

Interference effects in photoreflectance and contactless electroreflectance spectra of CdTe films grown on Si substrate

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We report the observation of oscillatory features (OFs) in the photoreflectance (PR) and contactless electroreflectance (CER) spectra of CdTe films grown on Si substrate, at energies below the band gap of CdTe. The simultaneous observation of OF in the reflectance (R) spectrum having the same period as those in the PR and CER spectra (as also their dependence on film thickness) provides a direct proof for optical interference effects as being the source of these features. However, in the present case the amplitude of the OF gets damped towards shorter wavelengths while remaining nearly wavelength independent in the longer wavelength region indicating a modulation mechanism different from those reported earlier. A series of experiments and simulations performed by us seem to indicate that while in PR the principal mechanism is the pump beam induced periodic temperature changes which in turn modulates the optical path length of the CdTe film, in CER the mechanism is the electric field induced modulation of the subband gap refractive index of the film through the electro-optic effect. The damping of the OF has been explained on the basis of subband gap absorption by the CdTe film. © 1997 American Institute of Physics. [S0021-8979(97)09009-9]

I. INTRODUCTION

Photoreflectance (PR) and contactless electroreflectance (CER)¹ spectroscopies are becoming widely used tools for studying the electronic energy levels of semiconductors and their heterostructures. A host of other physical properties which are either influenced by or influence the electronic structure of these materials have also been investigated by this technique.^{1,2} It has been extensively used in the study of thin multilayered semiconductor structures such as quantum wells and superlattices. However apart from the features due to direct interband transitions (DITs), a typical spectrum can have oscillatory features at energies higher than the DIT which can be either Franz–Keldysh oscillations^{2,3} or transitions associated with unconfined states⁴ in quantum wells. At energies below the fundamental gap it can have features due to impurities¹ and also oscillatory features (OFs) due to interference effects.^{5–7} In fact, in quantum wells and superlattices, interference effects play a major role in determining the lineshapes associated with the interband transitions.^{8–13} These OF often distort the lineshapes of the signals associated with interband transitions which makes it difficult to fit conventional lineshape functions to them and thereby one loses a lot of information. Thus the study of interference effects in these spectra is important for proper analysis and interpretation of the features seen in them.

Huang *et al.*⁵ were the first to show that the subband gap OF in a PR spectrum arises due to interference effects. They showed that the modulation of the refractive index of a doped substrate by the pump laser beam gave rise to a reflected beam at the film-substrate interface in phase with the laser chopping. This beam interfered with the beam reflected from the film-air interface giving rise to the OF. These features were then used by Kallergi *et al.*⁶ to measure homo-

layer thickness of GaAs films on doped GaAs substrates. Thereafter, Lipsanen *et al.*⁷ showed that one can observe such features even in case of films grown on undoped substrates with short subband gap PR tails. All that was required was that the film be sufficiently thick so that the period of the OF was small enough for some to be seen before they are damped out. Two modulation mechanisms were proposed for the change in the refractive index of the substrate. The first was the electric field induced changes in the subband gap dielectric function through the Franz–Keldysh effect. The field changes at the interface were produced either by electron-hole pairs generated by the pump laser beam reaching the substrate or by charges produced at the surface diffusing towards the interface. The second mechanism proposed was the pump beam induced modification of the occupancy of the impurity band tail states which in turn would modify the absorption and hence the refractive index of the substrate. Both these mechanisms give rise to strong damping of the OF away from the band gap towards lower energies which was consistent with their experimental observations.

In this article we report the observation of OF in the PR and CER spectra simultaneously with OF in the reflectance (R) spectra of CdTe films grown on Si substrate, at energies below the band gap of CdTe. Unlike the previously mentioned reports, we find that in these spectra the OF shows damping in the opposite direction (i.e., towards higher energies) and is practically photon energy independent at lower energies suggesting a different modulation mechanism than the two mentioned earlier. In order to estimate the magnitude of the changes in the optical properties of the sample required to produce the OF in PR and CER spectra we performed a series of simulations. Thereafter we considered various physical processes that could give rise to these changes and present the results of the experiments performed to resolve the modulation mechanism.

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II. EXPERIMENT

A conventional experimental arrangement¹ was used for obtaining the PR spectrum. It consisted of a 4 mW He-Ne laser (632.8 nm line) as the pump beam while the probe beam was obtained by dispersing light from a 150 W quartz-tungsten-halogen lamp using a 0.125 m monochromator with a 1 μm blazed grating. The detector used was a Ge photodiode. In the CER experiment, the front electrode consisted of a transparent conducting ZnO layer on glass, which was kept at a distance of 0.5 mm from the sample surface while the sample itself was fixed on the ground electrode using vacuum grease. A maximum peak to peak alternating voltage of 3.5 kV was applied to the front electrode (in 3.0×10^{-4} mbar vacuum) during the CER measurements. Phase sensitive detection of the PR and CER signals was made using a lock-in amplifier and the data was recorded on a computer. The reflectance of a Au coated mirror was used to make correction for the spectral response of the measurement system. For low temperature measurements the sample was cooled using a closed cycle He refrigerator. Other relevant details of the experimental setup have been described in Ref. 14.

