

## Infrared ellipsometry of GaAs epilayers on Si(100)

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Infrared spectroscopic ellipsometry is used to characterize the structure of molecular-beam-epitaxial grown GaAs layers on Si(100) before and after thermal cycle (TC) annealing. The dielectric function of the GaAs epilayer has been described by the sum of a factorized form and a classical Drude model in the spectral fitting procedure. The epilayer LO phonon frequency shifts toward lower frequency with increasing TC number while the opposite is seen for TO phonon. The shift of the LO mode indicates that the tensile stress increases with increasing TC number, while the shift of the TO mode is attributed mainly to the self-energy effect in GaAs:Si. Unequal thermal diffusion of  $\text{Si}_{\text{As}}^-$  and  $\text{Si}_{\text{Ga}}^+$  is indicated. © 2003 American Institute of Physics. [DOI: 10.1063/1.1561577]

The heteroepitaxy of GaAs on a Si substrate (GaAs/Si) has attracted much interest as this is a promising material combination for optoelectronic integrated circuits.<sup>1–3</sup> However, the lattice and thermal mismatches between the two materials typically present severe handicaps to obtaining defect-free layers.<sup>4</sup> Furthermore thermal annealing, which is a very effective means to realize low defect density GaAs epilayers on Si substrates, results in the increase of stress<sup>5</sup> and the diffusion of Si into the GaAs layer.<sup>6</sup> Although Raman measurements have been extensively used as a nondestructive probe to characterize the stress and the Si doping level of such GaAs material, it is difficult with this method to obtain information on the TO phonons because light scattering from TO phonons is not allowed in backscattering off a (100) face.<sup>7</sup>

Spectroscopic ellipsometry (SE) is another very powerful, nondestructive technique for the investigation of film structure, thickness, and optical properties.<sup>8</sup> Infrared spectroscopic ellipsometry (IRSE) enables the application of SE to wavelengths matching the optical phonon frequencies of both the TO and LO phonons as well as the free-carrier response of doped semiconductor materials.<sup>9</sup> In the present work, we have assumed for the IRSE analysis a four phase model [i.e., (1) air, (2) low Si concentration GaAs layer, (3) high Si concentration GaAs layer, and (4) Si substrate] and that the dielectric function can be described by a sum of a factorized form and a classical Drude model. Good agreement between the experimental and calculated spectra has been obtained. As a result, we found that the LO phonon shifts toward lower frequency with increasing thermal cycle (TC) number while interestingly the opposite effect was seen for the TO frequency. The high Si concentration GaAs layer adjacent to the GaAs/Si interface displays an increase of thickness and Si concentration with increasing TC number.

The 1  $\mu\text{m}$ -thick GaAs film was grown at 600 °C by molecular beam epitaxy on a (100)-oriented Si substrate with a 2° misorientation toward [110]. The TC annealing was per-

formed in vacuum with the sample surface covered with a  $\text{SiO}_2$  coated Si substrate. The temperature was raised to 850 °C, stabilized at that level for 5 min, and cooled to 300 °C in each cycle. Further details of the growth and TC annealing procedure can be found in Ref. 10. The samples, labeled by 1–5 in Table I, each had different anneal cycle numbers. Room-temperature IRSE spectra of the samples were measured in the range 50–400  $\text{cm}^{-1}$  at 2  $\text{cm}^{-1}$  resolution and 65° angle of incidence and using a rotating analyzer. The details of the measurement conditions are the same as those reported previously.<sup>11</sup>

The ellipsometric parameters  $\Psi$  and  $\Delta$  are defined as usual from the ratio  $\hat{\rho}$  of the complex reflection coefficients  $\hat{r}$  for  $s$  and  $p$  polarization

$$\hat{\rho} = \frac{\hat{r}_p}{\hat{r}_s} = \frac{|\hat{r}_p|}{|\hat{r}_s|} e^{i(\delta_p - \delta_s)} = \tan \Psi e^{i\Delta}. \quad (1)$$

