Electronic States in $\text{Cd}_{1-x}\text{Zn}_x\text{Te}/\text{CdTe}$ Strained Layer Coupled
Double Quantum Wells and Their Photoluminescence

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ABSTRACT

Experimental and theoretical investigation of electronic states in a strained-layer $\text{CdTe}/\text{CdZnTe}$ coupled double quantum well structure are presented. The optical properties of this lattice-mismatched heterostructure were characterized with photoluminescence (PL), PL excitation and polarization spectroscopies. Influence of electrical field on exciton states in the strained-layer $\text{CdTe}/\text{CdZnTe}$ coupled double quantum well structure is experimentally studied. The confined electronic states were calculated in the framework of the envelope function approach, taking into account the strain effect induced by the lattice-mismatch. Experimental results are compared with the calculated transition energies.

INTRODUCTION

An increasing amount of attention has recently been directed to structures employing strained layer quantum wells, coupled double quantum wells and superlattices because of their potential for optoelectronic devices applications. The studies of strained layer quantum structures grown using lattice mismatched materials has been widely developed for III-V semiconductors. Strained layer II-VI compounds heterostructures have not been studied as much as those from III-Vs, but they are a rapidly growing of semiconductor research. The wide gap II-VI compounds are direct bandgap materials, which makes them attractive for active optoelectronic devices. Most of the research on strained layer structures in the wide gap tellurium-based compounds has concentrated in two areas. The first area is the diluted magnetic semiconductors involving Mn in the $\text{Cd}(\text{Zn})\text{Te}$ system. The other area is CdTe/ZnTe and $\text{CdZnTe}/\text{ZnTe}$ quantum wells and superlattices. For the $\text{CdZnTe}/\text{CdTe}$ most of publications are related to structures with very small amounts of Zn (0.04 to 0.06) [1-5]. Recently, papers were published on growth and optical characterization of $\text{CdZnTe}/\text{CdTe}$ strained layer single quantum wells with a Zn concentration about 20% [6,7].

In this paper we investigate the photoluminescence, photoluminescence excitation, polarization and photocurrent spectra in $\text{Cd}_{1-x}\text{Zn}_x\text{Te}/\text{CdTe}$ symmetric coupled double quantum wells (CDQW) for the first time, to the best of our knowledge, in II-VI compounds. In symmetric, coupled double quantum wells (CDQW) the electron and hole subband levels are split into levels associated with symmetric and antisymmetric combinations of isolated single quantum well (SQW) wave functions. Thus, the isolated SQW heavy-hole levels are split into symmetric and antisymmetric heavy-hole levels associated, respectively, with symmetric and antisymmetric combinations of isolated SQW wave functions, while the light hole and electron subband levels are split similarly. The binding of an electron in a symmetric state and a heavy-hole in a symmetric state gives rise to a symmetric heavy-hole free-exciton (S-HHFE). Similarly, an antisymmetric heavy-hole free exciton (A-HHFE) is formed from an "antisymmetric" electron and an "antisymmetric" heavy-hole. The binding of a "symmetric" electron and a "symmetric" light-hole gives rise to a symmetric light-hole free exciton (S-LHFE), while an antisymmetric light-hole free exciton is formed from an "antisymmetric" light-hole and an "antisymmetric" electron. Our previous study on $\text{CdTe}/\text{Cd}_{1-x}\text{Zn}_x\text{Te}$ SQWs has shown that in this heterostructure system the band lineup is type I for heavy-holes and type II for light-holes. Excitonic transitions associated with

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heavy-holes are observed in PL and correspond to collapse of S-hhFE and A-hhFE. In PLE, with the detection locked on S-hhFE and A-hhFE in the wells, FE in the barrier layer are observed. The circular polarized excitation spectra have confirmed that all observed transitions are associated with heavy-holes. The photocurrent spectra (PCS) in CDQW are shown to be proportional to absorption spectra for the intrinsic optical transitions. Furthermore, the photocurrent technique does not require the removal of the substrate which is required for absorption measurements. The PCS measurements however involve electric fields that create Stark shifts, and changes in transition strength, and transition lifetime [8-12]. The confined states are calculated in the framework of the three-band envelope function method [17], taking into account the strain effect due to the lattice mismatch between the barrier and well layers. The binding energies of S-hhFE and A-hhFE are deduced from these calculations and experimental results.