The samples used in the study were CdTe films grown on $\langle 100 \rangle$ Si substrates by molecular beam epitaxy. The x-ray diffraction measurements show that the CdTe films are oriented in the $[111]$ direction. The epilayer thickness of the samples studied are approximately 11 and 15 μm . As such the sample surface appears very smooth. However considering the large lattice mismatch ($\approx 16.2\%$) between the film and the substrate, it is expected that the epilayer contains misfit dislocations.

III. RESULTS AND DISCUSSION

Figures 1(a), 1(c) and 1(e) show the experimental R , PR and CER spectra, respectively, of one of the samples. The feature near 0.82 μm in the PR and CER spectra is due to direct interband transition (DIT) at the fundamental gap of CdTe. Beyond 0.875 μm we see OF in all the spectra. Note that the normalized PR or CER spectrum ($\Delta R/R = I_0 \Delta R / I_0 R$, where I_0 represents the measurement system's spectral response, R the sample's reflectance and ΔR the change in reflectance due the external perturbation) can have OF simply because of its presence in $I_0 R$ even though the $I_0 \Delta R$ spectrum may not have any such OF. However we would like to emphasize that in the present case, the OF occurs in both the $I_0 R$ and the $I_0 \Delta R$ spectra.

The OF in the R spectrum is associated with optical interference. For photon energies smaller than the band gap of CdTe, light gets reflected from the air/CdTe as well as from the CdTe/Si interface. These two beams interfere and give rise to the OF in the reflectance spectrum. For photon energies higher than the band gap of CdTe, the light gets absorbed by the CdTe film, hence the beam reaching the CdTe/Si interface is strongly attenuated and the OF is damped out. This is evident in the spectrum shown in Fig. 1(a). By considering a model consisting of two dielectric layers with the top layer having a finite subband gap absorption coefficient (Urbach tail) we were able to fit the R spec-

