Electric field distributions in a molecular-beam epitaxy $Ga_{0.83}Al_{0.17}As/GaAs/GaAs$ structure using photoreflectance

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We have studied the photoreflectance (PR) spectra from a molecular-beam epitaxially (MBE) grown heterostructure consisting of 200 nm of $Ga_{0.83}Al_{0.17}As$, a 800-nm GaAs buffer layer on a semi-insulating (SI) ⟨100⟩ (LEC) GaAs substrate. By varying both the pump beam wavelength and modulation frequency we are able to identify the component layers, their quality, and the quality of the various interfaces. In this study we find evidence for a low density of interface states between the GaAs buffer layer and the GaAlAs layer, and a relatively large density of interface states, between the substrate and buffer layers. These states, previously observed by deep-level transient spectroscopy (DLTS) of doped structures, are presumably associated with the interface produced by MBE growth on etched and air exposed substrates. However, in our experiment since the substrate is semi-insulating and the buffer layer is undoped, it is difficult to resolve these states spatially by *C–V* techniques. Our results show that the PR technique can be used to characterize low conductivity or semi-insulating structures such as enhancement mode metal–semiconductor field effect transistor (MESFET) and high electron mobility transistor (HEMT) type devices and it may be useful for the *in situ* characterization of epigrown surfaces and interfaces.

I. INTRODUCTION

Photoreflectance,[1] a contactless form of electromodulation, is a powerful tool to study the interface electric field distribution in semiconductor structures.[2–5] In photoreflectance (PR) the electric field in the material is modulated by the photoinjection of electron–hole pairs by a pump beam chopped at frequency Ω_m. It has been demonstrated that PR is indeed a form of electroreflectance yielding sharp, third-derivative spectra in the region of interband transitions in bulk or thin-film semiconductors.[1–5] Since PR is the ac response of the system to the modulating electric field there is also important information in the other modulation parameters such as modulation frequency (Ω_m),[4,5] pump beam wavelength (λ_p),[6] pump beam intensity (I_p), etc.

We have studied the PR spectra at 300 K from a molecular-beam epitaxially (MBE) grown $Ga_{0.83}Al_{0.17}As$/GaAs/GaAs (epilayer/buffer/substrate) heterostructure as a function of λ_p (820–420 nm) and Ω_m (20–4000 Hz). The sharp spectral features have allowed us to observe the direct band gaps of the various components of the structure. These are designated E_0(A), E_0(B), and E_0(C) for the GaAlAs epilayer (region A), GaAs buffer (region B), and GaAs substrate (region C), respectively. For 420-nm pump radiation, which does not penetrate into either region B or C, we observe E_0(A) and E_0(B) but not E_0(C). All three peaks are seen for $\lambda_p = 620$ nm, which corresponds to an energy larger than E_0(A) and penetrates in region B but not into C. When the pump photon energy (1.51 eV) is well below E_0(A) photoexcited electron–hole pairs are created in both the GaAs buffer and substrate regions. In this case the spectrum exhibits primarily E_0(C) with a small contribution from E_0(B). In addition E_0(A) and E_0(C) have different variations with Ω_m; the dependence of E_0(B) is related mainly to the modulation mechanism of region A with some contribution from region C. We interpret these results as evidence for a low density of interface states between the GaAs buffer layer and the GaAlAs epilayer, and a relatively large density of states between the substrate and buffer.

II. EXPERIMENTAL PROCEDURE

The heterostructure used in this study consisted of a 200-nm $Ga_{0.83}Al_{0.17}As$ epilayer grown on a 800-nm GaAs buffer on a semi-insulating (SI) ⟨100⟩ liquid encapsulated Czochralski (LEC) GaAs substrate. All measurements were made at 300 K. The PR apparatus has been described in the literature.[7] However, in contrast to most previous PR experiments the source for λ_p was a Xenon arc filtered by a one-quarter meter monochromator instead of a He–Ne laser.[6] The intensity of the pump beam was ~2 mW. In all cases the observed line shapes were independent of I_p indicating modulation in the low-field regime. A two-phase lock-in amplifier was used to record the in-phase and out-phase components of the PR signal relative to the phase of the pump beam. The range of modulating frequency was limited by the properties of the mechanical chopper.

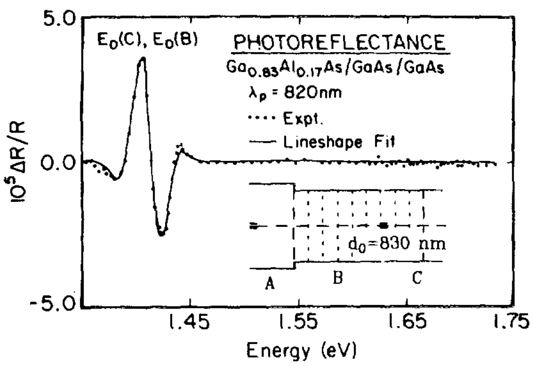

FIG. 1. Photoreflectance signal vs photon energy for GaAlAs/GaAs/GaAs structure (see the text) for a pump beam wavelength of 820 nm.