EXPERIMENTAL

The samples studied were nominally symmetric, coupled, $\text{CdTe}/\text{Cd}_{1-x}\text{Zn}_x\text{Te}$ double quantum well structures grown by molecular-beam epitaxy (MBE) on n^+ -type (100) GaAs substrates. It has been well documented that both (111) and (100) CdTe can be grown on GaAs(100) [13]. To ensure that the (100) orientation was obtained for the layers and to eliminate any possible confusion, we deposited approximately 30Å of ZnTe to initiate the (100) orientation.

Fig. 1. PL spectra from sample R813 and R835, which is a $\text{Cd}_{1-x}\text{Zn}_x\text{Te}$ epitaxy layer grown on n^+ -type (100) GaAs substrates under the condition similar to the growth of R813. The inset is a schematic of the band lineup.

Fig. 2. The "net" emission spectrum of the CDQW and its curve fitting.

After the initial 30Å of ZnTe was deposited, a $\text{Cd}_{1-x}\text{Zn}_x\text{Te}$ layer was grown ($x \sim 0.14$). The mismatch between $\text{Cd}_{0.86}\text{Zn}_{0.14}\text{Te}$ and GaAs is quite large ($\sim 13\%$). This leads to a very high dislocation density in the films. We have found, using both photoluminescence microscopy and X-ray diffraction, that the quality of the CdTe film increases with the thickness until the film is 3 to 4 μm thick [13c]. There may be some continued improvement in the film beyond this thickness but the improvement is small and it is difficult to verify. Therefore, the underlying CdZnTe buffer layers were grown to a thickness of 4 μm . The coupled quantum

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wells consisted of two CdTe quantum wells each with a thickness of 75 Å and a CdZnTe barrier. The thicknesses of the barriers were 13, 25, 50, and 75 Å. On top of the coupled quantum wells, a 0.5 μm cap layer of CdZnTe was grown. The buffer layer and CDQW structure are nominally not doped.

X-ray diffraction measurements were performed using a 4-bounce silicon monochromator with a resolution of 8 arcsec (the (115) was used as the asymmetric reflection). Both the lattice parameter and the full-width at half-maximum (FWHM) were determined for each sample. The Zn composition was obtained using the lattice parameter and Vegard's law. From the analysis of the X-ray data, the buffer and cap layers were relaxed.

Table 1. Parameter values used for calculations. $E_g = 1.606 + 0.494x + 0.294x^2$ (eV) (calculated using Hill's theory), $a(\text{Cd}_{1-x}\text{Zn}_x\text{Te}) = 6.481 - 0.3773(\text{Å})$ [15], $m_e^*(\text{Cd}_{1-x}\text{Zn}_x\text{Te}) = 0.099 + 0.017x$, $\gamma_1(\text{Cd}_{1-x}\text{Zn}_x\text{Te}) = 4.11 - 0.04x$, $\gamma_2(\text{Cd}_{1-x}\text{Zn}_x\text{Te}) = 1.08 - 0.3x$ [4]

	E_g [15] (eV)	Δ [16] (eV)	a_v [16] (eV)	a_c [16] (eV)	b [16] (eV)	a_0 [16] (eV)	C_{11} [16] (eV)	C_{12} [16] (eV)	E_{val}^* (eV)
ZnTe	2.394	0.91	0.79	-5.83	-1.26	6.1037	0.713	0.407	+0.03
CdTe	1.606	0.93	0.55	-3.96	-1.10	6.481	0.562	0.394	+0.21

