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Photoluminescence measurements for GaAs grown on Si(100) and Si(111) by molecular beam epitaxy

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Photoluminescence measurements have been used to characterize Si-doped GaAs layers, ranging in thickness from 1.1–8.1 μm, grown on Si(111) and misorientated Si(100) substrates by molecular beam epitaxy. 4.2 K PL spectra for GaAs/Si (100) show a strain-induced splitting between the heavy and light hole valence bands which corresponds to a biaxial tensile stress of 2.8 ± 0.15 kbar acting on the GaAs layer. Similar measurements for GaAs/Si(111) indicate that the GaAs layer is subject to a biaxial tensile stress of 3.9 ± 0.15 kbar at 4.2 K. Furthermore, the intensity and line shape of luminescence features for GaAs/Si(111) for the first time indicate a crystalline quality comparable with the best GaAs/Si(100) material.

The optical properties of GaAs layers grown on Si(100) substrates have previously been assessed by a number of experimental techniques, including photoluminescence (PL)[1–6] and Raman scattering measurements.[7,8] Low-temperature PL spectra for undoped[2] GaAs/Si(100) have revealed two intrinsic radiative transitions which reflect a strain-induced lifting of the valence-band degeneracy in the GaAs layer. The difference in energy between the electron to light hole, and electron to heavy hole transitions provides a measure of the in-plane stress. Furthermore, this stress is tensile in nature, and arises from the difference in thermal expansion coefficients between GaAs and Si. The anisotropy in the thermal expansion of GaAs grown on Si(100) has been clearly demonstrated by x-ray scattering measurements.[9] Strain relief mechanisms and the nature of dislocations in GaAs/Si heterostructures have also been investigated[10] using transmission electron microscopy. Relaxation of the thermally induced stress has been achieved by post-growth patterning of the GaAs epilayers with a chemical etchant.[4,5]

In this letter we present PL data for GaAs layers grown on both Si(100) and Si(111) substrates by molecular beam epitaxy (MBE). While the intensities and line shapes of the dominant recombination transitions provide a measure of the material quality, the energies of these features reflect the degree of stress present in each layer. In this way, we compare the thermally induced stress for GaAs layers grown on Si(100) and Si(111) substrates.

Both (100) and (111) orientated Si wafers were used as the substrate material for this study. The Si(100) substrates were *n*-type (P doped, $\rho \sim 2200\ \Omega$ cm), and misorientated by 3° towards the [011] direction, whereas the Si(111) wafers were *p*-type (B doped, $0.75 \leqslant \rho \leqslant 1.25\ \Omega$ cm). The substrates were chemically treated with a simple HF etch and reoxidation routine before In-free mounting onto Mo platters, and loading into a VG Semicon V80H MBE reactor. Further details concerning the Si substrate preparation and the MBE growth conditions have previously been reported in the literature.[11] Following the desorption of the oxide layer from the Si(100) samples, a 0.1 μm buffer layer was grown at 300 °C, at a rate of 0.5 μm/h. These buffer layer conditions have been previously investigated using both Raman scattering measurements[12] and spectroscopic ellipsometry.[13] The substrate temperature was then increased in the As_4 flux to 580 °C. During this temperature ramp the buffer layer ordered to yield a (2×4) single-domain GaAs(100) reconstructed surface. GaAs active layers (i.e., doped such that $N_{Si} \sim 2 \times 10^{16}$ cm^{-3}) were grown at 580 °C with a deposition rate of 1 μm/h. The total epitaxial thickness was varied in the range $1.1 \leqslant d \leqslant 8.1 \mu$m. Each of these GaAs/Si(100) layers was observed, by reflection high-energy electron diffraction (RHEED) measurements, to terminate growth with a single-domain GaAs(100) (2×4) reconstruction. Two approaches were taken towards the growth of GaAs/Si(111). The first involved repeating the above- mentioned two-step process for the (100) system, using an epitaxial thickness of 4.1 μm. The second approach did not use a buffer, but rather initiated growth at 1 μm/h. Two such "nonbuffered" layers were grown, one at 580 °C, and the other at 530 °C. Other details relating to the growth and characterization of these GaAs/Si(111) structures are presented elsewhere.[14] RHEED measurements indicated both $(\sqrt{19} \times \sqrt{19})$ and (2×2) surface phases. Since only a (2×2) structure is reported to exist on the GaAs(111) surface,[15] while both can exist on a GaAs$(\bar{1}\,\bar{1}\,\bar{1})$ surface, it is suggested that GaAs grows on Si(111) with a $(\bar{1}\,\bar{1}\,\bar{1})$ orientation. Electrical measurements, which make use of the fact that Si acts as a *p*-type dopant in GaAs(111) and *n*-type in GaAs$(\bar{1}\,\bar{1}\,\bar{1})$,[15] have also confirmed the growth of GaAs$(\bar{1}\,\bar{1}\,\bar{1})$ on Si(111).[14]

PL measurements were carried out at temperatures from 4.2 to 300 K inside an Oxford Instruments cryostat. A helium-neon laser provided 1 mW excitation at 632.8 nm. The luminescence was dispersed by a Coderg T800 triple spectrometer and detected by a GaAs photomultiplier, RCA type C31034, equipped with photon counting electronics. The experimental resolution remained better than 0.5 meV at all times.

