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THE PHOTOREFLECTANCE SPECTRA OF $Al_xGa_{1-x}As$/GaAs JUNCTIONS

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ABSTRACT

Layers of $Al_xGa_{1-x}As$, $0<x\leq0.4$, have been grown by liquid phase epitaxy on top of n-type GaAs(001) substrates. Films of n and p-type conductivity were obtained by doping with Sn and Ge, respectively. Besides the expected shift of the E_o transition with Al content, the structure and line shape of the photoreflectance (PR) spectra exhibit additional structures depending on Al content and type of conductivity. The results are correlated with low temperature photoluminescence spectra.

INTRODUCTION

The $Al_xGa_{1-x}As$/GaAs heterojunction is the basis of many optoelectronic devices. This devices, like optical modulators and semiconductor lasers have a daily appliance. A relatively new application of this heterojunctions is in the manufacture of periodical structures like multiple quantum wells and superlattices, which present a lot of exciting and new physical phenomena [1]. These systems and devices have been the subject of many studies both theoretical and experimental; however, apparently the photoreflectance study of the single heterojunction $Al_xGa_{1-x}As$/GaAs has been oversigth. Since the knowledge of the energies of important optical transitions in the band structure is essential for an adequate technological application, a fast and reliable characterization is necessary. The photoreflectance spectra provide the critical point energies with high resolution due to their characteristic 3th derivative line shape in the dielectric constant [2]. Even though the determination of the critical points energies is direct, a full interpretation of the photoreflectance spectra is not yet available at this time without correlation of the photoreflectance results with additional techniques.

Layers of $Al_xGa_{1-x}As$, $0<x\leq0.4$, were grown by liquid phase epitaxy (LPE) on top of GaAs(001) substrates. Films of n and p-type conductivity were studied. Besides the expected shift of the E_o transition with Al content, the structure and line shape of the room temperature photoreflectance (PR) spectra exhibited additional structures depending on Al content and type of conductivity. The relevant features are the following: 1) The PR spectra of p-$Al_xGa_{1-x}As$/GaAs contain the E_o transition of GaAs, whereas for n-type films no signal from the substrate is observed. 2) Narrowing of the E_o transitions of $Al_xGa_{1-x}As$ for p- and n-type films with increase of aluminum content. 3) Additional transitions at the low energy side of the E_o gap of $Al_xGa_{1-x}As$. The results are correlated with low temperature photoluminescence spectra.

EXPERIMENTAL DETAILS

The samples used in this study were single heterostructures of intrinsic, n- and p-type $Al_xGa_{1-x}As$ epitaxial layers grown by LPE on top of Si doped n^+-GaAs(001) ($n \sim 2x10^{18}$ cm^{-3}) substrates. The growth solution were saturated at 800 ^oC with 3 ^oC of initial supercooling and the temperature was lowered at a rate of 0.2 ^oC/min. The grown layers were around 1 μm thick. The Al composition in both undoped and doped $Al_xGa_{1-x}As$ layers was varied between 0.1 and 0.4, for n(p) type the impurity used was Sn(Ge) and the amount of Sn(Ge) in the solutions had a fixed value of 1.693% (0.034%) for all Al compositions. Room temperature photoreflectance spectra of $Al_xGa_{1-x}As$/GaAs(001) were obtained with a standard system [2] and He-Ne laser excitation.

DISCUSSION

The evolution of the photoreflectance spectra of the ternary alloy $Al_xGa_{1-x}As$ for n and p-type films compared with the

spectrum of the clean substrate is shown in figure 1. Some relevant features can be observed in the spectra: 1) The expected change in the fundamental gap energy with Al composition; 2) The appearance of the E_o transition of GaAs in the spectra of the p-type alloys while it is not present in the spectra of the n-type alloys; 3) The narrowing of the E_o transition of GaAs in the p-type spectra, and, 4) Additional features around the low energy side of the E_o transition of $Al_xGa_{1-x}As$. Regarding this last point, the origin of these features has not been determined; however they could be related to the presence of non identified impurities which are more efficiently incorporated during the growth process with increasing Al content. In this respect, it was reported very recently that impurities can give place to a PR signal in bulk GaAs [3]. A more detailed study of these features will be published elsewhere.

