Electromodulation spectra of a single $Al_xGa_{1-x}As/GaAs$ modulation-doped heterojunction: Experiment and theory

N. H. Lu and T. M. Hsu
Department of Physics, National Central University, Chung-li, Taiwan 32054, Republic of China
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Electroreflectance spectroscopy is applied to reexamine the theoretical model which has been devised to explicate the temperature-dependent photoreflectance spectra of single $Al_xGa_{1-x}As/GaAs$ modulation-doped heterojunctions. Building on the presumption that the modulation mechanism is mainly due to the electromodulation of the band bending in the buffer layer, we apply the Franz-Keldysh theory to simulate the photoreflectance and electroreflectance spectra at room temperature. As the sample temperature is decreased to 10 K in the photoreflectance experiment, there appears a large number of oscillations extending for more than ten periods. This phenomenon manifests existence of a fairly uniform electric field in the buffer layer.

I. INTRODUCTION

Selectively doping a semiconductor has proved to be a very powerful tool to achieve specific electronic functions. Two types of structures originating from such an idea have been exploited under flourishing research progress: a δ-doped structure and a modulation-doped heterojunction (MDHJ).[1,2] Although technological interest focuses mainly on their charge-transport properties, spectroscopic techniques have been demonstrated to be useful and sensitive characterization methods for investigating such structures. Seeing that it is easily implemented and displays sharp spectra without noticeable background even at room temperature, electromodulation (EM) spectroscopy plays an important role in probing the electronic and optical properties of semiconductor microstructures.[3-6] Owing to the close resemblance between the band structure of Si-δ-doped GaAs and that of a single $Al_xGa_{1-x}As/GaAs$ MDHJ, much attention has been paid recently to photoreflectance (PR) and electroreflectance (ER) studies of these two structures. The present paper aims to unveil the underlying modulation mechanism of PR and ER spectra of a single MDHJ.

In Si-δ-doped GaAs, the planar doping layer and the crystal surface are separated by undoped GaAs. Since the Fermi level at the surface is pinned around midgap either by intrinsic surface states or by states associated with native defects, this configuration ensures a uniform built-in electric field across the undoped region. The existence of the uniform electric field is confirmed by the extensive Franz-Keldysh oscillations (FKO's) appearing in PR and ER spectra.[7-11] Direct assessment of the two-dimensional electron gas (2DEG) in a δ-doped structure might be feasible by performing differential photoreflectance (DPR) measurement,[11,12] which is a modified form of the PR technique.

In contrast to the case of a δ-doped structure, the underlying modulation mechanism that dominates the PR line shape from the single MDHJ is still unknown. Since Glembocki's original demonstration of PR spectra from single $Al_xGa_{1-x}As/GaAs$ MDHJ's in 1985,[3] many attempts, including varying crystal temperature,[10,13,14] modifying PR configuration,[15,16] and performing theoretical calculations,[17,18] have been made to examine the nature of the PR spectra from single MDHJ's; however, no decisive conclusion has ever been reached up to the present.

Snow, Glembocki, and Shanabrook[19] calculated the dielectric function and measured the ER spectra of $Al_xGa_{1-x}As/GaAs$ MDHJ's. In their ER measurement, electrical contact was made between the 2DEG system and the front surface. By applying an ac voltage between the contact electrode and the 2DEG system, the channel carrier concentration n_s was modulated out of the field effect. Assuming that the ER modulation mechanism was the variation in n_s, they calculated the dielectric function based on a self-consistent calculation of the conduction-subband states and the bulklike valence-band states. Both the calculated spectra and the ER data reveal broad structures above the GaAs band gap. This kind of broad structure is a direct demonstration of the nature of the valence band, which allows many valence-band states to overlap with a single conduction-subband state. Notwithstanding the success of their theoretical approach in explicating the experimental ER data, it fails to explain the narrow oscillatory feature of the PR spectra on the same structure.

