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Band alignment in ZnCdTe/ZnTe and ZnCdSe/ZnSe SQW structures grown on GaAs(100) by MBE

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Abstract. MBE-grown ZnTe/CdZnTe/ZnTe and ZnSe/ZnCdSe/ZnSe strained single quantum well (SQW) structures with non-doping layers were investigated by cathodoluminescence (CL) and deep level transient spectroscopy (DLTS). Obtained DLTS and CL results were used for the estimation of the conduction band offset parameter Q_C.

1. Introduction

One of the major parameters of SQW structures is the energy band offset ΔE_C (conduction band), ΔE_V (valence band), which determines the heights of potential barriers for electrons and holes. However, these parameters for structures that we investigated are determined insufficiently reliably. Thus, the data of conduction band offset value, $Q_C = \Delta E_C/\Delta E_G$, ($\Delta E_G = \Delta E_C + \Delta E_V$ is gap discontinuity), for the $Zn_{1-x}Cd_xTe$/CdTe heterojunction are known from the literature being changed from 0.775 up to 1.2 [1, 2] and for $Zn_{1-x}Cd_xSe$/ZnSe one from 0.64 up to 0.83 [3], respectively. One of the reasons of such data scattering can be essential dependence of edges of allowed bands on built-in elastic strains. These strains appear due to mismatching of crystal lattice parameters and their distribution on layers depends on concrete structure composition.

2. Experiment

In this paper the band offsets in strained ZnTe/$Zn_{1-x}Cd_xTe$/ZnTe and ZnSe/$Zn_{1-x}Cd_xSe$/ZnSe SQW structures are experimentally determined by the low-temperature cathodoluminescence (CL) and electrical current deep level transient spectroscopy (DLTS) methods. Studied samples were grown by molecular beam epitaxy (MBE) on n^+-GaAs(100) substrates misoriented on 3° to a ⟨110⟩ direction. Main parameters of grown structures are given in the left part of Table 1. CL spectra were recorded at temperature of 14 K, electron energy of 10 keV, e-beam current density of 0.1 mA/cm^2 and an electron beam spot diameter of 1 mm. In the case of DLTS the thermal evaporation of indium on the GaAs substrate back and nickel on the ZnTe (ZnSe) cap layer was used to prepare diode-like structures. The area of the nickel electrodes was 1 mm^2. All samples had high electrical resistance because of self-compensation effects in the epitaxial layers. Capacity of structures did not change with a bias voltage. For this reason, traditional DLTS variant based on a relaxation of the structure capacity [4] could not be applied for study of our samples. We registered the electrical current relaxation through the structure (the current DLTS) using usual procedure of DLTS measurement in all other respects.

3. Results and discussion

CL spectra of SQW structures contained weak narrow emission lines from free and bound exciton emissions near band edge region of ZnTe (ZnSe) and also an intense I_{qw} line due to quantum well (QW) emission. Energy standing of the I_{qw} line depended on QW

Table 1. Parameters of studied structures with single $Zn_{1-x}Cd_xTe$ QW (samples 195–197) and $Zn_{1-x}Cd_xSe$ QW (samples 207, 209–211).

Sample numb.	%Cd in QW	L_w (nm)	E_{CL} (eV)	ΔE_{CL} (meV)	$E1$ (meV)	E_{e1} (mev)	E_{hh1} (mev)	Q_C
195	22	3.5	2.246	134	101	80	16	0.823±0.045
196	22	6.5	2.206	174	133	38	7.5	0.816±0.048
197	20	5.5	2.226	154	116	46	9	0.814±0.05
207	21	9	2.562	241	155	19	5.3	0.656±0.038
209	37	5	2.403	400	255	54	15.3	0.676±0.033
210	20	5	2.583	220	140	44.5	12.9	0.695±0.038
211	34	5	2.427	376	220	53	15	0.632±0.035

parameters. The I_{qw} intensity was 2–3 orders of magnitude more than intensity of near band gap emission lines. Full width on half maximum of I_{qw} lines was equal to 8–10 meV. This fact testifies to high enough quality of structures. Energy standings, E_{CL}, of the I_{qw} line maximums for all tested structures are listed in Table 1.

The DLTS spectra contained a peak from deep level with an activation energy $E2$ (samples 195–197, Fig. 1) or $E3$ (samples 207, 209–211, Fig. 2) and an intense peak $E1$ in low temperature region. At used minimal temperature of measurements (77 K) the recording of this peak was possible in emission rate windows providing relaxation time constant less than $5 \cdot 10^{-4}$ s.