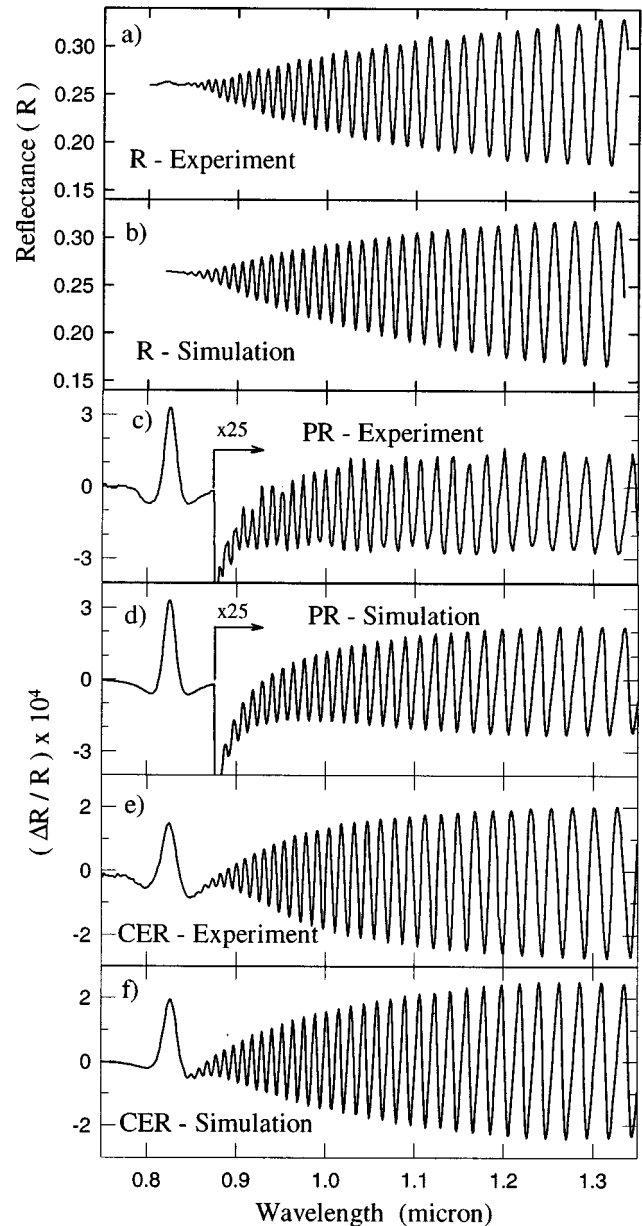


FIG. 1. (a) The experimental reflectance (R) spectrum of a CdTe film grown on Si substrate. (b) The simulated R spectrum which takes into account a finite subband gap absorption by the CdTe film. (c) Experimental photo-reflectance (PR) spectrum. (d) Simulated PR spectrum. The OF in PR was obtained by considering $\delta d_{\text{CdTe}} = 0.01 \text{ \AA}$ and $\delta n_{\text{CdTe}} = 0.0$ in the subband gap region. The simulated OF for $\delta n_{\text{CdTe}} = 2 \times 10^{-7}$ and $\delta d_{\text{CdTe}} = 0.0$ is identical. (e) Experimental contactless electro reflectance (CER) spectrum. (f) Simulated CER spectrum. The OF in CER was by obtained considering $\delta n_{\text{CdTe}} = 5.8 \times 10^{-6}$ and $\delta d_{\text{CdTe}} = 0.0$ in the subband gap region. The simulated OF for $\delta d_{\text{CdTe}} = 0.23 \text{ \AA}$ and $\delta n_{\text{CdTe}} = 0.0$ is identical. Note that both the above simulations reproduce the observed damping of the OF.

trum and obtain the parameters determining the subband gap absorption coefficient. The relevant formulas and parameters used for fitting are described in the Appendix. The calculated R spectrum is shown in Fig. 1(b). We note here that in the previous reports on this subject⁵⁻⁷ the systems studied were mainly AlGaAs, InGaAs and GaAs films on doped GaAs substrates with very small difference between the refractive indices of the film and the substrate, hence the OF in the R

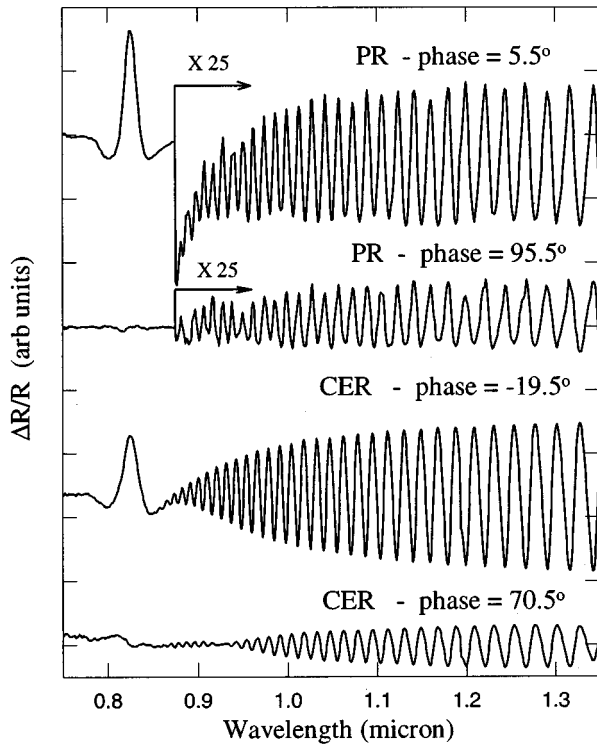


FIG. 2. The dependence of the signal amplitude of the DIT and the OF on the phase setting on the lock-in amplifier. The phase settings are those for which the DIT signal is a maximum or zero in PR and CER, respectively. Note that the OF signal does not go to zero for the phase settings at which the DIT signal is zero.

spectra of these samples was not seen. We see such feature even in the R spectrum in the present case essentially because of the large difference between the refractive indices of the film ($n_{\text{CdTe}} \sim 2.92-2.76$) and the substrate ($n_{\text{Si}} \sim 3.64-3.5$) in the λ range $0.875-1.35 \mu\text{m}$.

Owing to different physical processes giving rise to separate features in a PR spectrum, the lock-in amplifier phase setting at which the amplitude of a particular feature peaks is different.² Such a behavior is evident in the PR and CER spectra of our samples as shown in Fig. 2. We find that the DIT and the OF signals peak at 5.5° and 47.0° in PR and at -19.5° and -2.0° in CER, respectively, clearly indicating that these features have different physical origins. The fact that the periods of the OF in the PR and the CER spectra match the period of the OF in the R spectrum provides direct evidence for optical interference being the source of these features in the PR and the CER spectra. Also the frequency of the OF in all three spectra increases with CdTe film thickness (measurements on the thicker film have not been shown here) consistent with what is expected on the basis of optical interference.

PR and CER measurements on the Si substrates gave no signal, indicating that the modulation of the refractive index of the substrate cannot be responsible for the OF seen in these spectra.⁵ Therefore the OF in the PR and the CER spectra must arise because of a modification of the optical path length in the film which occurs in phase with the periodic perturbation viz the chopped pump laser beam in PR