The parameters  $\Psi$  and  $\Delta$  can be implicitly expressed as a function of the dielectric function  $\epsilon$  and thickness for the samples under study. The dielectric function of GaAs described in terms of the sum of a factorized model<sup>12</sup> and a classical Drude model<sup>13</sup> is written by

$$\epsilon = \epsilon_\infty \left[ \frac{\omega_L^2 - \omega^2 + i\omega\gamma_L}{\omega_T^2 - \omega^2 + i\omega\gamma_T} - \frac{\omega_p^2}{\omega(\omega + i\gamma_p)} \right], \quad (2)$$

where  $\epsilon_\infty$  is the high-frequency dielectric constant,  $\omega_L(\gamma_L)$ ,  $\omega_T(\gamma_T)$  and  $\omega_p(\gamma_p)$  are the frequencies (damping factors) of LO, TO phonons and charge carrier plasma, respectively. The plasma frequency  $\omega_p$  depends on the free-carrier concentration  $N$ ,  $\epsilon_\infty$ , and effective mass  $m^*$  of the free carriers. Although the sum of a harmonic Lorentz oscillator and the Drude model has been used to describe doped GaAs by several authors,<sup>9,14</sup> that approach fails to describe the typically asymmetric dielectric response function of multiple-mode materials, especially near a phonon mode frequency.<sup>15</sup> It will be mentioned later that the observed LO and TO phonon frequency shifts were attributable to two different effects when the cycle number was varied. Therefore, it is reasonable to assume different damping factors for LO and TO

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TABLE I. Best-fit model parameters of GaAs epilayer on Si(100) substrate determined by infrared spectroscopic ellipsometry. The  $\omega_{p1}(d_1)$  and  $\omega_{p2}(d_2)$  are plasma frequency (thickness) of low and high Si concentration regions, respectively. The 90% confidence limits are given with ( $\pm$ ).

Sample no.	Cycle number	Dislocation density ( $10^7 \text{ cm}^{-2}$ )	IRSE parameters									
			$\epsilon_\infty$	$\omega_{LO}$	$\gamma_{LO}$	$\omega_{TO}$	$\gamma_{TO}$ ( $\text{cm}^{-1}$ )	$\omega_{p1}$	$\omega_{p2}$	$\gamma_p$	$d_1$ $\mu\text{m}$	$d_2$ $\mu\text{m}$
1	0	13.4		290.5 $\pm 0.6$	3.5 $\pm 0.5$	265.6 $\pm 0.4$	2.6 $\pm 0.7$	47 $\pm 21$	210 $\pm 16$	141 $\pm 40$	0.98 $\pm 0.09$	0.24 $\pm 0.008$
2	1	3.9		290.2 $\pm 0.4$	3.4 $\pm 0.5$	265.8 $\pm 0.3$	2.4 $\pm 0.6$	68 $\pm 12$	224 $\pm 12$	170 $\pm 29$	0.99 $\pm 0.08$	0.31 $\pm 0.06$
3	3	2.7	10.52	289.7 $\pm 0.5$	2.4 $\pm 0.6$	266.2 $\pm 0.3$	2.8 $\pm 0.6$	99 $\pm 11$	332 $\pm 19$	216 $\pm 25$	0.85 $\pm 0.06$	0.32 $\pm 0.05$
4	5	2.0		289.1 $\pm 0.5$	2.2 $\pm 0.6$	266.3 $\pm 0.3$	2.7 $\pm 0.5$	99 $\pm 11$	335 $\pm 17$	171 $\pm 16$	0.83 $\pm 0.06$	0.34 $\pm 0.04$
5	7	1.7		288.2 $\pm 0.5$	1.4 $\pm 0.7$	267.5 $\pm 0.3$	3.0 $\pm 0.5$	128 $\pm 8$	383 $\pm 12$	169 $\pm 10$	0.48 $\pm 0.05$	0.66 $\pm 0.04$

phonons. In performing the fitting, parameters such as phonon frequency, damping factor, plasma frequency, and thickness were evaluated numerically by minimizing the fitted mean squares deviation with a regression program.