In figure 2 we compare spectra of intrinsic, p and n-type $Al_xGa_{1-x}As$ films with x=0.4. In the spectra of intrinsic and p-type films one can observe the presence of the E_o transition of GaAs, while it is not present for the n-type alloy. These results were obtained for all the films in the $0<x\leq0.4$ range indicating that for intrinsic and p-type layers there exists modulation of the electric field at the interface $Al_xGa_{1-x}As$/GaAs, giving place to the detection of the substrate PR signal. The modulation of the reflectivity was produced with a He-Ne laser (1.97 eV) and since the films are around 1 μm thick and the absorption coefficient at this energy for the widest gap alloy (x=0.4) is $\alpha=1.2\times10^4$ cm^{-1} [4], there is a small possibility for the light to reach the interface; so, the exciting process must be the transport of carriers to the interface, where they recombine at interface states modifying the intrinsic electric field. An additional evidence for this assignment is the presence of the photoreflectance substrate signal even when the excitation source is an Ar-ion laser tuned at 4880 Å, which is strongly absorbed within the surface region of the AlGaAs layer. An intense electric field in the interface, for the case of intrinsic and p-type AlGaAs films, can be the driving force for the transport of carriers to the heterojunction. Here, it must be taken into account that the n-type substrate had a carrier concentration $n=2\times10^{18}$ cm^{-3} and considering the expression for the screening length [5]:

$$L^2 = \frac{\varepsilon_s \varepsilon_0 k_B T}{e^2 n} \qquad (1)$$

we obtain a value of around 30 Å. In this expression ϵ_s is the dielectric constant of GaAs and the other parameters have the usual meaning. The small value obtained for the screening length is an indication

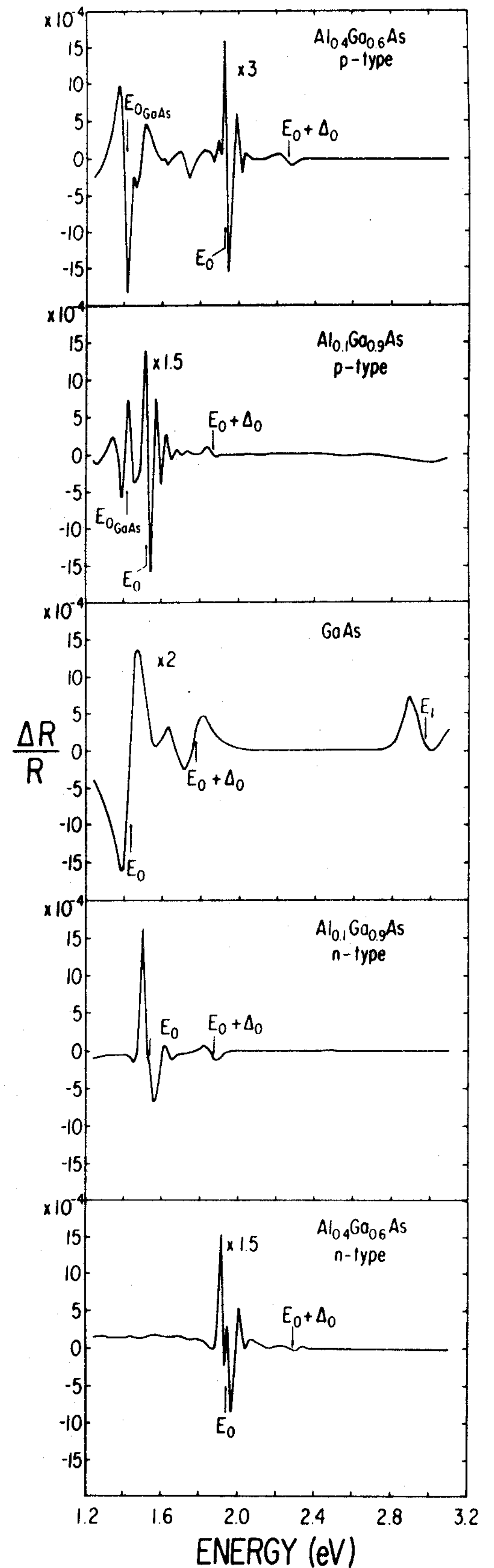

FIG. 1. Evolution of photoreflectance spectra with Al content for n and p-type $Al_xGa_{1-x}As$ epitaxial layers grown on GaAs(001).

of a strong electric field at the substrate surface.

In Fig. 3 we shown a schematic illustration of the band diagrams for the three cases; it can be observed that electrons and holes generated within the AlGaAs layer will be more likely pulled to the interface by the electric field for the cases of intrinsic and p-type alloys.

