Superficies y Vacío ***10***, *32-35, Junio 2000*

Influence of Si(110) misoriented substrates on the microstructure and photoreflectance of GaAs thin films deposited by MBE.

M. Meléndez-Lira, J. Luyo-Alvarado and M. López-López
Departamento de Física, Centro de Investigación y de Estudios Avanzados del IPN.
Apdo. Postal 14-740, México D.F., México 07000

M. A. Vidal
Instituto de Investigación en Comunicación Óptica, Universidad Autónoma de San Luis Potosí, S.L.P.,
Alvaro Obregón 64, San Luis Potosí, México 78000

We have grown GaAs layers by molecular beam epitaxy on Si(110) substrates with different tilted angles towards the [001] direction. The samples where characterized by atomic force microscopy (AFM), high resolution x-ray diffraction (HRXRD), and photoreflectance spectroscopy (PR). The surface morphology analysis by AFM showed that the surface roughness decreased as the off-angle increased. The dislocation density was obtained from the full width at half maximum of the HRXRD reflection peaks. By increasing the off-angle we observed a reduction in the dislocation density. The PR spectra showed the presence of oscillations above the band-gap energy value associated to built-in internal electric fields. The built-in electric field strength and the GaAs band-gap energy values were obtained by employing the Franz-Keldysh model. We obtained band-gap energy values that suggest the presence of residual strains in the films.

Keywords: MBE, heterostructures, GaAs on Si, X-Ray, photoreflectance.

1. Introduction

The epitaxial growth of GaAs on Si substrates has been actively studied because it opens the opportunity to integrate the electronic and optoelectronic capabilities of these two technologically mature materials [1,2]. Because the inherent chemical and physical characteristics of Si and GaAs it has been very complicated to obtain good quality material. Briefly, the factors responsible for this are: i) the silicon non-polar and the GaAs polar bond characteristics, ii) the 4.1 % lattice mismatch, and iii) the ~60% mismatch in thermal expansion coefficients [3]. These problems are reflected in the fact that GaAs/Si heterostructures have a high density of dislocations, beyond the useful range to produce reliable devices. In order to decrease the number of dislocations several approaches have been tried: i) substrate misorientation, ii) buffer layers employing strained layers superlattices and iii) post-annealing of the GaAs/Si heterostructure.[3] However, reduce the GaAs Dislocation density is still an open field. Most of the work employing misorientes substrates have been carried out employing Si(100) substrates or Si(110) with low angle tilting, we are extending the range of tilting angles by employing susbtrates up to 10 degrees.

In this work we report the optical and structural characteristics of GaAs films grown by molecular beam epitaxy (MBE) on misoriented Si(110) substrates. The studied samples were grown on substrates having 0 to 10 degrees of tilting towards the [001] axis. For comparison purposes a sample was deposited on a (110) Si substrate with 6 degrees of misorientation towards the $[1\bar{1}0]$ direction. The samples were studied employing high resolution X-ray diffraction (HRXRD), atomic force microscopy (AFM), and photoreflectance spectroscopy (PR). The results including surface roughness, band gap energies, the HRXRD full width at half maximum (FWHM) of the (220) GaAs diffraction peak and dislocation density showed a decreasing behavior with the Si substrate degree of inclination.

2. Experimental Details

Commercial Si(110) substrates with off-angles of 0, 2, 4, 6, 8 and 10° (± 0.2°) towards the [001] direction were employed in this work. In order to study the effect of the misorientation direction, a Si(110) substrate with an off-angle of 6° towards the orthogonal $[1\bar{1}0]$ direction was also used. The native surface oxide on the Si substrates was removed by dipping the substrates for 5 min in a 30% HF solution before the growth. Immediately after this procedure they were loaded into the MBE system. Before the growth the substrates were annealed at 1000 °C for 20 min. Then, the substrates surface was exposed to an As beam at a flux of 2×10^{-6} Torr at a temperature of 800 °C for 20 min. The GaAs growth was performed at a substrate temperature of 520 °C with a growth rate of 0.8 monolayer (ML) per second, the GaAs film thicknesses were around 1μm. The parameters of the studied samples are summarized in Table 1. The surface morphology was studied by AFM observations in air. The crystal quality of the samples was investigated by HRXRD, using a Philips Material Research Diffractometer, which has a four-crystal Bartels monochromator in the Ge (022) reflection mode, and uses a Cu anode as source of x-ray radiation. The diffractometer was set to select the Cu $K\alpha_1$ wavelength. The x-ray source was operated at 35 kV and 35 mA. Diffraction profiles were obtained from the (220) and (440) symmetric reflections for each sample. Room temperature photoreflectance spectroscopy measurements were carried out employing a standard setup with a He-Ne laser as source of modulation, the probe light was obtained from a tungsten-halogen lamp analyzed with a single monochromator.