We consider that more intense $E1$ peak is due to emission of electrons from the ground quantified level in the conduction band of the QW. The activation energy of the $E1$ in this case corresponds to the energy interval between the conduction band bottom in the barrier layer and ground quantified level in the QW. The activation energy of the traps bound with the low temperature $E1$ peak changed from 101 up to 255 meV for various structures (Tables 1, 2).

The values of the effective bulk carrier concentrations N_t, at $E1$ levels calculated by traditional method, are listed in Table 2. Taking into account that the capture of carriers occurs in the QW, it is possible to estimate the sheet concentration n_s of carriers captured on the ground quantified level as: $n_s = N_t \cdot L_w$, where L_w is the well width. The estimates show that in studied samples n_s does not exceed 1×10^{10} cm^{-2}. It means that in the QW the ground quantified level is filled only.

The CL and DLTS experimental results were used for the estimation of conduction band offset parameter:

$$Q_C = \Delta E_C/\Delta E_G = (E1 + E_{e1})/(\Delta E_{CL} - \Delta E_b + E_{e1} + E_{hh1}), \qquad (1)$$

where $E1$ is the DLTS activation energy of electron emission from the ground state e1 in QW, ΔE_{CL} is the energy shift of the QW emission line from the free exciton emission line in the barrier ZnTe (ZnSe); E_{e1}, E_{hh1} is the energy of the ground state for electrons in the conduction band and holes in the valence band, respectively; ΔE_b is changing of heavy hole exciton binding energies in the barrier layer and QW (see Table 1).

The energies E_{e1} and E_{hh1} were calculated by using known parameters of the QW (its width, $E1$, electron and hole effective masses in the QW and the barriers, Cd content) and taking the rectangular model of the QW with wide barriers and finite depth [5]. So, E_{e1} and E_{hh1} can be written as:

$$E_{e1} = F\{L_w, \Delta E_C\} = F\{L_w, E_{add} + E_{e1}\}, \qquad (2)$$

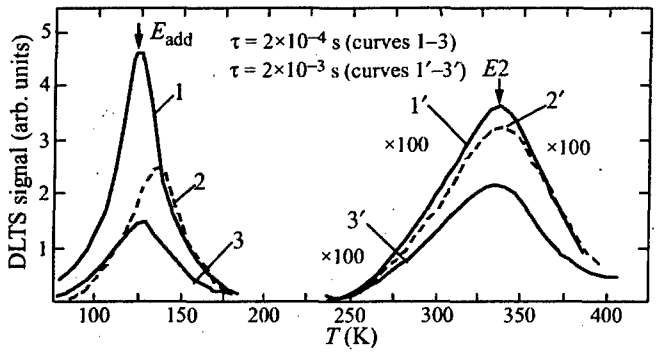

Fig. 1. DLTS spectra of the ZnTe/$Zn_{1-x}Cd_xTe$ structures No 195 (curves 1–1′), 196 (2–2′), 197 (3–3′) measured at the reverse voltage $V_r = -1$ V and the filling voltage $V_f = +1$ V.

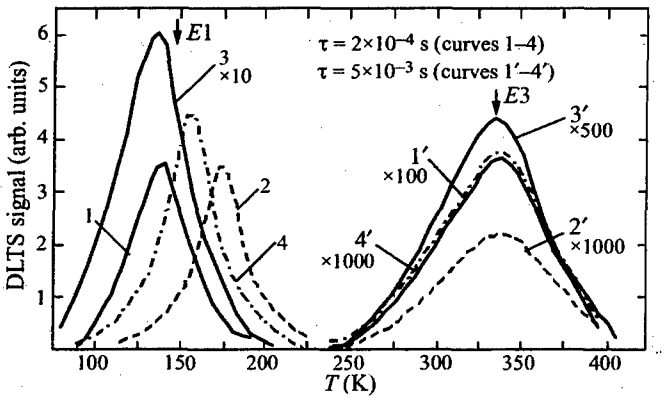

Fig. 2. DLTS spectra of the ZnSe/$Zn_{1-x}Cd_xSe$ structures No 207 (curves 1–1′), 209 (2–2′), 210 (3–3′), and 211 (4–4′) measured at the reverse voltage $V_r = -1$ V and the filling voltage $V_f = +1$ V.

$$E_{hh1} = G\{L_w, \Delta E_V\}G\{L_w, \Delta E_C(1 - Q_C)/Q_C\}$$
$$= G\{L_w, (E_{add} + E_{e1})(1 - Q_C)/Q_C\}, \quad (3)$$

where F and G are the transcendental functions.