Relative to the top of GaAs valence band given HAO theory

The optical spectra were measured in the back scattering direction at $\approx 26^\circ$ from the normal to the quantum well layer, with the sample mounted on a cold finger cooled by a closed-cycle helium cryostat down to 8.5K. The PL measurements were performed with an Ar⁺ laser for the Cd_{1-x}Zn_xTe barriers excitation (488nm line) or by a tunable Ti:Sapphire laser with Burleigh wavemeter model WA2000S for barrier excitation or directly the CdTe quantum well excitation. Luminescence spectra were recorded with a Jarell-Ash 0.75m monochromator equipped with a 1180 grooves/mm grating. The detection electronics consists of thermoelectrically cooled photomultiplier with a fast preamplifier connected to a dual-channel gated photon counting system controlled by a computer, which also controls the scanning monochromator Jarell-Ash and tunable Ti:sapphire laser. The circular polarization of luminescence and excitation spectra were measured using a highly sensitive and absolute apparatus involving a photoelastic modulator (PEM). The system was described in detail in a previous publication[14].

The photocurrent measurement was done on a Schottky barrier structure prepared by evaporating a semitransparent gold electrode (100 Å thick) on the Cd_{1-x}Zn_xTe cap layer. A second indium Ohmic contact was made at the back side of the n-type ($2-3 \times 10^{17}/\text{cm}^3$) GaAs substrate. The sample holder was mounted on a cold finger cooled by a close-cycle helium cryostat down to 9 K. The photocurrent spectra measurements were carried out using the tunable Ti:sapphire laser as the excitation source and a Keithley 236 Source Measure Unit for photocurrent measurement.

RESULTS AND DISCUSSION

Detailed results are only presented for the sample R813 ($x=1.42$, $L_b=75\text{Å}$) since the results were found to be similar for each CDQW investigated. Fig. 1 shows the PL spectra of R813 and R835, which is a Cd_{1-x}Zn_xTe epitaxial layer grown on n⁺-type (100) GaAs substrates under conditions similar to the growth of R813. The spectra were taken at T= 9.0 K, excited by the 488nm line of Ar⁺ laser. By comparison of these spectra, it is clear that only the peak

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A (at 1.5879eV) and peak B (at 1.6068eV) are from the CDQW structure. After curve fitting and removing the emission peaks from barrier layer, the "net" emission spectrum of the CDQW is plotted in Fig. 2. Our previous study on CdTe/Cd_{1-x}Zn_xTe SQWs[7] has shown that the binding energy of heavy-hole-free-exciton in a 75Å SQW is about 36.5meV. Using this value, peaks A and B falls into the region for S-hhFE and A-hhFE collapse respectively.

The PLE spectrum of peak A is shown in Fig.3. The PLE (dashed line) spectrum is taken with detection locked on the energy of 1.58543 eV, which detects emission from peak A in PL spectrum. The peak at 1.6105eV in the PLE spectrum indicates that the S-hhFE and A-hhFE in PL spectrum are well coupled to each other. The peak at 1.6842eV in the PLE spectrum is due to the FE formation in barrier layer. The PLE of peak B is also plotted (solid line) in Fig. 3, which shows a strong peak at the barrier FE energy. Note from Fig. 3 that both S-hhFE and A-hhFE in PL spectrum are strongly coupled to the barrier FE and S-hhFE and A-hhFE are well coupled to each other.

Table 2. Calculated and experimental transitions and their difference E_B for all samples studied. The x value is the mole concentration of Zink in the Barrier layer.