In a previous work,[20] we have not only studied the temperature effects on the PR spectra of single $Al_xGa_{1-x}As/GaAs$ MDHJ's, but also demonstrated that the narrow oscillatory PR signal comes mainly from the photomodulation of the built-in electric field across the space-charge layer. In attempts to further support this argument, here we will apply modulating voltage across the whole sample. We confirm that the oscillatory features are FKO's originating from the internal electric field within the buffer layer by comparing the photomodulated and electrically modulated reflectance spectra with the theoretical calculations. As the temperature is reduced to 10 K, the PR spectra also reinforces our point

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of view.

A theoretical approach based on the improved Fang-Howard solution,[21] which allows the variational wave function to penetrate into the barrier, is used to calculate the electric-field profile within the buffer layer. Taking advantage of the calculated field values, EM spectra are simulated with the WKB approximation developed by Aspnes and Frova.[20,22–25]

II. EXPERIMENT

The single MDHJ investigated in the present study is grown by molecular-beam epitaxy (MBE). The epitaxial structure consists of a 500-Å Si-doped $Al_{0.3}Ga_{0.7}As$ layer ($N_D=2\times10^{18}$ cm^{-3}), a 100-Å $Al_{0.3}Ga_{0.7}As$ spacer layer, and a 1-μm GaAs buffer layer. For the sake of applying an electric field across the whole sample, the selectively doped heterostructure is deposited on a p^+-GaAs substrate ($p\approx4.6\times10^{18}$ cm^{-3}). The absence of a GaAs cap layer is deliberately designed so that the buffer layer may be the only region that contributes to the GaAs signal.[18,26–29] In most of the cases, $Al_xGa_{1-x}As$/GaAs MDHJ is capped with a GaAs protection layer to prevent oxidation; however, in order to obtain the unambiguous information from the buried active layer, we recommend that MDHJ's without GaAs cap layers be demanded for studying the EM mechanism.

Experimental arrangements for PR and ER have been described elsewhere.[8,9,30] The modulation source in PR is a 5435-Å He-Ne laser, which is mechanically chopped at 210 Hz. The pump intensity is controlled by a neutral density filter. Using an Air Products De202 closed-cycle refrigerator, the crystal temperature can be reduced to 10 K.

The ER experiment is performed with an electrolyte ER technique. The sample is placed between two electrolytic chemical cells, and the electrolytes are used as contact electrodes. We use a saturated $Na_2S\cdot9H_2O$ solution as the rear surface electrode; on the other hand, 2.4-M $Na_2S\cdot9H_2O$ is used for the front surface electrode. The voltage is applied between the two electrolytic electrodes, thus resulting in an electric field across both surfaces of the sample. No dc bias is applied, and the modulating voltage is 0.5 V.

III. THEORY

A. Variational self-consistent scheme

The electric-field profile within the buffer layer of the single MDHJ is calculated self-consistently by the modified Fang-Howard wave function performed for the electric quantum limit; i.e., only one subband is occupied in the Hartree approximation.[21]

In actual samples the potential deep in the buried layer is quite complicated, since the boundary condition depends on the unknown charge redistribution near the epilayer/substrate interface. Therefore instead of trying to model this potential near the interface, we introduce an offset parameter E_{cf} to set the boundary condition. The quantity E_{cf} is defined as the energy difference between the conduction band and the Fermi level at the epilayer/substrate interface, as illustrated in Fig. 1. To take account of E_{cf}, we have modified the approach described in Ref. 21. For the convenience of comparison, the notations used here will follow those of Ref. 21 as closely as possible.

In the effective-mass formalism the envelope wave function of an electron confined in the z direction can be expressed as follows:

$$\Psi_{n,\mathbf{k}}(\mathbf{r})=\frac{1}{\sqrt{S}}\chi_n(z)\exp(i\mathbf{k}\cdot\mathbf{R}) , \tag{1}$$

in which n is a subband index and $\mathbf{k}$ a two-dimensional wave vector, and $\mathbf{r}=(\mathbf{R},z)$. The wave function $\chi_n(z)$ is given by the solution of the one-dimensional Schrödinger equation

$$\left[-\frac{\hbar^2}{2}\frac{d}{dz}\frac{1}{m(z)}\frac{d}{dz}+V(z)\right]\chi_n(z)=E_n\chi_n(z) , \tag{2}$$

where $m(z)$ is the position-dependent effective mass, and E_n corresponds to the energy of the bottom of subband n.