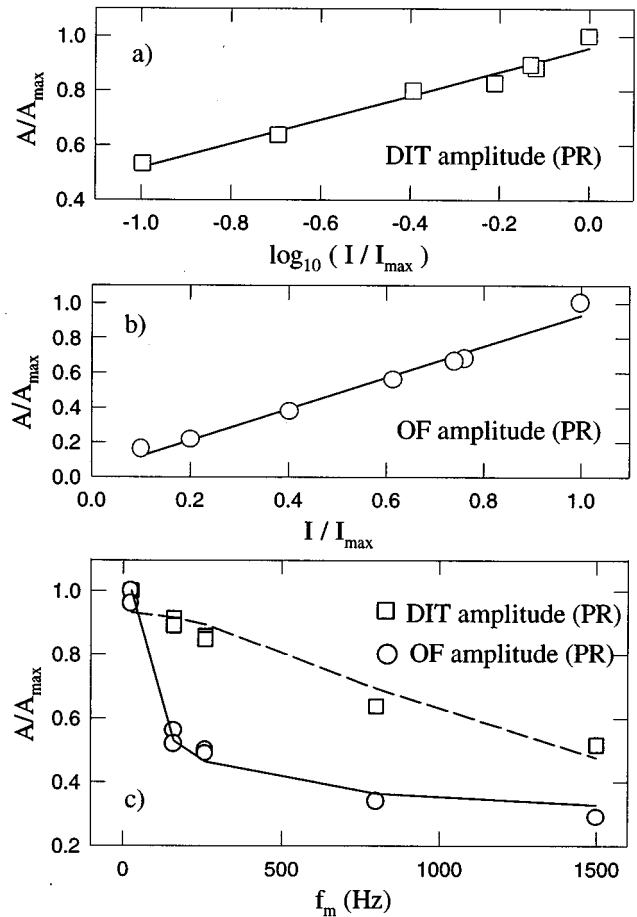


FIG. 3. (a) The linear dependence of the DIT amplitude (A) on the logarithm of the pump beam intensity (I) in PR. A_{max} and I_{max} correspond to the maximum amplitude and the maximum pump beam intensity, respectively. (b) The linear dependence of the OF amplitude (A) on the pump beam intensity (I) in PR. (c) The dependence of the DIT and the OF amplitude on the pump beam chopping frequency (f_m) in PR. The dashed line is a fit to the model of Shen *et al.* (see Ref. 2), while the continuous line represents the solution of Equation (1).

and the high alternating voltage in CER. The optical path length may change due to a change in the refractive index of the CdTe film (δn_{CdTe}), thickness of the CdTe film (δd_{CdTe}) or both. To estimate the magnitude of these changes we performed a series of simulations, the details of which are given in the Appendix. The relative λ independence of the OF amplitude at longer λ prompted us to consider, as a first approximation, a λ independent δn_{CdTe} . From the results, shown in Fig. 1(d) and Fig. 1(f), it is evident that the inclusion of a finite subband gap absorption can account for the observed damping of the OF at shorter λ . To estimate the upper limits on δn_{CdTe} and δd_{CdTe} only one was considered at a time. We found δn_{CdTe} (max) and δd_{CdTe} (max) to be 2×10^{-7} and 0.01 \AA in PR and 5.8×10^{-6} and 0.23 \AA in CER, respectively. A variety of physical phenomena can give rise to these small changes. However, band filling of the impurity states and Franz-Keldysh mechanisms for change in refractive index (which were the principal sources of modulation in the previous reports⁵⁻⁷) are ruled out in the present case since as explained earlier they cannot

account for the λ independence of the amplitude of the OF at longer λ . The following section describes the results of the experiments performed to determine the origin of these changes in δd_{CdTe} and δn_{CdTe} .

A. Photorefectance

It is known that the amplitude of the DIT transition scales logarithmically with the pump beam intensity because ΔR is proportional to the amplitude of the changing surface electric field, which in turn varies logarithmically with the pump beam intensity.¹⁵ A plot of the DIT amplitude versus logarithm of pump beam intensity in our case [Fig. 3(a)] clearly shows this behavior. However the amplitude of the OF does not follow this trend and instead scales linearly with the pump beam intensity as shown in Fig. 3(b). This indicates that the change δn_{CdTe} or δd_{CdTe} is not due to the pump beam induced changes in the electric field. An effect linear

with pump beam intensity would be refractive index modification by the pump beam generated plasma. However this mechanism has to be ruled out as our calculations show that such a phenomenon leads to a wavelength dependent change of δn_{CdTe} , varying by a factor of 2 in the range 1.0–1.35 μm , which clearly does not agree with our observation of near λ independence of the OF amplitude in this λ range.

Another possibility is heating of the sample due to the absorbed pump beam photons. To estimate the rise in temperature we consider a model consisting of a sample ($s \equiv \text{CdTe}$) of thickness d_s on a backing ($b \equiv \text{Si}$) placed in a fluid medium ($l \equiv \text{air}$) on which is incident a light beam of intensity I_0 ($\approx 3.2 \times 10^3 \text{ Wm}^{-2}$) chopped at a frequency f_m ($= 260 \text{ Hz}$). The solution due to Mandelis¹⁶ gives the amplitude of the change in temperature ΔT (complex quantity) at the surface to be

$$\Delta T = \frac{A}{\alpha_s^2 - \sigma_s^2} \left(\frac{(r-1)(h+1)e^{\sigma_s d_s} - (r+1)(h-1)e^{-\sigma_s d_s} + 2(h-r)e^{-\alpha_s d_s}}{(g+1)(h+1)e^{\sigma_s d_s} - (g-1)(h-1)e^{-\sigma_s d_s}} \right) \quad (1)$$