Band gap of the QW material and its change respect to band gap of the barrier material can be expressed through the energy standing, E_{CL}, of the QW emission line and its energy shift, ΔE_{CL}, from the free exciton emission line in the barrier ZnTe (ZnSe) (see Table 1) as:

$$E_G = E_{CL} + E^b_{hh} - E_{e1} - E_{hh1}, \quad (4)$$

$$\Delta E_G = \Delta E_V + \Delta E_C = \Delta E_V + E1 + E_{e1} = \Delta E_{CL} - \Delta E^b_{hh} + E_{e1} + E_{hh1}, \quad (5)$$

where E_{bhh} is the heavy hole exciton binding energy. Thus, it is supposed that the free exciton emission line formed by the heavy hole. Further, in calculations of E_G, it has been taken into account that the exciton binding energy, E^b_{hh}, is incremented approximately on 10 meV in the narrow QW when Bohr radius of the exciton (~5.5 nm for ZnCdTe and ~4 nm for ZnCdSe [7]) becomes comparable with well width. In case of the wide QW (9 nm, sample 207) the exciton binding energy is close to value 18 meV observed in the bulk ZnSe [5].

The numerical solution of combined equations (1–5) allows to calculate values E_{e1}, E_{hh1} and parameter Q_C using the experimental data from the CL and DLTS spectra without calculation of the built-in elastic strains. Observed such manner values Q_C are listed in

Table 2. Parameters of the deep levels detected by DLTS. E_t, N_t — activation energy and bulk concentration of the trap, $\sigma = \sigma_\infty \exp(\Delta E_b/kT)$ is the capture cross section, ΔE_b is the activation energy for capture of electrons, σ_∞ is the temperature independent prefactor of the capture cross-section.

Sample number	DLTS level	ΔE_t (eV)	Cross section, $\sigma_\infty \exp(\Delta E_b/kT)$ (cm^2)	N_t (cm^{-3})
195	$E1$	0.101±0.01	$6 \cdot 10^{-16}$	$3.3 \cdot 10^{15}$
	$E2$	0.58±0.02	$1.3 \cdot 10^{-16}$	$3.6 \cdot 10^{13}$
196	$E1$	0.133 ± 0.01	$2.6 \cdot 10^{-14}$	$2.6 \cdot 10^{15}$
	$E2$	0.58 ± 0.02	$3.4 \cdot 10^{-16}$	$3.4 \cdot 10^{13}$
197	$E1$	0.116 ± 0.01	$3.5 \cdot 10^{-14}$	$1.4 \cdot 10^{15}$
	$E2$	0.58 ± 0.02	$5 \cdot 10^{-16}$	$2.1 \cdot 10^{13}$
207	$E1$	0.155 ± 0.01	$2.8 \cdot 10^{-16}$	$1.8 \cdot 10^{15}$
	$E3$	0.72 ± 0.03	$8 \cdot 10^{-14}$	$3.5 \cdot 10^{13}$
209	$E1$	0.255 ± 0.015	$2.1 \cdot 10^{-15}$	$3.2 \cdot 10^{15}$
	$E3$	0.72 ± 0.03	$6.3 \cdot 10^{-14}$	$2 \cdot 10^{12}$
210	$E1$	0.140 ± 0.01	$5.4 \cdot 10^{-16}$	$6.1 \cdot 10^{14}$
	$E3$	0.72 ± 0.03	$5.6 \cdot 10^{-14}$	$8.7 \cdot 10^{12}$
211	$E1$	0.220 ± 0.015	$9 \cdot 10^{-16}$	$4.3 \cdot 10^{15}$
	$E3$	0.72 ± 0.03	$4.1 \cdot 10^{-14}$	$3.6 \cdot 10^{12}$

Table 1. We have found that $Q_C \approx 0.82$ for ZnTe/$Zn_{1-x}Cd_xTe$ structures at cadmium concentration of 0.2–0.22 in the QW and $Q_C = 0.66$ as an average value for ZnSe/$Zn_{1-x}Cd_xSe$ structures with $x = 0.2$–0.37.

4. Conclusion

Thus, in this work the signal caused by electrons emission from the ground quantified level in the conduction band ZnCdTe/ZnTe and ZnSe/ZnCdSe SQW structures was found by DLTS method. Activation energy of this level correlates with the energy standing of the QW emission line on CL spectra. The calculation procedure of the conduction band offset parameter Q_C based on experimental data from DLTS and CL at known QW width is offered.

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