Comparison of the Strain and Stress in Bonded and Epitaxial Gallium Arsenide on Silicon by Photoreflectance Spectroscopy Measurements

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ABSTRACT

The presence of an internal strain arising from the GaAs/spin-on-glass (SOG)/Si bonding procedure was investigated. In addition, the magnitude of any residual stress at room temperature and the mechanisms that may impose a stress, leading to elastic or plastic deformation of the bonded GaAs films, were identified.

A comparative study of biaxial strain and stress, as a function of temperature in the range of 80- 300 K, in a bonded 2 μm-thick GaAs/SOG/Si sample and in an epitaxial 2 μm-thick GaAs/Si sample, grown by molecular beam epitaxy (MBE), will be presented. The type and magnitude of strain were determined by photoreflectance spectroscopy. In the case of GaAs/SOG/Si, the strain in the GaAs layer was found to be negligible, with compressive character, at room temperature and tensile in all other measured temperatures, whereas for the epitaxial GaAs/Si, the strain was taking significant tensile values in all temperatures. Furthermore, the strain for both samples was increasing with temperature reduction, as it is expected for a thermal strain induced by the different thermal expansion coefficients of GaAs and Si.

The comparative study indicated clearly that the bonded GaAs/SOG/Si films are essentially strain-free at room temperature. This is a very important result for the good reliability of laser diodes that can be processed from such bonded GaAs material, which also has a crystal quality similar to that of the available GaAs substrates.

INTRODUCTION

The wafer scale integration of III-V optoelectronic devices with Si CMOS circuits can result into semiconductor components with improved performance and/or new functionalities [1]. Two alternative GaAs-Si material integration processes have been investigated for this purpose; the heteroepitaxial growth of GaAs-on-Si (GaAs/Si) and the low temperature bonding of GaAs and Si wafers using a spin-on-glass (SOG) intermediate layer (GaAs/SOG/Si). The presence of crystalline defects and internal strains in the III-V semiconductor films is critical for the reliability of fabricated laser diodes and thus it becomes very important to study these issues in the two alternative GaAs-on-Si structures.

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To estimate the internal strain in a 2 µm GaAs/SOG/Si sample (#133) as well as a reference 2 µm epitaxial GaAs/Si sample (#66), the energy band-gap shift from the gap of an unstrained GaAs substrate was determined, by the photoreflectance (PR) technique.

EXPERIMENTAL AND FITTING DETAILS

The experimental set-up for the PR measurement was essentially the same as described in literature. A laser beam, which is incident on the sample, modulates the optical response of the sample. The laser is chopped at a frequency ($f \approx$ 370 Hz was used), which is also used as the reference frequency to the Lock-in amplifier. The photodetector output signal is pre-amplified by a current amplifier.

Modulation spectroscopy, such as PR (ΔR/R) is expressed as the ratio of the reflectance change caused by modulation light –laser- (ΔR) to the reflectance (R). The normalized change in the reflectivity (ΔR/R) -in the low field-regime- can be written, according to Aspnes theory [2], as

$$\frac{\Delta R}{R} = \mathrm{Re}\left[\sum_{j=1}^{f} \frac{A_j e^{i\Phi_j}}{(E - E_{gj} + i\Gamma_j)^{n_j}}\right] \qquad (1)$$

where f is the number of the transitions to be fitted, A is the amplitude, Φ is a phase angle (interference effects), E is the photon energy, E_g is the energy-gap, and Γ is the broadening parameter due to carrier scattering processes. Parameter n refers to the type of optical transitions: n=2 and 2.5 for an excitonic and a three-dimensional one-electron transition, respectively. So, for a given transition, the fitting parameters are A, Φ, Eg and Γ. The PR spectra were considered to originate from three-dimensional one-electron transitions. Therefore n=2.5 and the PR line-shapes are modeled as

$$\frac{\Delta R}{R} = \mathrm{Re}\left[\sum_{j=1}^{f} \frac{A_j e^{i\Phi_j}}{(E - E_{gj} + i\Gamma_j)^{2.5}}\right] = \sum_{j=1}^{f} \frac{A_j \cos[\Phi_j + 2.5 ArcCos\kappa_j]}{((E - E_{gj})^2 + \Gamma_j{}^2)^{1.25}} \qquad (2)$$

where κ is the phase angle of the complex number [(E-Eg)-iΓ].

EXPERIMENTAL RESULTS AND DISCUSSION

All the PR spectra line-shapes retained their line-shape at every measured temperature, as the temperature was decreased from 296 K to 80 K and then it was increased back to 296 K. This is a rather important result, because it manifests that GaAs/SOG/Si does not undergo a plastic deformation, thus all the spectra line-shapes are reverted to their initial shape. Differences were only observed in the intensities of the spectra. The same behavior was also observed for the epitaxial 2 µm GaAs/Si sample (#66).