The good agreement obtained between measured and calculated IRSE spectra of samples 1 and 5 is shown in Fig. 1. The best-fit model parameters obtained in the simulation of  $\tan \Psi$  and  $\cos \Delta$  spectra are shown in Table I for all the samples. In the same table the epilayer dislocation densities determined by double-crystal x-ray diffraction measurement are also shown for comparison. In our fitting procedure, we have used a fixed value of 10.52 for  $\epsilon_\infty$ <sup>9</sup> and the same parameters in the factorized model were assumed for the top and interface layers to minimize the number of free parameters. In Fig. 1, the  $\tan \Psi$  base line for sample 5 is larger than that of sample 1 over the whole frequency range because the

carrier concentration of sample 5 is higher than that of sample 1.

It is interesting to note that the LO phonon shifts towards lower frequency with increasing cycle number, indicating that the stress of the GaAs layer increases with increasing cycle number  $N$ . The LO phonon shift with the biaxial strain can be written as<sup>16</sup>

$$\delta\omega(\text{LO}) = -3.9X = -4.9 \times 10^2 \epsilon_{\parallel}, \quad (3)$$

where  $X$  is the biaxial strain and  $\epsilon_{\parallel}$  is the in-plane lattice distortion. We have calculated  $\epsilon_{\parallel}$  using the LO frequency ( $291.5 \text{ cm}^{-1}$ ) for GaAs bulk<sup>9</sup> and plotted this distortion versus dislocation density as shown in Fig. 2(a). The strain is positive ( $\epsilon_{\parallel} > 0$ ) for both annealed and unannealed samples. This means that the GaAs epilayers are always under biaxial

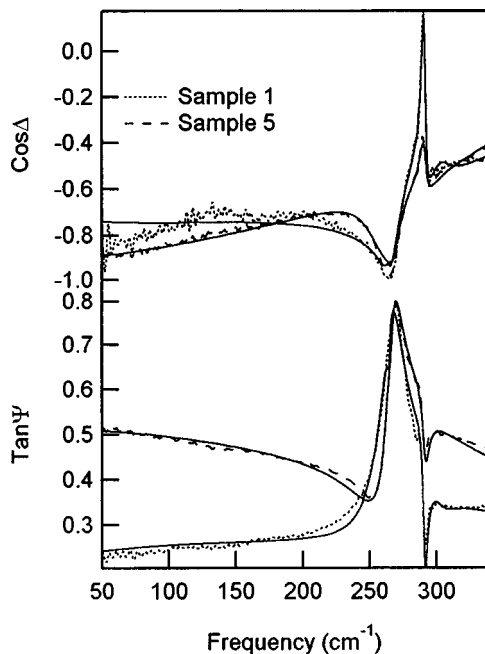


FIG. 1. Measured (dot line and dashed line) and fitted (solid lines)  $\cos \Delta$  (top) and  $\tan \Psi$  (bottom) infrared spectroscopic ellipsometry spectra of samples 1 and 5 at room temperature.

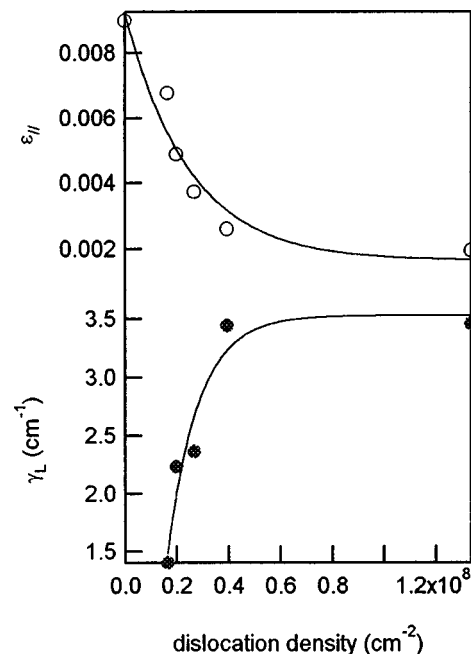


FIG. 2. Variation of the strain (top) and the damping factor of LO (bottom) with dislocation density.