$$A = \frac{\alpha_s I_0}{2\kappa_s}, \quad a_j = \sqrt{\frac{\pi f_m}{D_j}}, \quad D_j = \frac{\kappa_j}{\rho_j c_j}, \quad (j \equiv s, b, l),$$

$$\sigma_s = (1+i)\alpha_s, \quad r = (1-i)\frac{\alpha_s}{2a_s}, \quad h = \frac{a_b \kappa_b}{a_s \kappa_s},$$

$$g = \frac{a_l \kappa_l}{a_s \kappa_s}, \quad i = \sqrt{-1},$$

where α_s ($\approx 4.6 \times 10^6 \text{ m}^{-1}$) is the absorption coefficient of the sample at the wavelength of the incident light (0.632 μm), κ_j is the thermal conductivity, c_j is the specific heat and ρ_j is the density of the j th medium. Using the above formula and the relevant material parameters given in Table I, one gets $|\Delta T| \approx 0.005 \text{ K}$. Since the film (CdTe) thickness is much smaller than its thermal diffusion length ($\Lambda_{\text{CdTe}} = \sqrt{4\pi\kappa/\rho\sigma f_m} \approx 800 \mu\text{m}$) the temperature rise will be uniform throughout the film. This temperature rise can cause both δn_{CdTe} and δd_{CdTe} change given by

$$\delta n_{\text{CdTe}} = \left(\frac{\partial n_{\text{CdTe}}}{\partial T} \right) \Delta T \quad \text{and} \quad \delta d_{\text{CdTe}} = d_{\text{CdTe}} \beta \Delta T. \quad (2)$$

Using the value of $\partial n_{\text{CdTe}}/\partial T$ ($\approx 1.0 \times 10^{-4} \text{ K}^{-1}$)¹⁷ and that of the linear thermal expansion coefficient β for CdTe ($\approx 4.8 \times 10^{-6} \text{ K}^{-1}$ at room temperature)¹⁸ we get $\delta n_{\text{CdTe}} = 5.0 \times 10^{-7}$ and $\delta d_{\text{CdTe}} \approx 0.003 \text{ \AA}$. Thus we see that first for the same ΔT , the change δn_{CdTe} is more important with respect to the origin of the OF as compared to the change δd_{CdTe} and second the order of magnitude of δn_{CdTe} as estimated above matches well with the value estimated from the simulations.

To test the above hypothesis further, we studied the pump beam chopping frequency (f_m) dependence of the DIT and the OF signal amplitude. The results [Fig. 3(c)] show

that the amplitude of the OF falls off much faster with increasing f_m (at smaller frequencies) than that of the DIT. This again proves that the two features, the OF and the DIT, have different physical origins. In general the frequency dependence of the amplitude of the DIT signal arises from the finite trapping time of the photo generated carriers which affects the profile of the changing electric field at the surface. By fitting the model of Shen *et al.*² [dashed line in Fig. 3(c)] we estimate the trapping time to be 0.2 ms. On the other hand as shown by the continuous line in Fig 3(c), which represents the change in the OF signal amplitude with pump beam chopping frequency as estimated from Equation (1), matches very well with the experimental values giving clear indication that their origin is related to pump beam induced temperature variation. In the wavelength range 0.875–1.35 μm , $\partial n_{\text{CdTe}}/\partial T$ has very weak λ dependence¹⁷ and this matches well with our observation of λ independence of the OF amplitude at longer λ , while its damping at shorter λ is well explained on the basis of subband gap absorption by the CdTe film as shown in the simulated PR spectrum [Fig. 1(d)]. Thus the above results prove that pump beam induced temperature modulation is the source of the periodic changes in the optical path length leading to the OF in the PR spectrum. It also seems likely that out of the two temperature induced changes δn_{CdTe} and δd_{CdTe} , the former makes the dominant contribution to the change in the optical path length of the CdTe film.

B. Contactless electroreflectance

Since in CER there is no conduction current, joule heating of the sample is ruled out. Also as shown in Fig. 4(a), the amplitude of both the DIT and the OF signals scale linearly with applied high voltage. For the OF, this implies that

TABLE I. Thermal properties of the various media. These were used in Equation (1) for estimating $|\Delta T|$, the values were taken from Refs. 18 and 24.