Within the Hartree approximation, the total potential energy $V(z)$ can be expressed as

$$V(z)=V_bY(-z)-e\Phi_{\mathrm{s.c.}}(z) , \tag{3}$$

where $V_bY(-z)$ accounts for the conduction-band discontinuity at the heterointerface, while the self-consistent electrostatic potential $\Phi_{\mathrm{s.c.}}(z)$ is determined by solving Poisson's equation

$$\frac{d^2\Phi_{\mathrm{s.c.}}(z)}{dz^2}=\frac{4\pi e}{\kappa}\left[\sum_i n_i\chi_i^2(z)-\rho(z)\right] , \tag{4}$$

with κ the static dielectric constant, n_i the areal electron concentration in the ith subband, and $\rho(z)$ the space-charge density of the ionized impurities. In most applications, the MBE-grown pure GaAs is lightly p-type doped,

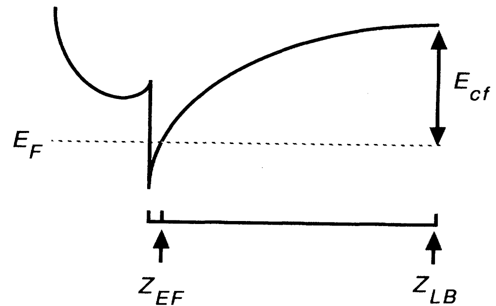

FIG. 1. Schematic conduction-band diagram of a single modulation-doped heterojunction. E_{cf} represents the potential-energy difference between the conduction-band edge and the Fermi level E_F at the epilayer/substrate interface. Z_{EF} designates the corresponding space position of E_F, Z_{LB} the space coordinate of the buffer/substrate interface. The electromodulation of the band structure is assumed to be mainly across the region between Z_{EF} and Z_{LB}.

so that $\rho(z)$ can be replaced by the ionized acceptor contribution $-N_A^-(z)$ in calculating the electrostatic potential in the buffer layer. In consequence, $\Phi_{s.c.}(z \geq 0)$ can be written as

$$\Phi_{s.c.}(z \geq 0)=\delta\Phi_{el\text{-}el}(z \geq 0)+\delta\Phi_A(z \geq 0) , \quad (5)$$

where $\delta\Phi_{el\text{-}el}(z \geq 0)$ and $\delta\Phi_A(z \geq 0)$ represent the electrostatic potentials due to the electrons and the ionized accepters in the channel, respectively.

Considering the nonvanishing amplitude of the wave function in the barrier with potential-energy height V_b, the ground-state trial wave function can be described by

$$\chi_1(z)=\begin{cases} M\exp(\kappa_b z/2) , & z \leq 0 \\ N(z+z_0)\exp(-bz/2) , & z \geq 0 , \end{cases} \quad (6)$$

where M, N, z_0, κ_b, and b are variational parameters related to one another through the continuity conditions at the interface $z=0$ and the wave-function normalization condition.

Imposing the continuity conditions at the heterointerface on $\chi_1(z)$ and $(1)/[m(z)](d/dz)\chi_1$, one can have

$$M=Nz_0 \quad (7)$$

and

$$z_0=\frac{2}{b+\kappa_b\dfrac{m_w}{m_B}} , \quad (8)$$

where m_w and m_B denote the effective masses in the well and barrier regions, respectively. Under the requirement that $\chi_1(z)$ be normalized, we obtain

$$N=\left[\frac{b^3}{2}\right]^{1/2}\times\frac{1}{\left[1+bz_0+\frac{1}{2}b^2z_0^2\left[1+\dfrac{b}{\kappa_b}\right]\right]^{1/2}} . \quad (9)$$

Granted that the ground subband energy E_1 depends much less on κ_b than on b, we may readily have $\kappa_b=2\sqrt{2m_bV_b/\hbar^2}$ and use b as the single variational parameter.