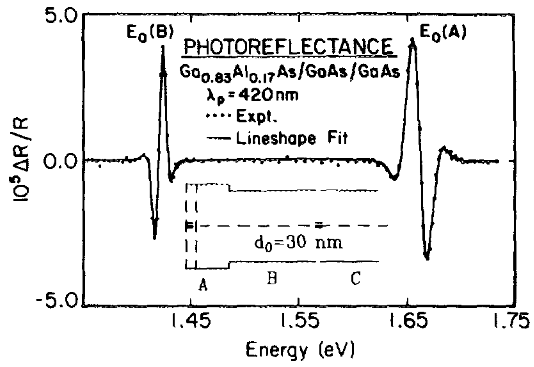

FIG. 3. Photoreflectance signal vs photon energy for GaAlAs/GaAs/GaAs structure (see the text) for a pump beam wavelength of 420 nm.

III. RESULTS AND DISCUSSION

Shown by the dotted line in Fig. 1 is the PR spectrum with $\lambda_p = 820$ nm and $\Omega_m = 200$ Hz. For this value of λ_p the GaAlAs is transparent and the penetration depth (d_0) in GaAs is 830 nm.[8] The solid line is a least-squares fit to the Aspnes low-field third-derivative functional form for a direct band gap.[9]

$$\Delta R/R = \mathrm{Re}[Ae^{i\phi}(E - E_0 + i\Gamma)^{-5/2}], \quad (1)$$

where A is the amplitude, φ is a phase factor, E is the photon energy, E_0 is the energy gap, and Γ is the broadening parameter. The line shape fit yields E_0 and Γ as well as the amplitude A.

In Eq. (1) the amplitude A can be expressed as[9]:

$$A \propto e^2\hbar^2F^2/8m_r^* \quad (2)$$

where F is the modulating electric field, m_r^* is the reduced interband effective mass in the direction of $\overline{F}$, and F is a function of pump beam parameters such as λ_p, Ω_m, and I_p. Thus, Eqs. (1) and (2) demonstrate that PR signals contain information not only in the sharp, derivativelike spectral features but also can be used as an optical probe of interface electric fields.

The spectrum of Fig. 1 exhibits structure in the vicinity of the direct band gap of GaAs but no signal is observed in the region of the GaAlAs gap. The line shape fit indicates that there are two oscillators which we denote as E_0(C) and E_0(B), the latter being only ~18% of the former. The energies and broadening parameters are 1.413 eV, 11 meV and 1.420 eV, 4 meV for E_0(C) and E_0(B), respectively. These values are comparable to those observed in other electromodulation experiments.[1,10,11] The features E_0(C) and $E_0(B)$ originate in the GaAs substrate and buffer, respectively. The narrower linewidth for the latter peak is probably due to the better quality of MBE grown material in relation to bulk GaAs.

Displayed by the dotted line in Fig. 2 is the experimental PR spectrum for $\lambda_p = 620$ nm and $\Omega_m = 200$ Hz. In this case d_0(GaAlAs) = 420 nm (Ref. 12) and d_0(GaAs) = 240 nm.[8] Thus, electron–hole pairs are created in regions A and B but not C. The solid line is a least-square fit to Eq. (1). In addition to E_0(C) and E_0(B), which have a ratio of ~1/3, we also observe E_0(A) at an energy of 1.662 eV with $\Gamma = 8$ meV. The position of E_0(A) enables us to determine the Al composition.[12,13]

The experimental data for $\lambda_p = 420$ nm and $\Omega_m = 200$ Hz is shown by the dotted line in Fig. 3. Since d_0(GaAlAs) = 30 nm (Ref. 12) for this pump wavelength photoexcited carriers are created only in region A and not B or C. The solid line is a least-square fit to Eq. (1). Only two peaks, E_0(B) and E_0(A) are observed in this experimental condition. We can detect no substantial evidence for E_0(C) in the line shape ~1.42 eV.

In Fig. 4 we have plotted the modulation frequency (Ω_m) dependence of the amplitude of the in-phase component of the various PR structures. Since $\lambda_p = 420$ nm produces E_0(A) and E_0(B) with no evidence for E_0(C), the data for the former two peaks were evaluated at this pump wavelength. We have detected no spectra with only E_0(C) and

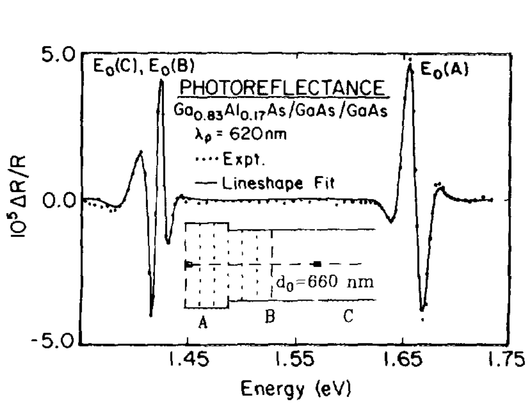

FIG. 2. Photoreflectance signal vs photon energy for GaAlAs/GaAs/GaAs structure (see the text) for a pump beam wavelength of 620 nm.