3. Results and discussion

It has been reported, Ref [3], that in order to obtain good quality GaAs/Si material it is necessary to increase the number of type I dislocations, because contrary to type II dislocations, they are more efficient in accommodating the mismatch and are kept near the interface. One of the approaches to reduce the number of type II dislocations is to increase the number of nucleation centers by using misoriented substrates. This is the approach taken here, which involves the use of Si (110) substrates cut with inclinations between 0 and 10°. As will be shown below the use of misoriented substrates improved the characteristics of the GaAs/Si system.

A representative X-ray diffractogram for samples studied is shown in figure 1. Figure 2(a) presents the FWHM results from the (220) and (440) GaAs diffraction peaks. We clearly observe a reduction in the FWHM values as the substrate inclination degree increases. The values beyond 4° are around 300 arcsec, which are similar to the results obtained for optimized GaAs growth on Si (100) substrates [4]. The dislocation density obtained from the FWHM values is shown in Fig. 2(b). We observe a monotonic decrease in the dislocation density as the off angle increases. The lowest value obtained is about 3×10^7 cm^{-2} for an off-angle of 8°.

Figure 3 shows AFM images from the samples OD1, 6D1 and 6D11, corresponding to samples grown on Si(110) with 0° and 6° towards [001], and 6° towards $[1\bar{1}0]$, respectively. We clearly observe that substrate misorientation angle is very important to reduce surface roughness, but also that depending on the substrate cut direction there is a big effect on the surface roughness. This could be associated with the density and geometry of Si dangling bonds exposed to the incoming Ga and As atoms: when substrate inclination increases a higher number of ledges is formed; the ledges act as nucleation centers for two-dimensional growth[5]. Figure 4 summarizes the rms roughness values for each sample as obtained from AFM. It is evident that the minimum roughness value is obtained for sample 6D1.

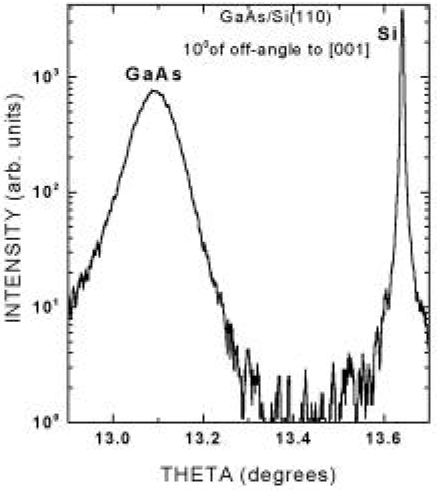

Fig. 1. Typical double crystal X-ray diffractogram of studied samples.

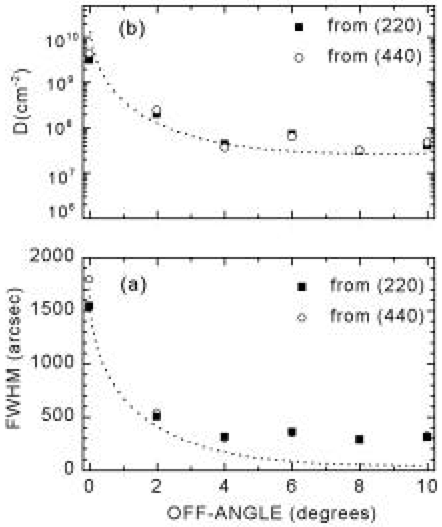

Fig. 2 (a) Full width at half maximum (FWHM) values of the HRXRD profiles from the GaAs(220) and (440) reflections as a function of the substrate tilting angle towards the $[1\bar{1}0]$ direction. (b) Dislocation density in the GaAs films obtained from the data in (a).