Substituting Eq. (6) into Eq. (4) and using Eq. (5), we can solve $\delta\Phi_{el\text{-}el}$ in the active region,

$$\delta\Phi_{el\text{-}el}(z \geq 0)=\frac{4\pi e}{\kappa}n_1N^2[(\alpha_0z^2+\beta_0z+\gamma_0)\exp(-bz) -\gamma_0+(\delta_0-c)z] , \quad (10)$$

where $\delta\Phi_{el\text{-}el}(0)=0$ has been taken as a boundary condition, c is a constant to be determined, and

$$\alpha_0=\frac{1}{b^2} , \quad \beta_0=\frac{2z_0}{b^2}+\frac{4}{b^3} , \quad \gamma_0=\frac{z_0^2}{b^2}+\frac{4z_0}{b^3}+\frac{6}{b^4} , \quad \delta_0=\frac{z_0^2}{b}+\frac{2z_0}{b^2}+\frac{2}{b^3} . \quad (11)$$

For typical values of residual acceptor doping on MDHJ structures, the acceptor depletion width may exceed the buffer layer thickness, so that the active region is fully depleted and the electric-field strength is finite at the buffer/substrate interface. For that reason, instead of applying the usually adopted boundary condition $(d\Phi_{s.c.}/dz)|_{z\to\infty}=0$, we introduce E_{cf} to take account of the finite field at the buffer/substrate interface

$$-e\Phi_{s.c.}(z=L_B)=E_F+E_{cf} , \quad (12)$$

where L_B is the buffer layer thickness. The integration of the two-dimensional density of states in the conduction band using Fermi-Dirac statistics gives

$$n_1=\frac{k_bTm_1}{\pi\hbar^2}\ln\left[1+\exp\left[\frac{E_F-E_1}{k_BT}\right]\right] , \quad (13)$$

with which E_F can be calculated.

Integrating Poisson's equation for $\delta\Phi_A(z)$ from the heterointerface to the buffer/substrate interface by incorporating with the prescribed boundary conditions yields

$$\delta\Phi_A(z \geq 0)=\frac{4\pi e}{\kappa}N_A\left[\frac{z^2}{2}-\xi z\right] , \quad (14)$$

with

$$\xi=\frac{1}{L_BN_A}\left\{\frac{\kappa}{4\pi e^2}(E_F+E_{cf}) -n_1N^2[\gamma_0-(\delta_0-c)L_b]\right\}+\frac{L_B}{2} , \quad (15)$$

where we have assumed that the residual acceptors are totally ionized. The numerical values for ξ and c are calculated iteratively until E_F converges. Finally, we can determine b by numerically minimizing

$$\langle\chi_1|-\frac{\hbar^2}{2}\frac{d}{dz}\frac{1}{m(z)}\frac{d}{dz}-\tfrac{1}{2}e\delta\Phi_{el\text{-}el}(z)-e\delta\Phi_A(z)|\chi_1\rangle . \quad (16)$$

B. Modulated reflectance

In the presence of a uniform electric field, the variation of the dielectric function for an M_0-type critical point can be expressed as[30,31]

$$\Delta\epsilon(E,\Gamma,F)=\frac{B(\hbar\theta)^{1/2}}{E^2}[G(\eta,\Gamma)+iF(\eta,\Gamma)] , \quad (17)$$

where E is the photon energy, B is a constant related to the optical matrix element,

$$\eta=\frac{E_g-E}{\hbar\theta} , \quad (18)$$

and

$$\hbar\theta=\left[\frac{e^2\hbar^2F^2}{2\mu}\right]^{1/3} , \quad (19)$$

with μ the reduced interband effective mass in the field direction. In the case of Lorentzian broadening, the broadened electro-optic functions $F(\eta,\Gamma)$ and $G(\eta,\Gamma)$ can be derived analytically:[31]