Material	Thermal conductivity ($\text{W m}^{-1}\text{K}^{-1}$)	Specific heat ($\text{J Kg}^{-1}\text{K}^{-1}$)	Density (Kg m^{-3})
CdTe	7.0	87.0	5.87×10^3
Si	140.0	700.0	2.33×10^3
Air	0.026	1040.0	1.29×10^0

δn_{CdTe} or δd_{CdTe} must also scale linearly with applied field. Furthermore, the OF amplitude is nearly wavelength independent at longer wavelength. There are two possible electric field related physical phenomena that may give rise to such changes having weak wavelength dependence. Since the film is preferentially $\langle 111 \rangle$ oriented there is a possibility of strain induced by the applied external field (F) through the piezoelectric effect. In such a case the change in the film thickness is given by^{19,20}

$$\delta d_{\text{CdTe}} = \frac{2e_{14}d_{\text{CdTe}}F}{\sqrt{3}C_{44}} \left(\frac{C_{11} + 2C_{12} - 2C_{44}}{C_{11} + 2C_{12}} \right), \quad (3)$$

where e_{14} ($= 0.031 \text{ C m}^{-2}$) is the piezoelectric stress coefficient, C_{11} ($= 5.33 \times 10^{10} \text{ N m}^{-2}$), C_{12} ($= 3.65 \times 10^{10} \text{ N m}^{-2}$) and C_{44} ($= 2.04 \times 10^{10} \text{ N m}^{-2}$) are the elastic moduli of CdTe.¹⁸ Using the above equation we see that for a change $\delta d_{\text{CdTe}} = 0.23 \text{ \AA}$ the field change required would be $1.67 \times 10^4 \text{ V cm}^{-1}$, which is much larger than what we expect in the present experimental arrangement. The second possibility is the change of refractive index δn_{CdTe} because of the electro-optic effect. In the class of semiconducting compounds, with respect to the electro-optic effect, CdTe has the highest figure of merit defined as $n^3 r_{41}$, where n is the refractive index and r_{41} is the largest nonzero electro-optic tensor element. The change δn_{CdTe} is proportional to²¹

$$\delta n_{\text{CdTe}} \approx \frac{n_{\text{CdTe}}^3 r_{41} F}{2}. \quad (4)$$

In the case of CdTe the quantity $n^3 r_{41}$ varies between $(101.6 - 107.2) \times 10^{-10} \text{ cm V}^{-1}$ in the wavelength range $(0.875 - 1.35 \text{ }\mu\text{m})$ ²¹ so the field change required for $\delta n_{\text{CdTe}} = 5.8 \times 10^{-6}$ is $\approx 1.1 \times 10^3 \text{ V cm}^{-1}$. Thus for the same value of the change in electric field, the change δn_{CdTe} is much more significant (with respect to the origin of the OF) than the change δd_{CdTe} . The weak λ dependence²¹ of $n^3 r_{41}$ is in accordance with our observation of near λ independence of the OF amplitude at longer λ while its damping at shorter λ is well explained on the basis of subband gap absorption by the CdTe film as shown in the simulated CER spectrum [Fig. 1(f)]. The quantity $n^3 r_{41}$ is expected to reduce at low temperature mainly due to reduction in n_{CdTe} (Ref. 17) and this should decrease the OF amplitude at low temperatures. The results of the low temperature CER measurements presented in Fig. 4(b) clearly show that the OF signal amplitude decreases at low temperatures. Note however that at low temperatures the amplitude of the DIT signal [Fig. 4(a)] increases significantly due to a reduction in the phenomono-

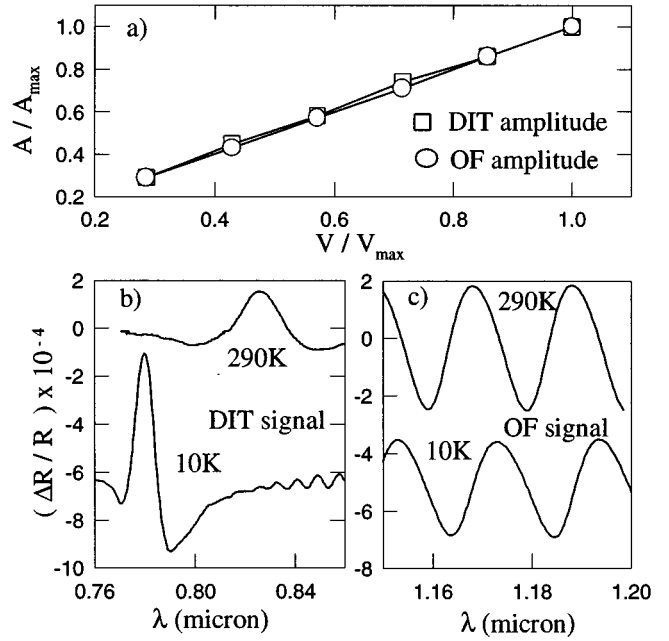


FIG. 4. (a) The linear dependence of the DIT and the OF signal amplitude (A) on the applied high voltage (V) in CER. A_{max} and V_{max} correspond to the maximum signal amplitude and the maximum applied voltage, respectively. (b) Temperature dependence of the DIT signal amplitude. (c) Temperature dependence of the OF signal amplitude. The baseline of the 10 K spectra have been shifted down for clarity.

logical broadening parameter Γ [see Eq. (8)]. Thus the most likely source of the change in the optical path length leading to the OF in CER seems to be the electro-optic effect induced refractive index change of the CdTe film.