Sample		Transition Type	Calculated Subband Gap (eV)	Experimental Emission Peak Energy (eV)	Exciton Binding Energy (meV)
R810	$x=0.134$	S-hhFE	1.61688	1.58281	34.07
	$L_b=13 \text{ \AA}$	A-hhFE	1.6003	1.56704	33.26
R811	$x=0.143$	S-hhFE	1.6198	1.58308	36.72
	$L_b=25 \text{ \AA}$	A-hhFE	1.63183	1.60601	25.82
R812	$x=0.133$	S-hhFE	1.62217	1.58638	35.79
	$L_b=50 \text{ \AA}$	A-hhFE	1.628	1.60674	21.26
R813	$x=0.142$	S-hhFE	1.62382	1.58876	35.06
	$L_b=75 \text{ \AA}$	A-hhFE	1.62665	1.60691	19.74

The circularly polarized PLE of peak A in PL spectrum is shown in Fig. 4, which clearly shows that both peak A and peak B in PL spectrum have heavy-hole polarity.

Table 1 lists all the physical parameters used to calculate the confined electronic states in the CDQW. The calculation shows that in all of 4 samples studied, there is only one confined level for electrons in the SQW and it is split into two levels, one symmetric and the other antisymmetric. The two heavy-hole levels in the SQW are similarly split into four sublevels, two of which are associated with symmetric combinations of isolated single quantum well (SQW) wave functions and the other two are associated with antisymmetric combinations of SQW wave functions. Light-holes are not confined in CdTe layer due to the strain effect. The only two allowed transitions are between first symmetric electron level (s-e1) and first symmetric heavy-hole level (s-hh1); and first antisymmetric electron level (a-e1) and first antisymmetric heavy-hole level (a-hh1). Subtracting the peak energy of peak A and B in Fig. 1 from calculated (s-e1 - s-hh1) and (a-e1 - a-hh1), the binding energies for S-hhFE and A-hhFE in sample R813 ($x=1.42$, $L_b=75\text{\AA}$) are deduced to be 35.06meV and 19.74meV

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respectively. Table 2 lists the results of calculations and measurements for all the samples studied. Note in Table 2 that for a given sample, $E_B(\text{S-hhFE}) > E_B(\text{A-hhFE})$, as is expected since S-hhFEs are more confined than A-hhFEs: Heavy-holes and electrons associated with symmetric combination of SQW wave functions lie lower in energy than heavy-holes and electrons associated with antisymmetric combination of SQW wave functions.

Fig. 3. PL excitation spectra of R813. Dashed line using peak A and solid line using peak B PL

Fig. 4. Circular polarization spectrum of R813.

Fig. 5. PC spectra of R813 under negative biases. a: S-hhFE transition energy and b: A-hhFE transition energy.

Fig. 6. PC spectra of R813 under positive biases. The inset shows physical structure of the electrodes.

The PC spectrum was obtained by measuring the PC with the electric field applied perpendicular to the quantum wells, as a function of the wavelength of incident light focused on semitransparent gold electrode, or near the Au contact. The variable wavelength IR source was a Ti: sapphire laser. The observation of a photocurrent requires that the excitation light create free carriers and that transport of the carriers occur in the electric field. The photocurrent most probably arises from carriers tunneling the barrier between the wells. The measured photocurrent spectra for sample R813, plotted versus energy in Fig. 5 and Fig. 6 for different applied voltage exhibit appearing (splitting) peaks with increasing applied voltage. In

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Fig. 5 for voltage +2.5 V and +5 V, only two peaks are observed with trace of shoulders on the low energy side. With increasing field more peaks appear as we can see from PC spectrum for +7.5 and +10 volts. These additional peaks are probably due to symmetry-forbidden transition under flat-band conditions. The arrows show transition energies at zero field for the S-hhFE and A-hhFE excitons respectively.

We compare the photocurrent and photoluminescence spectra of CDQW at 9.2 K for sample R813 ($x=1.42$, $L_b=75\text{\AA}$). The comparison of PC spectra and the photoluminescence spectra revealed a significant exciton peak shift toward the lower energy. The identifications of PC peaks require comparison their energies to transition energies predicted in envelope function calculations including electric field effect. The detail of analysis of PC spectra in comparison with PLE and PL spectra's will be discussed in separate publication.

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