$$F(\eta,\Gamma)+iG(\eta,\Gamma)=2\pi[\exp(-i\pi/3)Ai'(x)Ai'(w)+wAi(x)Ai(w)] - \left[\frac{-\eta+(\eta^2+\Gamma_0^2)^{1/2}}{2}\right]^{1/2}+i\left[\frac{\eta+(\eta^2+\Gamma_0^2)^{1/2}}{2}\right]^{1/2}, \quad (20)$$

where Γ represents the phenomenological broadening energy

$$x=\eta+i\Gamma_0=\frac{E_g-E}{\hbar\theta}+i\frac{\Gamma}{\hbar\theta}, \quad (21)$$

and

$$w=x\exp(-i2\pi/3). \quad (22)$$

The terms Ai and Ai' are the Airy function and its derivative, respectively.

In a fairly uniform electric field, the FKO will extend up to a large number of periods if the collision broadening is not significant. As a result, the exhibition of interference between heavy- and light-hole signals will be evident. For the purpose of making a quantitative comparison with the experimental data, the field-induced change of the dielectric function should be rewritten:[9,32,33]

$$\Delta\epsilon(E,\Gamma,F)=\sum_j\frac{B_{jh}(\hbar\theta_{jh})^{1/2}}{E^2}[G(\eta_{jh},\Gamma)+iF(\eta_{jh},\Gamma)], \quad (23)$$

where $j=l$ or h represents the contribution from the light or heavy hole.

Considering that in the PR technique the internal electric field will be modulated from F in the dark to $F-\delta F^{\mathrm{PR}}$ under illumination, Shen and Pollak[24] propose

$$\Delta\epsilon^{\mathrm{PR}}(E,\Gamma,F,\delta F^{\mathrm{PR}})=\Delta\epsilon(E,\Gamma,F)-\Delta\epsilon(E,\Gamma,F-\delta F^{\mathrm{PR}}). \quad (24)$$

In the ER method, the electric field is modulated between $F+\delta F^{\mathrm{ER}}$ and $F-\delta F^{\mathrm{ER}}$; therefore, the variation in the dielectric function turns out to be[23,34]

$$\Delta\epsilon^{\mathrm{ER}}(E,\Gamma,F,\delta F^{\mathrm{ER}})=\Delta\epsilon(E,\Gamma,F+\delta F^{\mathrm{ER}}) -\Delta\epsilon(E,\Gamma,F-\delta F^{\mathrm{ER}}). \quad (25)$$

If the perturbation $\Delta\epsilon$ is spatially dependent and $|\Delta\epsilon|\ll|\epsilon|$, the effective change of the dielectric function is given by[20,22-25]

$$\langle\Delta\epsilon\rangle=-2iK\int_0^\infty\Delta\epsilon(z)\exp(2iKz)dz, \quad (26)$$

with $\Delta\epsilon(z)$ from Eq. (24) for PR, from Eq. (25) for ER, and K is the complex propagation vector of the probe light in the solid. The electromodulated reflectance can then be calculated,[9,22,30]

$$\Delta R/R=\mathrm{Re}[\exp(i\phi)(\alpha-i\beta)\langle\Delta\epsilon\rangle], \quad (27)$$

where ϕ is a phase factor, and α and β are the Seraphin coefficients.[34]

IV. RESULTS AND DISCUSSIONS

Figure 2 shows the room-temperature ($T=300$ K) PR and ER spectra of the investigated sample, the layer sequence of which is also depicted in the inset. Both line shapes display narrow oscillatory features of comparable periods above the GaAs fundamental gap. The appearance of the large-period oscillations beyond ≈ 1.8 eV is associated with the $Al_{0.3}Ga_{0.7}As$ layer.

