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A RAMAN STUDY OF EPITAXIAL GaAs LAYER ON Si [100] SUBSTRATE

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ABSTRACT

A bevel has been etched in a GaAs epitaxial film grown on Si substrate, so that Raman spectrum of GaAs layers can be measured as a function of distance from the GaAs/Si interface. The amount of strain and disorder in the GaAs film has been estimated from the GaAs longitudinal optical phonon lineshape and frequency. Both the strain and the amount of disorder were found to decrease with increase in the distance from the interface.

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Recently there has been much interest in GaAs epitaxial films grown on Si substrate. This is due to the many potential applications which can result from combining the fast speed and excellent electro-optic properties of GaAs with the highly developed Si technology.¹⁻⁴ Two major problems have been encountered in the growth of high quality GaAs films on Si substrates. First there is a 4.1% lattice mismatch between the two materials, and secondly the random occupation of the Ga and As sublattices leads to the presence of anti-phase domains. The first effect results in high densities of dislocations and possibly also strain in the GaAs films. The anti-phase domains contain large amounts of antisite defects at the domain boundaries. Raman scattering has been useful in the study of defects in GaAs caused by ion-implantation, polishing, and high-energy neutron and electron irradiations.⁵⁻¹⁰ We report here the first Raman study of epitaxial films of GaAs grown on Si. From this study we determined the crystallinity and strain in the GaAs film as a function of its distance from the interface.

Our sample was a 2.3 micron thick GaAs film grown by molecular beam epitaxy (MBE) on a Si substrate oriented 4° off the [100] direction towards the [110] axis. To avoid the formation of islands, the first few hundred Angstroms of GaAs was grown at $T < 350^\circ\text{C}$. This thin layer of GaAs was amorphous. After the Si surface was completely covered by GaAs, the substrate temperature was increased to 600°C . Two layers of strained InGaAs-GaAs superlattice, each of 5 periods, were included in the GaAs film as shown in the inset of Fig. 1. The

strained superlattices bent the dislocations and drastically reduce the density of the dislocations which can propagate through the superlattice. A small angle bevel was etched by gradually dipping the sample into $\text{NH}_4\text{OH}:\text{H}_2\text{O}_2:\text{H}_2\text{O}$ (1:1:20) to expose the GaAs layers near the interface as shown in the inset of Fig. 1. To maintain a uniform etching rate, the sample passes over deionized water before touching the etchant.

Raman experiment was performed at room temperature in the $x(yz)\bar{x}$ back-scattering geometry, where x,y,z refer to the [100], [010] and [001] crystallographic axes respectively. A SPEX double spectrometer and a multichannel detector, which is similar to that described in Ref. 11 was used to analyze the Raman signal. Typically 300 mW of Ar^+ laser power ($5145 \text{ \AA}$) was focussed with a cylindrical lens to a spot of about $10 \times 40 \text{ (micron)}^2$ on the sample with the longer side parallel to the edge of the bevel. The GaAs lattice temperature at the focus was estimated to be 360 K.

Raman spectra were obtained successively by translating the sample in a direction perpendicular to the bevel edge with a micrometer. From the known bevel angle and distance of laser focus to the bevel edge, the thickness of the GaAs film probed by the laser can be calculated. The accuracy of this thickness measurement is about $300 \text{ \AA}$. When the focus was scanned towards the bevel edge from the GaAs side, the GaAs Raman signal decreased while the Si optical phonon (at 519.5 cm^{-1}) intensity increased (see Fig. 1). Since the laser beam has to penetrate the GaAs film to reach the Si substrate, we can determine the

absorption coefficient of the GaAs film from the variation of the Si phonon intensity provided that this absorption coefficient is not varying with the GaAs film thickness. The solid curve in Fig. 1 shows a fit to the experimental points with a constant GaAs penetration depth of 1580 ± 20 Å. This value is consistent with that of bulk GaAs.¹²

The GaAs LO phonon intensity in Fig. 1 was actually the sum of the Raman scattering from GaAs layers at different depths from the interface up to the surface. To determine the Raman spectra of the GaAs layers as a function of its distance to the interface, we have adopted the following procedure. First the Raman spectrum of GaAs was measured with the laser focus at a spot as close as possible to the edge of the bevel. This is taken to be the Raman spectrum of the GaAs layer at the interface. The laser focus is then translated by a few hundreds of Angstrom away from the interface. The resultant Raman spectrum is then the sum of the Raman spectrum from the GaAs nearest to the interface plus that from an additional overlayer. By subtracting one Raman spectrum from the other, we obtain the Raman spectrum of the additional layer. The attenuation of light due to absorption in the GaAs film has to be corrected for in this subtraction process. This process can be continued until the spot reaches the surface of the GaAs film. Fig. 2 shows the normalized GaAs LO phonon lineshape of GaAs layers at different distances to the interface obtained in this way. When the layers are far away from the interface, their LO phonon spectra are narrow, symmetric and Lorentzians in shape. After correction for the instrumental response, the intrinsic GaAs LO phonon linewidth

is about 2 cm^{-1} for layers farther than half micron from the interface. The GaAs LO phonon peaks become broader and more asymmetric when the layers are closer to the interface. Fig. 3(a) shows the asymmetry and broadening of the GaAs LO phonon as a function of the layer distance to the interface.