The energy difference between the transition of the bonded or GaAs/Si samples that corresponds to the band-gap and the energy band-gap of the GaAs substrate can be obtained by fitting the PR line-shapes, using the Eq. (2). From elastic theory, we can estimate the value of the internal strain from the band-gap change. The change of the band-gap energy ΔE_g ($m_j = \pm 3/2, \pm 1/2$) associated with the two valence band states ($J = 3/2$, $m_j = \pm 3/2, \pm 1/2$) becomes [3]:

$$\Delta E_g(m_J = \pm\frac{3}{2}) = 2a(1-\frac{C_{12}}{C_{11}})\varepsilon \quad -b(1+\frac{2C_{12}}{C_{11}})\varepsilon = -6.28\varepsilon \text{ (eV)} \qquad (3)$$

$$\Delta E_g(m_J = \pm\frac{1}{2}) = 2a(1-\frac{C_{12}}{C_{11}})\varepsilon \quad +b(1+\frac{2C_{12}}{C_{11}})\varepsilon = -12.8\varepsilon \text{ (eV)} \qquad (4)$$

For a tensile strain, the quantity ε, by definition, assumes a positive value, while ε is defined to be negative for compressive strain. Quantities a and b are known as hydrostatic and shear deformation potentials, respectively. In Eqs. (3) and (4), $a = a_c + a_v = -8.7$ eV and $b = -1.7$ eV are the values which have been used for the strain estimation. Furthermore, $C_{11} = 11.88\times10^{11}$ dyne/cm^2 and $C_{12} = 5.38\times10^{11}$ dyne/cm^2 are the elastic stiffness coefficients. When strain is tensile, the conduction band shifts to lower energies in regard with the unperturbed conduction band. The shift is in absolute value greater than that of ±3/2 and ±1/2 valence bands, so the energy-gap decreases. On the other hand, when the strain is compressive, the conduction band shifts to higher energies and no matter how the valence bands shift, the energy band-gap is increased. Consequently, the energy band-gap is mainly depended by the conduction band gap shift.

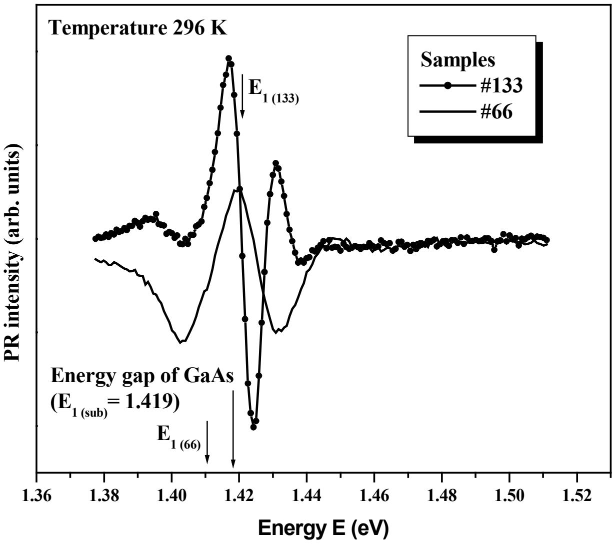

FIGURE 1. Experimental photoreflectance spectra at 296 K. The band-gap of sample #133 coincides with that of the unstrained GaAs substrate. Arrows have been inserted in the figures to indicate the band-gap values, as follows: $E_{1(133)}$= energy-gap of sample #133, $E_{1(66)}$= energy-gap of sample #66, $E_{1(sub)}$= energy-gap of GaAs (substrate).

Figure (1) shows the experimental PR spectrum of the samples #133 and #66 at 296 K. Arrows have been inserted in the figures to indicate the band-gap values, as follows: $E_{1(133)}$= energy-gap of sample #133, $E_{1(66)}$= energy-gap of sample #66, $E_{1(sub)}$= energy-gap of GaAs (substrate). From the fit of Eq. (3) to the PR spectra the energy position of the first (E_1) has been determined for each sample. These values have to be compared to the measured values from the strain free GaAs (substrate). For estimating the internal strain in samples #133 and #66, the corresponding energy band-gaps shift was determined. Since the energy position of the transition (E_1) is the energy band-gap of each sample, the energy difference between this transition and the value of the band-gap of the GaAs substrate corresponds to the energy band-gap change due to the biaxial strain. Therefore, for the strain estimation we used Eq. (3) when the sample has bigger band-gap energy than the GaAs substrate (compressive strain) and Eq. (4) for the reverse case (tensile strain). Since we can determine the strain ε, the stress σ ($dyne/cm^2$) can also be calculated from Eq. (5).

$$\sigma = \frac{(C_{11}+2C_{12})(C_{11}-C_{12})}{C_{11}}\varepsilon \Rightarrow \sigma = 12.38\times 10^{11}\varepsilon \quad (dyne/cm^2) \qquad (5)$$

It was observed that the strain for both the 2 μm GaAs/Si and 2 μm GaAs/SOG/Si samples was increased with temperature reduction. However, the strain in the bonded GaAs film was always significantly lower compared to the epitaxial sample (#66). The estimated values of strain are accurate within $\pm 0.2\times 10^{-3}$. In Fig. (2), the PR spectrum of the GaAs/SOG/Si sample (#133) at 296 K can be seen along with the theoretical fitting. The energy position of the first transition (E_1) has been determined by fitting the data points using Eq. (3).