Caution must be exercised in comparing the present ER result with that of Snow, Glembocki, and Shanabrook.[19] In their ER experiment, modulation of n_s was made possible by applying an ac voltage between the semitransparent gate and the 2DEG system. With this technique, the ER spectrum exhibits a broad structure above the band gap. On the other hand, in the present study the modulating voltage is applied between the front and back sides of the sample as against that of Snow, Glembocki, and Shanabrook. By solving the Poisson's and continuity equations for electrons and holes, Bottka *et al.*[35] deduced that the oscillations as observed in their ER measurement, the contact mode of which is similar to ours, are FKO's originating primarily from the region in the GaAs buffer layer. Consequently, we ascribe the narrow oscillatory structures appearing in our ER to the electric-field modulation in the buffer layer.

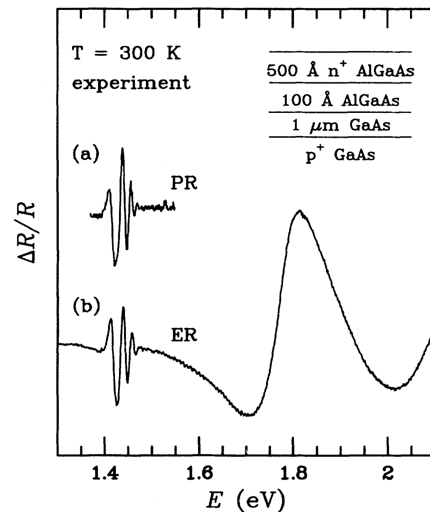

FIG. 2. Experimental photoreflectance and electroreflectance spectra at $T=300$ K. Also shown in the inset is the layer sequence of the sample.

In PR, chopped illumination will create electron-hole pairs. When photoinjected electrons and holes travel within a space-charge region, they will be accelerated in opposite directions by the electric field. The separation of charges will screen and reduce the internal field, with the result that the band bending of the semiconductor can be photomodulated. For a single MDHJ, we assume that the photomodulation of the internal electric field is across the sample. In this way, the resulting modulated reflectance spectra can be calculated with the built-in and photoreduced field profiles.

In order to make headway toward modeling the EM spectra from a single MDHJ, we suppose that all quantized subbands below the Fermi level are occupied by electrons over the temperature range studied. This supposition will contradict the real case only slightly.[36] As a consequence, the incident photons will cause electronic transitions from the bulklike valence-band states to the quite delocalized conduction-band states above the Fermi level rather than pump electrons into the confined subband states below the Fermi level. Accordingly, the conventional three-dimensional Franz-Keldysh theory can be resorted to in this study.

Even at room temperature, most channel electrons will occupy the lower subband states, whose wave functions are distributed near the quasitriangular notch potential.[36] Therefore, the band structure close to the $Al_xGa_{1-x}As$/GaAs heterointerface on the GaAs side could hardly be electromodulated at low and moderate modulating levels. In computing the integral of Eq. (26), we substitute the corresponding space position of the Fermi level Z_{EF}, as sketched in Fig. 1, for the lower integration limit. Further presuming that reflections from regions deep behind the epitaxial layers are negligible in comparison with those from the buffer layer, we replace the upper integration limit of Eq. (26) with the space coordinate at the buffer/substrate interface Z_{LB}. To be brief, we have assumed that the GaAs EM signal is due mainly to the electromodulation of the internal electric field in the region between Z_{EF} and Z_{LB}.

Recently, Baliaev, Scolfaro, and Leite[37] applied the Franz-Keldysh theory to calculate the DPR spectra from Si-δ-doped GaAs. Their calculated result is in qualitative agreement with the experimental data. In a sense, our approach in calculating $\langle \Delta\epsilon \rangle$ parallels what they proposed.

Given that $n_s = 9\times10^{11}$ cm^{-2}, $N_A = 10^{14}$ cm^{-3}, $\delta F^{PR} = 3$ kV/cm, and $\delta F^{ER} = 2$ kV/cm, we can simulate the EM spectra of Fig. 2. The calculated results are plotted in Fig. 3.