Figure 1 contains PL spectra, measured at $T = 4.2$ K, for GaAs layers of different thicknesses grown on Si(100). The PL intensity is observed to increase, while the full

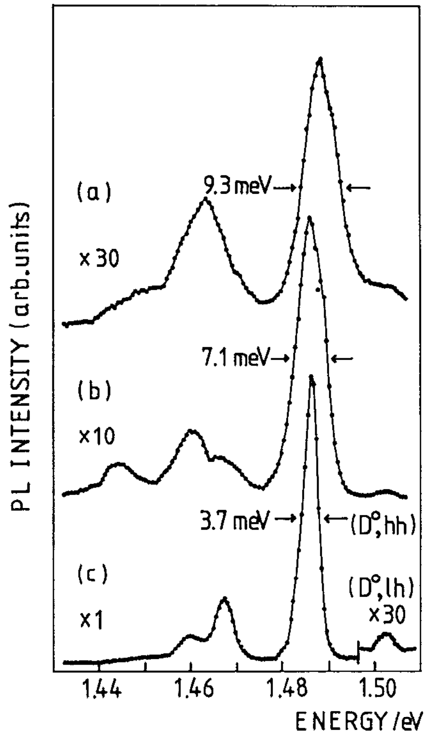

FIG. 1. 4.2 K PL spectra for (a) 1.1 μm GaAs/Si(100), (b) 2.1 μm GaAs/Si(100), and (c) 4.6 μm GaAs/Si(100).

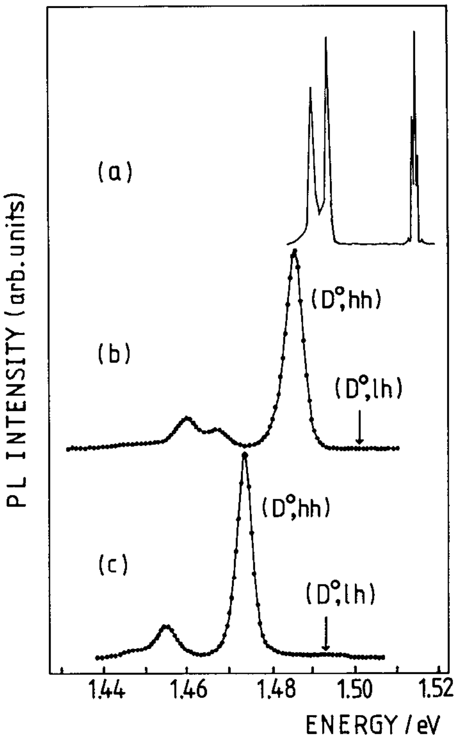

FIG. 2. Comparison between PL spectra for (a) 10 μm GaAs/GaAs(100), (b) 4.1 μm GaAs/Si(100), and (c) 4.1 μm GaAs/Si(111); all spectra measured at $T = 4.2$ K and normalized to unit height.

width half maximum (FWHM) value of the dominant recombination feature decreases, with increasing GaAs thickness. The PL peak energies agree well with values reported in the literature.[1-3,5,6] In particular, the 4.6 μm GaAs/Si(100) structure shows PL transitions at 1.502(5) eV, (D^0,lh), and 1.486 eV, (D^0,hh), which correspond[2] to recombination involving excitons bound to Si donors and the $m_j = \pm 3/2$ (light hole) and $m_j = \pm 1/2$ (heavy hole) valence-band states. The PL peaks at 1.486 and 1.460 eV have previously[5] been associated with transitions from the conduction band to neutral carbon acceptors, and from the Si donors to Si acceptors, respectively, for GaAs doped to the same extent. The FWHM of the 1.468 eV luminescence feature is 3.7 meV, which compares very favorably with a FWHM of 2.9 meV found[2] for high quality undoped GaAs grown on Si(100). Figure 2 compares the PL spectrum obtained from a 10-μm-thick GaAs layer ($\mu_{77\,\mathrm{K}} \geqslant 150\,000$ $\mathrm{cm}^2\,\mathrm{V}^{-1}\,\mathrm{s}^{-1}$) grown on GaAs(100), with PL spectra for 4.1-μm-thick GaAs layers grown on Si(100) and Si(111) substrates. The GaAs/Si(100) structure was grown at 580 °C, while the GaAs/Si(111) epilayer was grown at 530 °C. In addition to lifting the valence-band degeneracy, the strain in the GaAs/Si layers has moved the PL features to lower photon energies. Moreover, the PL spectrum for GaAs/Si(111) has been shifted considerably more than the corresponding spectrum for GaAs/Si(100), and the valence-band splitting has also increased, with the (D^0,*l*h) transition now occurring at 1.493 eV and the (D^0,hh) transition at 1.474 eV. This suggests that the degree of stress exerted on the GaAs epilayers by the Si substrate, due to the difference in thermal expansion coefficients between GaAs and Si, depends on the orientation of the substrate. Similar PL spectra were obtained for the GaAs/Si(111) layers grown at 580 °C, indicating that the observed shifts in PL transition energies between GaAs/Si(100) and GaAs/Si(111) are not due to the 50 °C difference in growth temperature. It is worth noting that for GaAs layers grown on Si(100) substrates there is little variation in the PL transition energies for thicknesses ranging from 1.1 to 8.1 μm. In comparison, a large increase in the number and size of microcracks has been observed[5] for GaAs layers thicker than 4.1 μm, which has in turn shed doubt[16] on the validity of Hall measurements for GaAs/Si structures with GaAs thicknesses exceeding 4.1 μm. Luminescence and conventional double-crystal x-ray diffraction measurements are dominated by the material quality between these microcracks and so indicate that the GaAs crystallinity continues to improve with thickness, at least for thicknesses up to 8.1 μm.