Figure 5 presents the results of room temperature PR spectroscopy for the whole set of samples. The rougher samples, (a) 0D1 and (b) 6D11, have a low value of the signal to noise ratio. These spectra were scanned and averaged three times more than the others. The spectrum for sample 0D1 is broad and quite asymmetric (Fig. 5(a)).

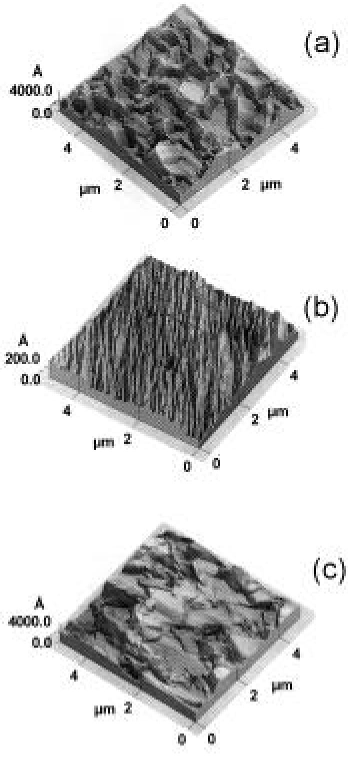

Fig. 3 Atomic force microscopy images of the surface of GaAs layers grown on Si(110) substrates with tilting angles of: (a) 0°, (b) 6° towards the [001] direction, and (c) 6° towards the $[1\bar{1}0]$ direction.

Table 1: Roughness, banda gap and built-in internal electric fields strength values for the studied samples.

Sample	Substrate orientation	rms roughness (Å)	E_g (eV)	F 10^6(V/m)
0D1	Si(110)	664	1.419	-
2D1	Si(110)2°→[001]	449	1.399	3.8±0.2
4D1	Si(110)4°→[001]	105	1.409	3.5±0.6
6D1	Si(110)6°→[001]	47	1.399	4.6±0.2
8D1	Si(110)8°→[001]	165	1.405	3.14±0.01
10D1	Si(110)10°→[001]	182	1.392	3.8±0.2
6D11	Si(110)6°→[1 $\bar{1}$ 0]	625	1.398	3.20±0.01

rms roughness: root mean square roughness values
E_g: band gap energy
F: built-in internal electric field strength

It could be argued that the asymmetry is due to the presence of residual strain, but the high density of dislocations in these sample rules out this possibility. The broad PR signal is related to the low structural quality of this sample. In order to obtain the band gap value from this spectrum we used the third derivative formalism [6]. However, in order to obtain a complete fit to this experimental spectrum, besides the GaAs band-gap transition, an additional low energy signal would be necessary. This energy signal lower than the band gap energy feature could be associated to the presence of an impurity level in GaAs [7]. The presence of this impurity related signal is in agreement with the presence of a high number of type II dislocations in sample 0D1, which may constitute channels for Si diffusion into the GaAs film. The diffusion of impurities is influenced by lattice defects, such as vacancy, interstitial, and dislocations.[8] The result of the fitting is shown as empty circles in Fig. 5(a), and the GaAs band gap value obtained for sample 0D1 is presented in Table 1. PR spectra for samples 2D1 to 10D1, figures 5(b) to 5(f), presented a higher value of the signal to noise ratio associated with an increased structural quality for these samples. Apparently, from the point of view of PR spectroscopy these samples are similar, showing a broad signal below the expected energy for bulk GaAs, and oscillations above this transition. However, a closer examination allows us to get more information about differences among these samples. The presence of a splitting around 1.4 eV is clear, that could be related to residual strain in the films, a similar splitting has been reported by Dimoulas *et al*.[9]. It has been shown that residual strain in the GaAs/Si system is mostly due to the difference in the thermal expansion coefficients between GaAs and Si producing a tensional state in the GaAs films [10]. This tension could cause the observed splitting, however further work is required to completely understand the origin of this feature.