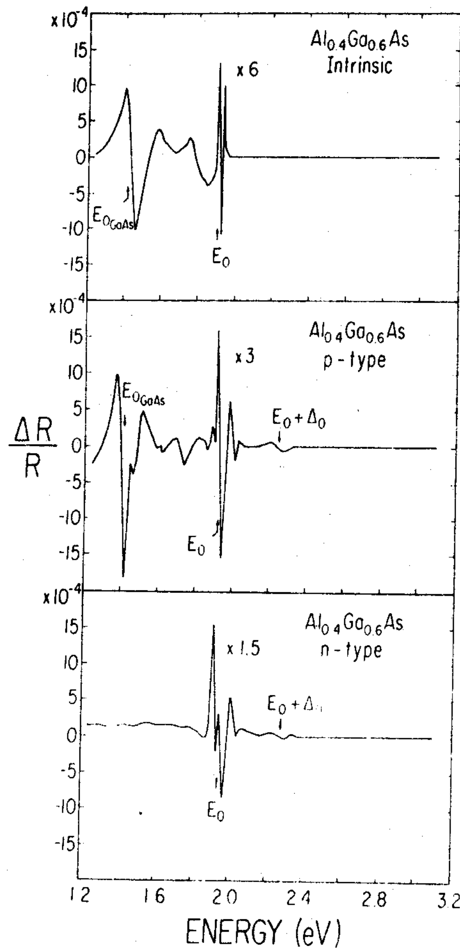

FIG. 2. Photoreflectance spectra of intrinsic, n- and p-type Al_xGa_{1-x} As films,note the presence of the E_o transition from the GaAs substrate in the p-type and intrinsic samples.

The analysis of the photoreflectance line shape was performed using the theory of Aspnes [6]. The line shape is given by:

$$\frac{\Delta R}{R} = \frac{C}{\left[(E - E_0)^2 + \Gamma^2 \right]^{\frac{n}{2}}} \bullet \cos\left(\theta - n \tan^{-1} \frac{\Gamma}{E - E_0} \right) \quad (2)$$

where n = 3.5, 3 and 2.5 for 1, 2 and 3-dimensional critical points. More recently

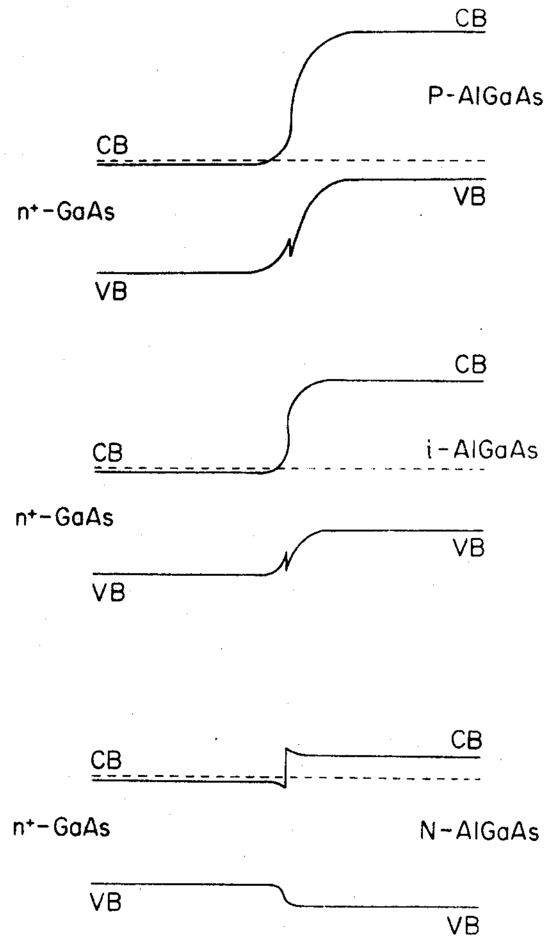

FIG. 3. Schematic representation of the band diagrams for the diferent heterojunctions.

