid thermal annealing (RTA). The forbidden transverse optical phonon is observed in the GaAs layers especially near the interface. In the as-grown state, the Raman frequency of the longitudinal optical phonon shifts toward higher frequency near the interface. This blue shift indicates the existence of the compressive stress due to the lattice mismatch between GaAs and Si. On the other hand, after the RTA, the Raman peak shifts toward lower frequency. This red shift indicates that the tensile stress exists near the interface because of the difference in thermal expansion. The stress change indicates the relaxation of the lattice mismatch stress near the interface by formation of dislocations during the RTA.

Recently there has been much interest in GaAs epitaxial films grown on Si substrates for its many potential applications. However, some problems prevent the formation of good GaAs layers. Large lattice mismatch of about 4% causes compressive stress in a GaAs layer near the heterointerfaces, and the difference in thermal expansion causes tensile stress in a GaAs layer. These stresses produce high density of dislocations. Generation of antiphase disorder (APD) degrades the crystalline quality. Fairly good crystallinity of a GaAs layer has been obtained by several growth methods, e.g., fabrication of buffer layers and use of off (100) oriented Si substrates. Noge et al. have previously reported that the preheating of a Si substrate at 1000 °C for 30 min prevents the formation of the APD. It has been reported that thermal annealing improves the crystalline quality of GaAs on Si. In particular, rapid thermal annealing (RTA) is more effective to improve it than conventional furnace annealing.

Raman spectroscopy has been applied to evaluate the crystalline quality of GaAs layers on Si. In order to get the information of various distances from the interface, beveled samples were prepared by angle etching or by slowly moving a shutter in the front of the sample during molecular beam epitaxy (MBE) growth. Different thickness samples also give the depth profile. In this communication, we investigate the depth profile of the crystalline quality of beveled MBE GaAs layers on Si with micro-Raman spectroscopy.

The MBE GaAs layers used in this study were grown on just (100) oriented Si substrates in a V. G. Semicon V80H system. The substrate was preheated under ultrahigh vacuum at 1000 °C for 30 min to prevent the formation of APD. Further growth procedures have been shown in Ref. 5. The MBE GaAs layer was single domain and intentionally doped with Si to about 10²⁰ cm⁻³. The thicknesses of the GaAs layer and the Si substrate were 2 and 250 μm, respectively.

RTA was performed at 800 °C for 6 s with or without SiO₂ encapsulation. Some MBE GaAs layers were coated with a ~350-nm-thick SiO₂ layer before the RTA by the spin-on method. Other GaAs layers were faced to another GaAs substrate during the capless RTA (proximity capping method). The samples were irradiated by halogen lamps in a quartz tube in flowing N₂.

The micro-Raman experiment was performed at room temperature in a backscattering geometry using NR-1100 (Japan Spectroscopic Co. Ltd.) with a double monochromator. An Ar⁺ laser beam (λ=514.5 nm) was focused onto a spot of about 1 μm in diameter. Beveled samples were prepared by a mechanical lapping to investigate the depth profile of the crystalline quality of the GaAs layer. The lapping angle was about 1°. The lapping damage at the surface region was removed by etching with an NH₄OH:H₂O₂:H₂O solution. The distance from the interface was calculated from the bevel angle and the difference between the illuminated position and the GaAs/Si interface. It should be noted that the observed Raman signal is the sum of the Raman scattering from positions within a finite depth from the illuminated surface. The penetration depths of the Ar⁺ laser (λ=514.5 nm) in GaAs and in Si are about 0.1 and 1 μm, respectively.

Figure 1 shows the Raman spectra of the GaAs layer at three distinct distances from the GaAs/Si interface. The transverse-optical (TO) phonon is forbidden by a selection rule in this scattering geometry, while the longitudinal-optical (LO) phonon is permitted. Consequently, a high relative intensity of the TO phonon indicates disorder, such as misfit dislocations, threading dislocations, APD, and impurity, in the sample. At present, we feel that we do not have enough data to identify the type of dominant disorder.
Figure 1. Raman spectra of the GaAs layer at three distinct distances from the GaAs/Si interface.

Figure 2 shows the depth profiles of the relative intensity of the TO phonon. The solid line, the dashed one, and the dash-dotted one represent the intensities in the as-grown sample, the SiO$_2$ capped sample after the RTA, and the sample after the capless RTA, respectively. In all the samples, the ratio decreases drastically within 0.3 μm from the interface. This suggests that the disorder is localized near the interface. The capless RTA increases the ratio but not the RTA with the cap.

It should be noted that the relative TO intensity observed near the interface is larger than the reported values, which are generally less than 0.1. The GaAs layer of the present sample was grown on just a (100) Si substrate without any buffer layer. Most reported GaAs layers, however, were grown on Si substrates with a buffer layer or on misoriented Si substrates. The observed high TO intensity is ascribed to the sample growth method adopted in this study. However, the reason for the increase in the TO intensity by the capless RTA is not clear.

Next we consider the change of peak shifts in Raman spectra. Figure 3 shows the LO phonon peak shifts from the surface LO peak as a function of distance from the interface. The solid line shows the peak shift of the as-grown sample. Near the interface, the LO peak shifts toward higher frequency (blue shift). The dashed and dotted lines show the LO phonon peak shifts of the samples after the RTA with or without the SiO$_2$ cap, respectively. Both shift toward lower frequency (red shifts). All the observed peak shifts decrease toward the surface where no significant peak shift is observed compared with bulk GaAs.

From the observation of the characteristic blue shift of the LO phonon, it is found that the compressive stress caused by the lattice mismatch is dominant in the as-grown state. This shows that the mismatch stress is not fully relieved in this sample growth. The existence of the compressive stress in GaAs films on Si has been reported by several researchers, but the blue shift observed here is considerably larger than the previously reported values (less than 1 cm$^{-1}$). This will also be due to the difference of the growth method.

On the other hand, absence of the blue shift after the RTA indicates that formation of dislocations during the RTA relaxed the stress due to the lattice mismatch near the interface. It seems that the observed red shifts are ascribed to the tensile stress caused by the difference in thermal linear expansion coefficient and to relaxation in the q vector selection rule. The observed red shift of about 3 cm$^{-1}$ is larger than the peak shift expected from the diff...
ference in the thermal expansion of GaAs and Si (about 1 cm\(^{-1}\)). Thus the observed red shift cannot be explained considering only the difference in thermal expansion.

If the red shift is caused by the relaxation of the \(q\) vector selection rule, the peak should broaden.\(^{15}\) However, no significant variation of a linewidth of the LO phonon peak was observed among all the samples, although it is difficult to deduce the accurate linewidth because of weak intensity near the interface. Since the TO phonon is clearly observed near the interface, a certain amount of red shift will be created by disorder.

In conclusion, crystal quality of MBE GaAs layers on Si have been investigated with micro-Raman spectroscopy before and after the RTA. The higher intensity ratio of forbidden TO phonon was observed near the GaAs/Si interface. In the as-grown state, the Raman frequency of the LO phonon shifts toward higher frequency near the interface. This blue shift indicates the existence of the compressive stress due to the lattice mismatch between GaAs and Si. On the other hand after the RTA, the Raman peak shifts toward lower frequency. This red shift indicates that the tensile stress exists near the interface because of the difference in thermal expansion. The stress change indicates the relaxation of the lattice mismatch stress near the interface by the formation of dislocations during the RTA.

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