On the other hand, the oscillations above the GaAs band-gap energy observed in Fig. 5, are associated with internal electric fields produced by the Franz-Keldysh effect. The FK oscillations extrema are marked with empty circles in figure 5. We employed the Franz-Keldysh (FK) asymptotic theoretical model to analyze these oscillations

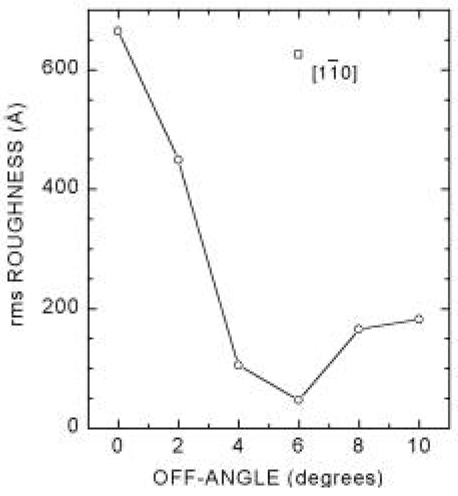

Fig. 4 Variation of the surface rms roughness as a function of substrate tilting angle, as obtained from AFM analysis. The square symbol corresponds to the rms roughness value for sample 6D11, tilted 6° towards the [1 $\bar{1}$ 0] direction.

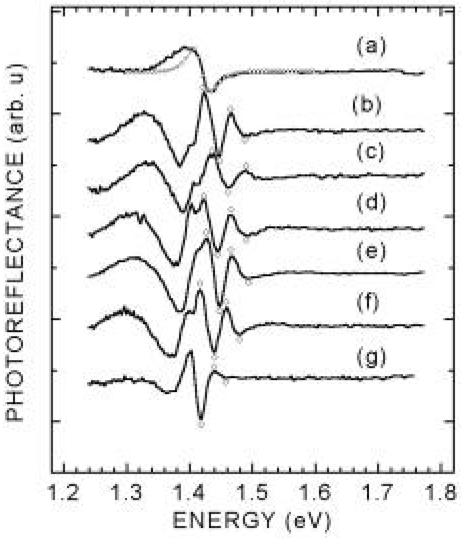

Fig. 5 PR spectra of GaAs layers grown on Si(110) substrates with tilting angles of: (a) 0°, (b) 2°, (c) 4°, (d) 6°, (e) 8°, and (f) 10° towards the [001] direction, and (g) with an off-angle of 6° towards the [1 $\bar{1}$ 0] direction. Empty diamonds correspond to the FK oscillations extrema employed to obtain the built-in internal electric field strength.

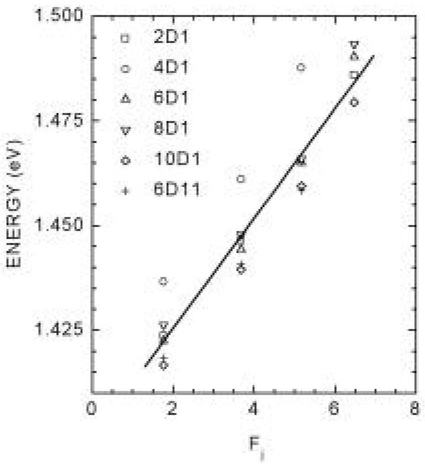

Fig. 6 Linear fittings, for the extrema energies in the PR spectra, to the asymptotic Franz-Keldysh model through Eq. (4).

extrema:[11]

$$\frac{\Delta R}{R} \propto \cos\left(\frac{2}{3}\left[\frac{E-E_g}{\hbar\Omega}\right]^{\frac{3}{2}} + q\right) \qquad (1)$$

where E_g is the semiconductor band gap, q a phase factor and $\hbar\Omega$ a characteristic electro-optic energy given by :

$$\hbar\Omega = \left(\frac{e^2 F_{\text{int}}{}^2 \hbar^2}{8m}\right)^{1/3} \qquad (2)$$

e is the electron charge, F_{int} the internal electric field strength, and $m$is the interband reduced mass involved in the transition. Then, according to Eq. (1), the FK oscillations extrema occur at energies given by

$$\frac{2}{3}\left[\frac{E_j - E_g}{\hbar\Omega}\right]^{\frac{3}{2}} + q = jp, \text{where}\cdots\cdots j = 1,2,.. \qquad (3)$$

Equation (3) can be rearranged as:

$$E_j = \hbar\Omega F_j + E_g \qquad (4)$$

where

$$F_j = \left[\frac{3}{2}p\left(j-\frac{1}{2}\right)\right]^{2/3} \qquad (5)$$

in Eq. (5) we set $q=p/2$ as corresponds to a 3-dimensional critical point.