The effect of biaxial tensile stress in the (100) plane is normally dealt with in terms of a hydrostatic tensile stress component together with a uniaxial (100) compressive stress component. The change in the band-edge transition energies $\delta(E_c - E_{\mathrm{lh,hh}})$ is then given by[17]

$$\delta(E_c - E_{\mathrm{lh,hh}}) = 3a(S_{11} + 2S_{12})X - a(S_{11} + 2S_{12})X \pm b(S_{11} - S_{12})X,$$

where S_{11},S_{12} are elastic compliances and a,b are deformation potentials corresponding to hydrostatic and tetragonal distortions, respectively. X is the stress acting on the layer. Hence, the changes in transition energies are given by

$$\delta(E_c - E_{lh}) = 2a(S_{11} + 2S_{12})X - b(S_{11} - S_{12})X, \qquad (1)$$

$$\delta(E_c - E_{hh}) = 2a(S_{11} + 2S_{12})X + b(S_{11} - S_{12})X. \qquad (2)$$

Similarly, biaxial tensile stress in the (111) plane can be decomposed into a hydrostatic component together with a uniaxial component acting along the (111) direction. This leads to

$$\delta(E_c - E_{lh}) = 2a(S_{11} + 2S_{12})X - (1/2\sqrt{3})dS_{44}X, \qquad (3)$$

$$\delta(E_c - E_{hh}) = 2a(S_{11} + 2S_{12})X + (1/2\sqrt{3})dS_{44}X, \qquad (4)$$

where S_{44} is an elastic compliance and d is the deformation potential for a trigonal distortion.

From Eqs. (1) and (2), the valence-band splitting for GaAs/Si(100) is equal to $2b(S_{11} - S_{12})X$. Using values[18] of $S_{11} = 12.6\times10^{-4}$ kbar^{-1}, $S_{12} = -4.23\times10^{-4}$ kbar^{-1}, $a = -8.3$ eV, and $b = -1.7$ eV, together with the experimentally determined valence-band splitting of 16 ± 0.5 meV, we find that the biaxial tensile stress X is 2.8 ± 0.15 kbar for GaAs/Si(100) at liquid-helium temperatures. Likewise, for GaAs/Si(111) the valence-band splitting from Eqs. (3) and (4) is equal to $(1/\sqrt{3})dS_{44}X$, where[18] $S_{44} = 18.6 \times 10^{-4}$ kbar^{-1} and $d = -4.55$eV. In this case, the measured valence-band splitting is 19 ± 0.5meV, which provides us with a value of 3.9 ± 0.15 kbar for the biaxial tensile stress exerted on GaAs layers grown on Si(111) substrates.

The PL spectrum for GaAs/Si(111) in Fig. 2 was obtained from a sample consisting of a 4.1-μm-thick GaAs layer deposited at 530 °C without the use of a low-temperature buffer layer. The FWHM of the (D^0,hh) transition is 4.1 meV, while x-ray diffraction measurements yield a FWHM for the GaAs layer of ~215 arcsec. These values compare well with 3.7 meV and ~ 250 arcsec obtained from our best GaAs/Si(100) material.

In conclusion, PL measurements have been used to compare the thermally induced stress present for GaAs layers grown on both Si(100) and Si(111) substrates. The energy splitting between the $(D^0,l\text{h})$ and (D^0,hh) transitions, at $T = 4.2$K, reflects a biaxial tensile stress of 2.8 ± 0.15 kbar for GaAs/Si(100), and a stress of 3.9 ± 0.15 kbar for GaAs/Si(111). We believe that this is one of the first reports of luminescence from GaAs deposited directly on Si(111) by MBE. Recently, there has been renewed interest in (111) growth, with (111) quantum well lasers exhibiting[19] lower threshold current densities than similar (100) laser structures. Hence, a more detailed study of the growth of GaAs on Si(111) is currently in progress.

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