The sample substrate is a Zn-doped GaAs wafer with doping level $\approx 4.6\times10^{18}$ cm^{-3}, in which the relative position between the Fermi level and the conduction band can be closely approximated by Boltzmann statistics. At the interface, as the epitaxial layer is growing on top of the substrate, the Fermi level of the two structures must be kept aligned. Neglecting the band bending in the substrate, the parameter E_{cf} will increase from 1.371 eV at $T = 300$ K to 1.504 eV at $T = 10$ K. The quantity E_{cf} will affect the homogeneity and the magnitude of the electric field within the buffer layer. In principle, a larger E_{cf} will build a more uniform and stronger built-in electric field in the active region if other structure and material parameters can be controlled.

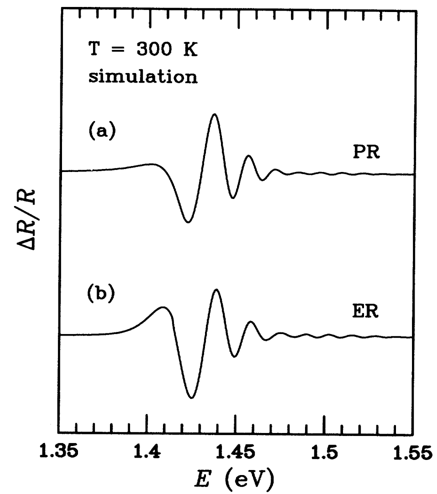

FIG. 3. Calculated photoreflectance and electroreflectance spectra at $T = 300$ K.

Figure 4 displays the 10-K PR spectrum, which manifests a large number of FKO's. Such PR features have been observed in a fairly uniform surface electric field.[7–11,32,38,39] As mentioned previously, the GaAs PR feature is assumed to be due primarily to the photomodulation of the internal electric field in the region between Z_{EF} and Z_{LB}. According to our calculation, the electric-field strength decreases very slowly from 14.79 kV/cm at Z_{EF} to 13.33 kV/cm at the buffer/substrate interface as $T = 10$ K, with the result that a rather uniform electric field is built in the GaAs buffer layer outside the notch region. The temperature dependence of Γ is also a

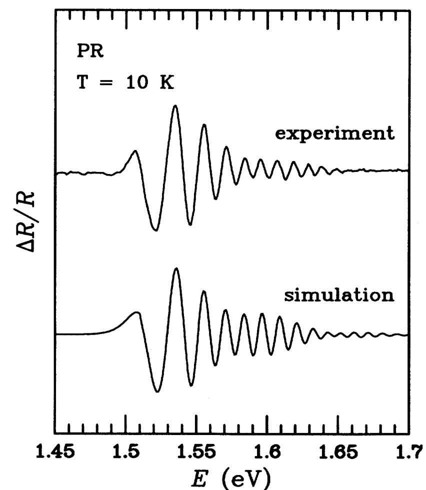

FIG. 4. Experimental and calculated photoreflectance spectra at $T = 10$ K.

factor that influences the damping behavior of the envelope function of the FKO. In the calculations we take $\Gamma = 7$ meV at $T = 10$ K and $\Gamma = 10$ meV at $T = 300$ K.

V. SUMMARY

Electromodulation techniques are very versatile optical methods for investigating selectively doped semiconducting structures. On account of the complicated line shapes, however, much effort is required to make a correct interpretation of their results. It is our intention to put forward a mathematical model which can be used to simulate the EM spectra of single MDHJ's. By comparing the calculated results with the experimental data, we can see that the theoretical scheme described here satisfactorily reaches the goal. In fact, this method also works out well in fitting the temperature-dependent PR line shapes of single $Al_xGa_{1-x}As/GaAs$ MDHJ's with different tailored structures.[20] Based on the results advanced in our earlier study and in present studies, we conclude that the underlying modulation mechanism which dominates the EM spectra of single MDHJ's is due to the electromodulation of the internal electric field in the buffer layer.

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