Figure 6 presents the linear fittings of the extrema of the FK oscillations according to Eq. 4. The built-in electric field strengths for the studied samples obtained from the slope in Eq. (4) are presented in Table I. The GaAs interband reduced mass employed included the heavy hole and electron contributions. The GaAs energy gap value obtained by this method for each sample is also given in this table. The obtained values for the band-gap energy are consistently lower than the commonly accepted value of 1.41 eV for GaAs. The lower band-gap values could reflect a tensional state of the GaAs films on the Si(110) misoriented substrates, as explained above. The internal electric field strengths are in the order of 3×10^6 eV, and could be related to the residual strains in the films through piezoelectric effects but a contribution from the band-offset at the GaAs/Si interface and the GaAs surface can not be ruled out.

Conclusions

We have studied the structural and optical properties of GaAs layers grown by MBE on Si(110) substrates tilted towards the [001] direction. AFM results showed a decrease in the rms surface roughness values from 664 Å for an off-angle of 0º to 47 Å for an off-angle of 6º. A HRXRD analysis showed a reduction of more than two orders of magnitude in the dislocation density in the films as the off-angle was increased from 0º to 6º. This improvement in the crystal quality could be caused by the presence of steps on the tilted substrates, which may act as nucleation sites for the GaAs epitaxial growth. GaAs films grown on Si(110) substrates tilted towards the $[1\bar{1}0]$ direction presented a poor crystal quality, showing that the geometry of the steps plays an important role to improve the epitaxy. The PR study revealed the presence of built-in internal electric fields in the films. The obtained band-gap energy values suggested the presence of residual strains in the layers.

Acknowledgments

The authors acknowledge the technical support provided by A. Guillen, Z. Rivera, R. Fragoso, Hector Silva, and Laura López. This work was partially supported by CONACyT-México.

References

[1]. H.K Choi, C.A Wang, and N.H. Karam, Appl. Phys. Lett. **59**, 2634(1991).
[2]. R.M. Sieg, S.A. Ringel, S.M. Ting, S.B. Samavedam, M. Currie, T. Langdo and E.A. Fitzgerald, J. Vac. Sci. Technol. B **16**, 1471(1998).
[3]. S.F: Fang, K. Adomi, S. Iyer, H. Morkoç, H. Zabel, C. Choi and N. Otsuka, J. Appl. Phys. **68**, R31(1990) and references therein.
[4]. A. Georgakilas, P. Panayotatos, J. Stoemenos, J.-L. Mourrain, A. Christou, J. Appl. Phys. **71**, 2679(1992).
[5]. L.T.P. Allen, E.R. Weber, J. Wahburn, Y.C: Pao. Appl. Phys. Lett. **51**, 670 (1987)..
[6]. D.E. Aspnes , in Handbook on Semiconductors, edited by T.S. Moss(North-Holland, New York, 1980), Vol. 2
[7]. J. Luyo-Alvarado, M. Meléndez-Lira, M. López-López, I. Hernández-Calderón, M.E. Constantino, H. Navarro-Contreras, M.A. Vidal, Y. Takagi, K. Samonji, and H, Yonezu. J. Appl. Phys. **84**, 1551(1998).
[8]. Y.C: Chen, J. Singh, and P.K. Bhattacharya, J. Appl. Phys. **74**, 3800(1993).
[9]. A. Dimoulas, P. Tzanetakis, A. Georgakilas, O.J. Glembocki, and A. Christou, J. Appl. Phys. **67**, 4389(1990).
[10]. N. Lucas, H. Zabel, H. Morkoç and H. Unlu, Appl. Phys. Lett. **52**, 2117 (1988).
[11]. D.E. Aspnes, A.A. Studna, Phys. Rev. B **7**, 4605(1973).