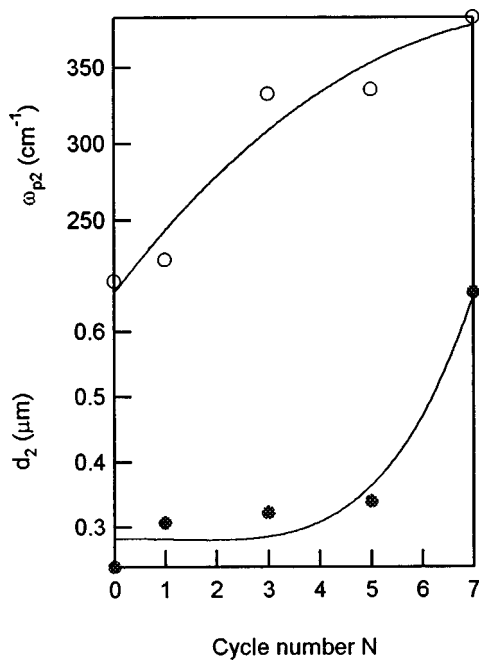


FIG. 3. Variation of the plasma frequency (top) and the thickness of interface (bottom) with cycle number.

tensile stress and that the strain increases with decreasing dislocation density, because the misfit strain is partially relaxed by dislocation formation.<sup>17</sup> Ardila *et al.*<sup>17</sup> found that the stress ( $\epsilon_{\parallel}$ ) for dislocation-free GaAs epilayers on Si is about 0.0045 using Raman spectroscopy. Because our result for the as-grown sample is twice as large as their result for their seed layer, we estimate the strain for dislocation-free material is 0.009 in our case. It is clear from Fig. 2 that the strain rapidly increases in the near dislocation-free range. Another interesting parameter is the LO damping factor, which decreases with decreasing dislocation density (see Fig. 2). This result suggests that the LO damping factor can be used to evaluate crystal quality. An opposite shift to that for the LO phonon frequency was found for the TO mode (see Table I). This behavior for the TO phonon is most likely due to the self-energy effect in GaAs:Si<sup>18</sup> dominating over strain effects.

In Fig. 3 we have plotted the plasma frequency and the thickness of interface layer versus TC number. It can be seen that the plasma frequency continuously increases with increasing TC number, and, up to a certain point, the thickness of the interface layer remains constant at about 0.3  $\mu\text{m}$ , which is the same result as obtained by secondary ion mass spectroscopy.<sup>6</sup> However, after the fifth annealing cycle the thickness abruptly increases. Given that Si is known to be

amphoteric, the concentration of  $\text{Si}_{\text{Ga}}^{+}$  thus increases with increasing TC number during the initial annealing stage. However, when the total Si concentration exceeds  $10^{18} \text{ cm}^{-3}$ , the  $\text{Si}_{\text{As}}^{-}$  concentration rises exponentially<sup>19</sup> leading to the interesting conclusion that the diffusion of the  $\text{Si}_{\text{As}}^{-}$  centers occurs more rapidly than does that of the  $\text{Si}_{\text{Ga}}^{+}$  centers.

In summary, an evaluation of the far infrared features of a GaAs epilayer on a Si(100) substrate has been performed using IRSE. Regardless of how much annealing was performed, the GaAs epilayer consisted of a low Si concentration region towards the top of the epilayer and a relatively high Si concentration region near the GaAs/Si interface. The LO phonon shifted towards lower frequency with increasing cycle number, while the opposite was found for the TO phonon. These two observations indicate the LO phonon is more affected by strain while the TO phonon is more strongly influenced by Si concentration. The Si concentration and thickness of the interface region also increased with increasing TC number and the measurements indicate unequal diffusion rates for  $\text{Si}_{\text{As}}^{-}$  and  $\text{Si}_{\text{Ga}}^{+}$ .

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