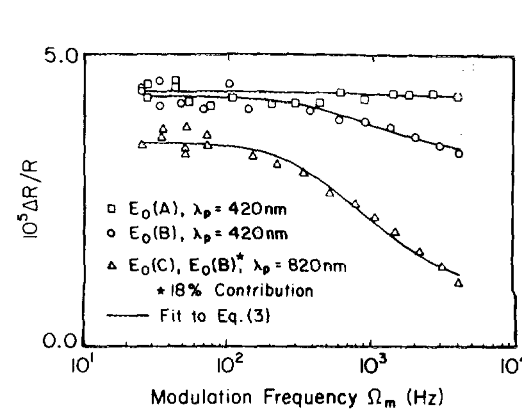

FIG. 4. Photoreflectance signal vs pump beam modulation frequency.

TABLE I. Values of τ_1, A_1, and A_0 for $E_0(A)$, $E_0(B)$, and $E_0(C)$.

Feature	τ_1 (ms)	A_1	A_0
$E_0(A)^a$	$\lesssim 0.04$	0	4.2
$E_0(B)^a$	0.32	1.0	3.2
$E_0(C)^{b,c}$	0.33	2.7	0.8

[a] $\lambda = 420$ nm.
[b] $\lambda = 820$ nm.
[c] Small contribution from $E_0(B)$.

hence for this feature the variation with Ω_m was recorded using $\lambda_p = 820$ nm since $E_0(B)$ produces only an 18% contribution.

The dependence of $\Delta R/R$ with Ω_m can be accounted for on the basis of the following considerations. The chopped pump radiation can be considered as a square-wave source. These charges are then free to fill traps and modify the electric field strength. We assume that these excess carriers change the built-in field in a response time much faster than the shortest characteristic time of our modulation ($\sim$0.04 ms).[1] When the light is switched off, the trap population and hence electric-field strength are restored with a characteristic time τ. For chopping frequency Ω_m can be shown that the Fourier transform of the in-phase component of the PR intensity, $[\Delta R(\Omega_m)/R]_{\text{in phase}}$, is given[14,15]:

$$[\Delta R(\Omega_m)/R]_{\text{in-phase}} = \sum_{i=1}^{n} [\Delta R(0)/R]_i f(\Omega_m \tau_i), \quad (3a)$$

$$f(\Omega_m \tau_i) = \{1 + 2\pi^2(\Omega_m \tau_i)^2[1 - \exp(-1/2\Omega_m \tau_i)]\}/[1 + 4\pi^2(\Omega_m \tau_i)^2] \quad (3b)$$

when τ_i is the characteristic time constant of the ith trap state and $[\Delta R(0)/R]_i$ is the PR signal produced by the modulation of the ith trap state in the limit of $\Omega_m \tau_i \ll 1$. It can be shown that in order to employ the principle of superposition of the contribution of states with different trap times it is necessary to consider the in-phase component of $\Delta R(\Omega_m)/R$, not the amplitude.[14,15]

If we assume that

$$\Omega_{\max} \tau_i \ll 1, \quad \text{for } i \geqslant 2,$$

where $\Omega_{\max}$ is the maximum Ω_m, then Eq. (3a) can be written in the simplified form

$$[\Delta R(\Omega_m)/R]_{\text{in-phase}} = A_1 f(\Omega_m \tau_1) + A_0, \quad (3c)$$

where $A_1 = [\Delta R(0)/R]_1$, and A_0 represents the contribution of states with faster than τ_1. Since the maximum Ω_m in our experiment is 4000 Hz the fastest τ_1 we can detect is $\sim$0.04 ms. States with faster trap times make a small contribution to the out-of-phase signal in the frequency range of our investigation.

The solid lines in Fig. 4 are least-squares fit of Eq. (3c) to the experimental data. The observed values of τ_1, A_1, and A_0 are listed in Table I. The $E_0(A)$ feature has essentially a flat response in our range of Ω_m indicating a trap state whose $\tau \lesssim 0.04$ ms. The values of A_1 and A_0 for $E_0(B)$ indicate that the main mechanism for the modulation of this structure is from these fast states with some contribution from a 0.3-ms state. The latter is the modulation mechanism for $E_0(C)$ and probably originates in the interface state between the buffer and substrate.

In conclusion we have used the PR technique to characterize an undoped GaAlAs/GaAs/GaAs heterostructure. By varying both the wavelength of the pump beam and its modulation frequency, we are able to identify the component layers, their quality and the quality of the various interfaces. We believe that this technique applied to undoped or low conductivity structures to be complementary to electrical modulation techniques, e.g., electroreflectance, deep-level transient spectroscopy, etc., which are usually applied to conducting structures.

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[15] In Eq. (1b) of Ref. 5, $\Delta R(\Omega_m)/R$ is the magnitude of the PR signal, which is the square root of the sum of the squares of the in-phase and out-phase signals. This quantity does not obey the principle of superposition. Thus, it is rigorously correct only for a single trap state. For multiple trap states it is necessary to evaluate the frequency dependence of the in-phase component (with respect to the pump beam) in order to employ the superposition of different contributions.