In a perfect crystal only zone center ($q=0$) phonon modes are observed in one-phonon Raman scattering due to quasi-momentum conservation. The phonon lineshapes are usually Lorentzian with the phonon linewidths determined by the phonon lifetime. In a disordered crystal, however phonons can be localized to regions of extent L . As a result quasi-momentum conservation is relaxed.^{7,8,9} and the LO phonon Raman peak becomes asymmetric and shifted towards lower frequency. On the other hand compressive stress can shift the LO phonon towards higher frequency.^{8,12,13,15} Thus the LO phonon lineshape and peak positions contain information on both the crystal quality and on the amount of strain in the GaAs film. We adopt this spatial correlation model to interpret our experimental results.^{7,9} In this model, L can be deduced from one of these quantities: shift in LO phonon frequency, LO phonon width or the asymmetry of LO phonon lineshape. Fig. 3(b) shows the correlation lengths of the GaAs film as a function of distance to the interface deduced from the linewidth and the asymmetry. Both show the same increase in the correlation length as the GaAs film become farther from the GaAs/Si interface.

We found that the GaAs LO phonon frequency is blue-shifted for GaAs layers nearer to the interface opposite to the

prediction of the spatial correlation theory. We attribute this difference to the presence of compressive strain in the GaAs layers near the interface due to the lattice mismatch between GaAs and Si. To determine the magnitude of this strain we assume an uniform and isotropic two-dimensional, strain for simplicity. We also assume that the GaAs film free surface is unstrained and use its LO phonon frequency as reference ω_0 . From the phenomenological theory in Ref. 8,13,14,15 the strain induced frequency shift $\Delta\omega$ is given by: $\Delta\omega / \omega_0 = -1.3 X$, where X is the strain. Fig. 3(b) shows the variation in the compressive strain as a function of distance from the interface. The strain measured in our sample is much smaller than the 4% strain expected from the lattice mismatch. This suggests that the strain in GaAs films on Si is relieved by dislocations. For GaAs layers more than $\sim 2000 \text{ \AA}$ away from the interface, the strain is below our measurement sensitivity.

A very small TO phonon Raman peak was also observed in our sample. Since the TO phonon is forbidden by selection rule in our scattering geometry, we have interpreted this peak as due to disorder induced scattering. The intensity of the TO phonon relative to the LO phonon increases towards the interface. This is consistent with our result that disorder increases for GaAs layers closer to the interface.

In conclusion, we have used the Raman scattering from a bevel etched on the GaAs film grown on Si substrate by MBE to examine the GaAs quality as a function of its distance to the interface. The lattice spatial correlation, and strain were deduced from the LO phonon lineshapes and frequency shifts. We

found that both the strain and the disorder in the GaAs film decreased in the first 2000 Å to a level below the sensitivity of the Raman measurement.

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Figure Captions

Fig. 1 Variation of the Si optical phonon and GaAs LO phonon intensities with the thickness of the GaAs film. The solid curve is a fit to the Si phonon intensity calculated by assuming that the GaAs film has an absorption length of 1580 Å. The broken curve is for guidance of eyes only. The GaAs LO phonon intensities have been multiplied by a factor of 12 in order to plot them on the same scale as the Si phonons. The inset shows the sample geometry.

Fig. 2 The Raman spectra of GaAs layers at different distances to the interface obtained by taking the difference of two Raman spectra measured from two adjacent spots along the bevel.

$\circ$
 A: 0 - 500 Å
 $\circ$
 B: 500 - 800 Å
 $\circ$
 C: 800 - 1000 Å
 $\circ$
 D: 1000 - 1500 Å
 $\circ$
 E: 1500 - 2100 Å
 $\circ$
 F: 2100 - 5200 Å

Fig. 3 (a) Linewidth, frequency shift and asymmetry of GaAs LO phonon as a function of distance to the interface. These results have been obtained from Raman spectra of the GaAs LO phonon measured with better resolution than those shown in Fig. 2. The inset shows quantitatively the definition of the parameters Γ_A and Γ_B and the asymmetry parameter: Γ_A/Γ_B .

(b) The strain and spatial correlation lengths of GaAs film as a function of distance to the interface deduced from Fig. 3 (a).

Fig.1

Fig. 2

Fig. 3

Fig. 4

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