Raccah et. al. proposed for the PR line shape the following Relation [7]:

$$\frac{\Delta R}{R} = \frac{1}{E^2} \sum_{M=1}^{3} a_M L^{(M)}(n, E) \quad (3)$$

with

$$L^{(M)}(n,E) = \frac{1}{\left[(E - E_0)^2 + \Gamma^2 \right]^{(M-n)/2}} \bullet \cos\left(\theta - (M-n) \tan^{-1} \frac{\Gamma}{E - E_0} \right) \quad (4)$$

where n = 1/2 corresponds to a 3-d critical point. In both models θ represents a phase factor and Γ the line broadening parameter. We performed a least squares line-shape fitting for the PR spectra of GaAs and $Al_xGa_{1-x}As$ around E_o. The fittings correspond to three different approaches :

1) Determination of the band gap energy, amplitude, phase and line broadening parameter following the Aspnes relation of a 3-d critical point, figures 4a and 5a. 2) Employing the Raccah et. al. expression for a 3-d critical point with 5 adjustable parameters: 3 amplitudes, phase and line broadening. The results are shown in Figs. 4b and 5b. The E_O value was obtained by the three-point method of Aspnes. 3) Considering a linear combination of 1, 2 and 3-d critical point line shapes given by Aspnes with E_O as obtained by the three-point method, giving a total of 9 adjustable parameters. The results are shown in figures 4c and 5c. The purpose of this approach is discussed later.

Inspection of the fittings for GaAs and AlGaAs given by the first two approaches gives comparable results. Since the Aspnes relation required less adjustable parameters and in the case of GaAs gave a better fitting, it can be considered more convenient for analysis of line shapes. It is clear that increasing the number of adjustable parameters could improve the fitting. However, this has to be done very carefully, otherwise it can result in good looking fittings with parameters which actually do not have any relation with the physics of the experiment, even when it could be argued that the extra parameters are properly included. An extreme case of adding adjustable parameters is illustrated in Figs. 4c and 5c by considering approach 3), which obviously has no physical meaning. For the case of GaAs the first approach gave the following values: E_O=1.432 ev; θ=2.39 and Γ=0.095. For the second approach, employing E_O=1.415 eV, it was obtained a value of θ=1.27 and Γ=0.070. The difference between the band gap energies from both methods is 1%. The differences of phase and broadening parameters are larger; however, the way they contribute to each model can be the source of the discrepancies.

Franz-Keldysh oscillations can be produced in photoreflectance spectra in the presence of strong intrinsic electric fields. These type of oscillations are clearly present in the p-type alloy spectra, Fig. 1. Using the proposed expression for the asymptotic behavior of the oscillations [8] we obtained a value for the internal electric field of $F = 3.04 \times 10^6$

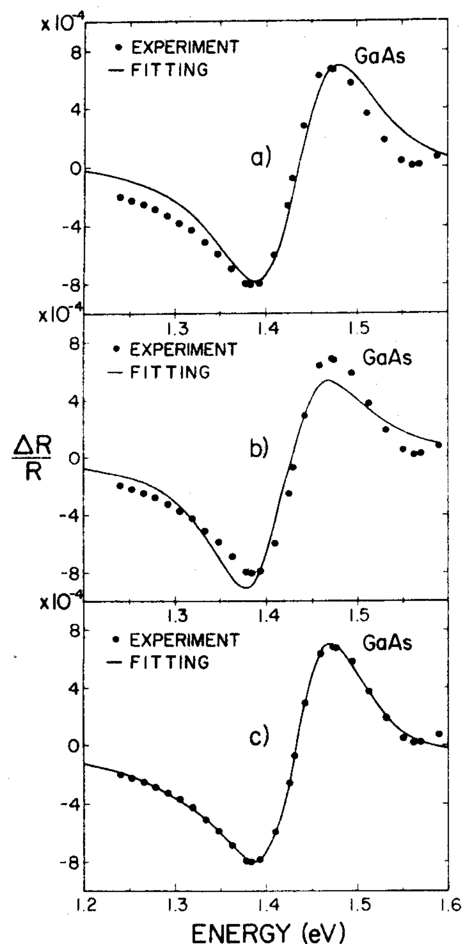

FIG. 4. Fitting around E_O of GaAs substrate using the expressionsof a) Aspnes,ref. [6], and,b) Raccah, ref. [7], c) see explanation in the text.