IV. CONCLUSION

In conclusion, we have provided direct evidence for optical interference being the source of the subband gap OF seen in the modulated reflectance spectra of multilayered semiconductor structures. Since in the present case, the λ dependence of the OF amplitude cannot be explained on the basis of Franz-Keldysh or impurity band filling mechanisms reported earlier in connection with the OF in PR, we performed detailed experiments to determine the modulation mechanism. The results indicate that for the CdTe/Si structure used in our experiments, the pump beam induced temperature modulation resulting in refractive index changes is the most likely modulation mechanism giving rise to the OF in PR, while in CER the OF arise due to the electric field induced changes in the refractive index through the electro-optic effect. We have also been able to account for the damping of the amplitude of the OF in the modulated reflectance spectra at shorter λ on the basis of a finite subband gap absorption.

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APPENDIX

The structure considered for modelling the OF in the R spectrum consists of an absorbing dielectric film (CdTe \equiv medium 2) on a nonabsorbing dielectric substrate (Si \equiv medium 3) suspended in a isotropic, homogenous medium (air \equiv medium 1). Its reflection coefficient is given by

$$R = \frac{1}{2} (r^s r^{s*} + r^p r^{p*}), \quad (5)$$

where r^s (r^{s*}) and r^p (r^{p*}) are the complex (complex conjugate) amplitude reflection coefficients for s and p polarized incident light for the total structure and are in turn given by²²

$$r^{s,p} = \frac{r_{12}^{s,p} + r_{23}^{s,p} e^{i4\pi d(u_2 + iv_2)/\lambda}}{1 + r_{12}^{s,p} r_{23}^{s,p} e^{i4\pi d(u_2 + iv_2)/\lambda}}, \quad (6)$$

where λ is the wavelength of the incident light in air, and d is the CdTe film thickness. The quantities $r_{12}^{s,p}$ and $r_{23}^{s,p}$ are complex amplitude reflection coefficients at the air/CdTe and CdTe/Si interfaces, respectively. These along with the quantities u_2 and v_2 depend on the real (n) and the imaginary (k) parts of the refractive indices of the various media, and the angle of incidence (θ_1) of the light beam in air. The detailed formulae relating these quantities are taken from Ref. 22. Then n and k values of Si and CdTe depend on λ as detailed below.

The wavelength dependent values of n_{CdTe} and n_{Si} were estimated by fitting a smooth function [$n = a_1 \exp(-a_2\lambda) + a_3$] to the data listed in Ref. 17. For the k values we made the following two assumptions:

- (i) In the wavelength range of interest (0.875–1.35 μm) Si has a finite imaginary part of refractive index (7.8×10^{-3} to $< 1.5 \times 10^{-6}$).¹⁷ However this value is too small to make a significant difference to the reflectivity of CdTe/Si interface and so it is taken to be zero.
- (ii) We see in Fig. 1(a) that as one approaches the band gap of CdTe from the longer wavelength side, the amplitude of the OF is progressively damped essentially due to absorption of light by the CdTe film. The listed values¹⁷ of CdTe k_{CdTe} are not sufficiently large to account for this damping. As such the film is expected to have enhanced subband gap absorption due to defects resulting from the large lattice mismatch with the substrate. Therefore to obtain k_{CdTe} vs λ we have considered an average subband gap absorption coefficient (α) consisting of an Urbach tail²³ and a parabolic background of the form

$$\alpha = \alpha_0 \exp\left[\gamma\left(\frac{1.24(1/\lambda - 1/\lambda_0)}{k_B T}\right)\right] + a\lambda^2 + b\lambda + c \quad (\lambda \text{ in } \mu\text{m} \text{ and } k_B T \text{ in eV}), \quad (7)$$

where k_B is the Boltzmann constant, T is the temperature, $1.24/\lambda_0$ is band gap energy (eV) of CdTe and $1.24/\lambda$ is the incident photon energy (eV). The parameters α_0 , γ , a , b and c are constants. k_{CdTe} is related to α by $k_{\text{CdTe}} = \lambda \alpha / 4\pi$.

The value of λ_0 is estimated by fitting the PR and CER feature due to the direct interband transition (DIT) at the

fundamental gap of CdTe (for $\lambda < 0.875 \mu\text{m}$) using the conventional third derivative functional form (TDFD)¹

$$\Delta R/R = \text{Re}\left(\frac{A e^{i\phi}}{(E - E_0 + i\Gamma)^m}\right) \quad (8)$$

where A is a constant, ϕ is a phase factor, Γ is the phenomenological broadening parameter $E = 1.24/\lambda$ and $E_0 = 1.24/\lambda_0$. The index m depends on the dimensionality of the critical point and is 2.5 in the present case (the fundamental gap of CdTe is a 3D critical point). A linear term is added to the above equation to account for the nonzero background. The fitted value of E_0 and Γ are found to be 1.497 eV and 0.034 eV, respectively.