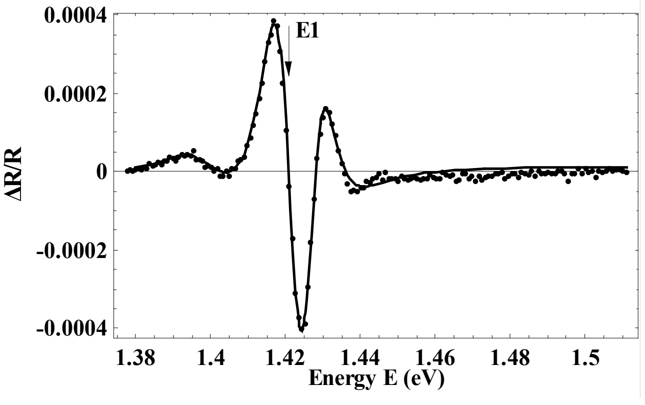

FIGURE 2. PR spectrum of the GaAs/SOG/Si sample #133 at 296 K temperature. The solid line is the theoretical fitting to the data points (solid circles). The E_1 corresponds to the band-gap determined by the fitting.

In Fig. (3), the PR spectrum of the epitaxial GaAs/Si sample (#66) at 296 K can be seen along with the theoretical fitting.

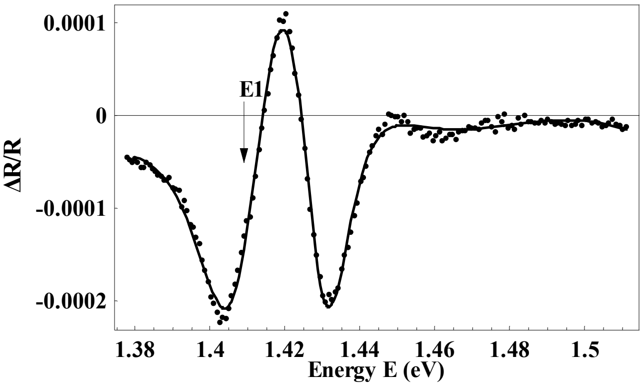

FIGURE 3. PR spectrum of the GaAs/Si sample #66 at 296 K temperature. The solid line is the theoretical fitting to the data points (solid circles). The E_1 corresponds to the band-gap determined by the fitting.

From the calculated values of strain, the strain of sample #133 was found to be slight compressive at room temperature. It must be pointed out that the estimated small value of compressive strain in the bonded 2 μm GaAs film is within the error of the calculation method, which is mainly determined from the error of the monochromator. The latter is due to the limited resolution of the monochromator, which is estimated to be 2 meV in the spectral range of 1.42 eV. A comparison with the epitaxial GaAs film indicates clearly that the bonded film is essentially strain-free at room temperature. This is a very important result for the good reliability of laser diodes that can be processed from bonded GaAs material.

In Fig. (4), the temperature variation of the stress in both the bonded GaAs/SOG/Si and the epitaxial GaAs-on-Si samples can be seen. An increase of the biaxial stress as a function of decreasing temperature was observed in both the bonded GaAs/SOG/Si and the epitaxial GaAs-on-Si samples. This indicates that in both cases the tensile stress is a thermal stress created by the different thermal expansion coefficients of GaAs and Si.

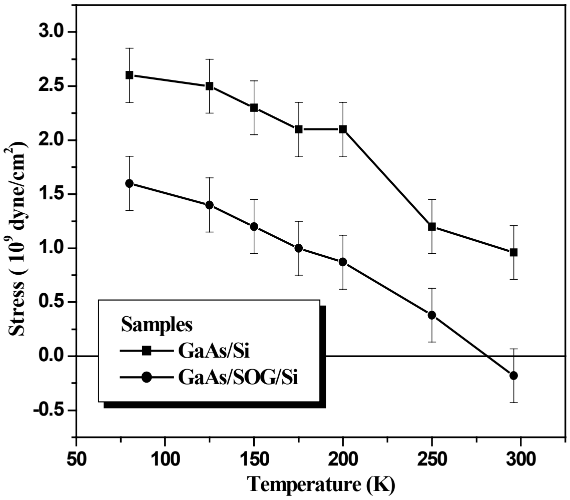

Figure 4. Stress in the 2 μm GaAs films of bonded GaAs/Si (#133) and heteroepitaxial GaAs/Si (#66), in the temperature range of 80-296 K. Error bars for stress are ± 2.5 10^8 dyne/cm^2.

CONCLUSIONS

Using PR spectroscopy we have determined the type of strain in a 2 μm GaAs/SOG/Si sample (#133), which was found to be almost unstrained at room temperature and tensile in all the lower temperatures. On the contrary, the type of strain was found to be tensile in an epitaxial 2 μm GaAs/Si film in all the temperature range. From the strain calculations, we see a similar increase of the biaxial strain, as a function of decreasing temperature, in both the bonded and the epitaxial GaAs/Si samples. This is due to the thermal stress created by the different thermal expansion coefficients of GaAs and Si.

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