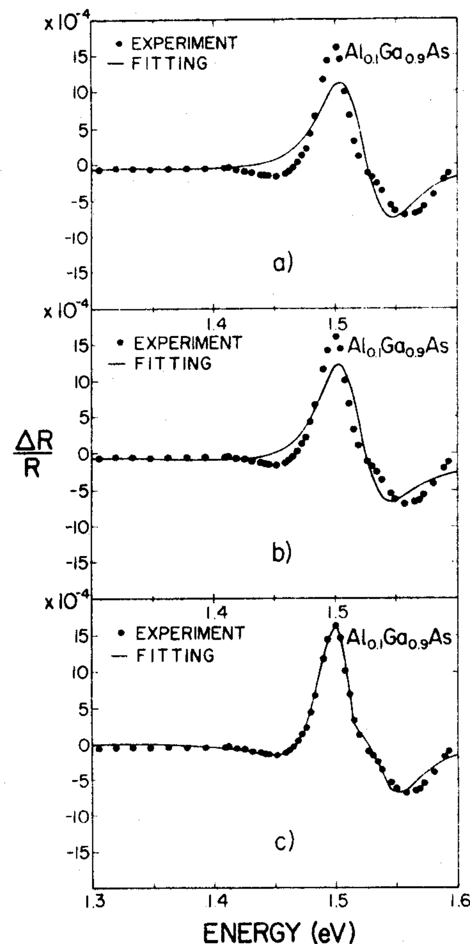

FIG. 5. Fitting around E_O of the n-type film $Al_xGa_{1-x}As$ using the expressions of a) Aspnes, ref. [6], and, b) Raccah, ref. [7], c) see explanation in the text.

V/m [9] which can be considered within the strong field regime [8]. Since the AlGaAs films were only sligthly doped, it seems misleading to assign these oscillations to the surface of the alloy, so they can be attributed to the junction region, indicating the existence of a strong electric field at the interface, in agreement with our previous discussion.

The experimental values for E_o found in photoreflectance and low temperature photoluminescence versus nominal Al concentration were consistently smaller compared to data reported in the literature [4,10]. From these results it was clear that the Al incorporation was smaller than the nominal concentration expected from the growth solution, this effect being stronger for higher nominal Al concentrations. Using the E_o experimental values and the data of Bosio et. al. [10] for the dependence of the E_o gap as a function of composition we determined the Al concentration of the films. The results are shown in Tables I and II. The results found by photoreflectance and low temperature photoluminescence are very similar, typically within 1%, indicating the capability of both techniques for a fast and accurate determination of alloy composition. Furthermore, this agreement gives us confidence in the value of E_o from photoreflectance spectra obtained by the Aspnes theory.

CONCLUSIONS

We have measured the photoreflectance spectra of intrinsic, p and n-type $Al_xGa_{1-x}As$ epitaxial films grown by LPE on n-type GaAs(001). The spectra showed the expected shift of the E_o transition with the increasing of Al content. Additional transitions at the low energy side of the E_o gap of $Al_xGa_{1-x}As$ are tentatively attributed to not yet identified impurities. The presence of the E_o transition of the GaAs substrate in intrinsic and p-type AlGaAs films is attributed to the modulation of the electric field at the layer/substrate interface caused by the transport of carriers generated in the AlGaAs layer. The appearence of Franz-Keldysh oscillations are attributed to the existence of a strong electric field at the interface. For the case of the p-type $Al_xGa_{1-x}As$ film an electric field of $3x10^6$ V/m was determined. It was found that the actual concentration of Al in the alloys is less than the nominal one, the difference being bigger at higher Al concentrations. The actual Al content obtained by using the E_o value from photoreflectance and low temperature photoluminescence are consistent within 1%.

TABLE I. Parameters for p-type $Al_xGa_{1-x}As$

X_N (%Al)	E_o^{PL} (eV)	X_{PL} a) (%Al)	E_o^{PR} (eV)	X_{PR} (%Al)
10	1.62	8	1.53	7
20	1.73	17	1.68	18
30	1.89	26	1.82	28
40	2.03	36	1.93	36

a) Following ref. [10].
PL: Photoluminiscence at 14 K.
PR: Photoreflectance at 300 K.

TABLE II. Parameters for n-type $Al_xGa_{1-x}As$

X_N (%Al)	E_o^{PL} (eV)	X_{PL} a) (%Al)	E_o^{PR} (eV)	X_{PR} (%Al)
10	1.62	8	1.51	7
20	1.77	18	1.66	17
30	1.89	26	1.78	25
40	2.05	37	1.94	36

a) Following ref. [10].
PL: Photoluminiscence at 14 K.
PR: Photoreflectance at 300 K.

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