The remaining parameters d , θ_1 , α_0 , γ , a , b and c are obtained by fitting the experimental R data with our model. The values of d and θ_1 are found to be 11.55 μm and 7.6° , respectively, and are consistent with what we expect from experimental considerations. The fit gives the values of α_0 and γ for the subband gap absorption coefficient (in the wavelength range 0.875–1.35 μm) as follows

$$\alpha(\text{cm}^{-1}) = 4.175 \times 10^3 \exp\left[0.4283\left(\frac{1.24/\lambda - 1.497}{0.025}\right)\right] + 4.34 \times 10^3 \lambda^2 - 1.153 \times 10^4 \lambda + 7.751 \times 10^3 \quad (\lambda \text{ in } \mu\text{m}).$$

The fact that the value of the absorption coefficient given by the above equation is much higher than that obtained from the data listed in Ref. 17 and the high value of Γ is consistent with our expectation of defects in the film.

The OF in the PR and CER spectra for λ greater than 0.875 μm can be simulated by calculating the difference in the reflectance of the sample as seen by the probe beam under two conditions: (i) with the modulating perturbation on (pump laser beam in PR and high voltage in CER), and (ii) with the perturbation off, i.e.,

$$\frac{\Delta R}{R} = \left(\frac{R_{\text{pertb. on}}}{R_{\text{pertb. off}}}\right) - 1. \quad (9)$$

The expression for $R_{\text{pertb. off}}$ is also given by Equations (5)–(8) with n_{CdTe} replaced by $n_{\text{CdTe}} + \delta n_{\text{CdTe}}$ or d replaced by $d + \delta d_{\text{CdTe}}$ or both as the case may be. The full simulated spectrum is given by a sum of the above equation and the TDFD equation given earlier. At this stage all the required parameters apart from δn_{CdTe} or δd_{CdTe} are already available from fitting the R spectrum. The magnitudes of these two quantities were determined by comparing the results of the simulations with the experimental PR and CER spectra. The simulated spectra are shown in Figs. 1(d) and 1(f).

¹F. H. Pollak and H. Shen, Mater. Sci. Eng. **R10**, 275 (1993).

²H. Shen and M. Dutta, J. Appl. Phys. **78**, 2151 (1995).

³D. E. Aspnes, in *Handbook of Semiconductors*, edited by M. Balkanski (North Holland, Amsterdam, 1980), Vol. 2.

⁴C. Parks, A. K. Ramdas, M. R. Melloch, G. Steblovsky, L. R. Ram-Mohan, and H. Luo, Solid State Commun. **92**, 563 (1994).

⁵D. Huang, D. Mui, and H. Morkoc, J. Appl. Phys. **66**, 358 (1989).

⁶N. Kallergi, B. Roughani, J. Aubel, and S. Sundaram, J. Appl. Phys. **68**, 4656 (1990).

⁷H. K. Lipsanen and V. M. Airaksinen, Appl. Phys. Lett. **63**, 2863 (1993).

- ⁸X. L. Zheng, D. Heiman, B. Lax, and F. A. Chambers, *Appl. Phys. Lett.* **52**, 287 (1988).
- ⁹P. C. Klipstein and N. Apsley, *J. Phys. C* **19**, 6461 (1986).
- ¹⁰R. A. Batchelor and A. Hammet, *J. Appl. Phys.* **71**, 2414 (1992).
- ¹¹A. P. Thorn, A. J. Shields, P. C. Klipstein, N. Apsley, and T. M. Kerr, *J. Phys. C* **20**, 4229 (1987).
- ¹²M. Nakayama, I. Tanaka, T. Doguchi, and H. Nishimura, *Jpn. J. Appl. Phys.* **29**, L1760 (1990).
- ¹³A. J. Shields and P. C. Klipstein, *Phys. Rev. B* **43**, 9118 (1991).
- ¹⁴S. Ghosh and B. M. Arora, *Advances in Instrumentation*, Proc. of International Conf. on Instrumentation (New Age, Bangalore, 1996).
- ¹⁵R. E. Wagner and A. Mandelis, *Phys. Rev. B* **50**, 14 228 (1994).
- ¹⁶A. Mandelis, *J. Appl. Phys.* **54**, 3404 (1983).
- ¹⁷*Handbook of Optical Constants of Solids*, edited by E. D. Palik (Academic, New York, 1985).
- ¹⁸*Landolt-Börnstein New Series*, edited by O. Madelung (Springer, New York, 1987).
- ¹⁹J. Singh, *Physics of Semiconductors and their Heterostructures* (McGraw-Hill, New York, 1993).
- ²⁰W. G. Cady, *Piezoelectricity*, 1st ed (McGraw-Hill, New York, 1946).
- ²¹A. Yariv, *Optical Electronics*, 4th ed. (Saunders, Philadelphia, 1991).
- ²²M. Born and E. Wolf, *Principles of Optics*, 6th ed. (Pergamon, New York, 1989).
- ²³G. Burns, *Solid State Physics* (Academic, New York, 1990).
- ²⁴*CRC Handbook of Chemistry and Physics*, edited by R. C. Weast (CRC, Boca Raton, FL, 1978).