ABSORPTION AND PHOTOLUMINESCENCE OF ZnSe/Zn$_x$Cd$_{1-x}$Se SUPERLATTICES AND QUANTUM WELLS UNDER HYDROSTATIC PRESSURE

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We present absorption measurements of a pseudomorphic Zn$_{0.75}$Cd$_{0.25}$Se/ZnSe superlattice and a Zn$_{0.91}$Cd$_{0.09}$Se/ZnSe single quantum well under high hydrostatic pressure applied by a diamond anvil cell. Excitonic transitions as 1s-heavy hole and 1s-light hole between the first bound states or minibands as well as transitions in the buffer material are visible. Transition energies are well understood by calculations of the band structure near Γ. The observed energy distance between photoluminescence and hh-absorption signal gives information on exciton localization. Whereas this distance is nearly pressure independent in the buffer, there is a significant increase at pressures $P > 5$ GPa for quantum structures.

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1. Samples and experimental set up

The presented structures were grown on (001)-GaAs substrates by MBE. A Zn$_{0.75}$Cd$_{0.25}$Se/ZnSe superlattice (SL) (10 ZnCdSe-wells, $d_w = 1.4$ nm, separated by ZnSe, $d_b = 3.3$ nm) was prepared on a 600 nm ZnSe-buffer. The single quantum well (SQW), $d_w = 10$ nm, is embedded in ZnSe. It was grown on a 500 nm ZnS$_{0.05}$Se$_{0.95}$ layer, which is unstrained on GaAs. The thickness of both structures was kept below the critical thickness to avoid plastic relaxation. The substrate was selectively etched off by a mixture of 82% NaOH and 18% H$_2$O$_2$ (30%). For high pressure measurements at 2 K we used a gasketed Syassen–Holzapfel-type diamond anvil cell (DAC) with liquid helium as pressure transmitting medium and ruby fluorescence for pressure calibration.

2. Optical transition energies: simple calculations

2.1. Strain effects on the band structure

First the hydrostatic and biaxial strain (ε_{hyd}, ε_{bi}) of each layer i with thickness d^i of a quantum structure was calculated at a given hydrostatic pressure P. In order to derive ε_{hyd} from P we used the well-known Murnaghan equation

$$\varepsilon_{hyd} = \left(1 + \frac{B_0'}{B_0}P\right)^{-1/(3B_0')} - 1. \tag{1}$$

The bulk module $B_0 + PB_0'$ of ternary compounds was linearly interpolated from binary compounds (Table). Under pure hydrostatic pressure the isotropic lattice constant is given by $a_{hyd}^i = a_0(1 + \varepsilon_{hyd})$. The biaxial strain of each layer i is given by

$$\varepsilon_{bi}^i = \frac{\bar{a} - a_{hyd}^i}{a_{hyd}^i}, \tag{2}$$

where $\bar{a} = \sum_i a_{hyd}^i d^i$ an averaged lattice constant. If samples are etched off the substrate, $\bar{a}$ is close to the isotropic lattice constant of the buffer. The strain-dependent energy shift of valence and conduction band energies at the Γ-point in the (001)--plane were calculated by Pollak [1]

$$E_{cb} = E_0 + \delta E_{cb},$$

$$E_{vb}^{hh} = \delta E_{vb} + \delta E_s,$$

$$E_{vb}^{lh} = \delta E_{vb} - \frac{1}{2}(\Delta_0 - \delta E_s) + \frac{1}{2}\sqrt{\Delta_0^2 + 2\Delta_0\delta E_s + 9\delta E_s^2} \tag{3}$$

with the abbreviations

$$\delta E_{cb/vb} = a_{c/v}\left[3\varepsilon_{hyd} + \left(2 - \frac{2C_{12}}{C_{11}}\right)\varepsilon_{bi}\right], \qquad \delta E_s = -b\left(1 + \frac{2C_{12}}{C_{11}}\right)\varepsilon_{bi}$$

with E_0 — gap energy; Δ_0 — split off energy; a_v, a_c, b — deformation potentials.

TABLE

Material parameters of cubic crystals ([†] derived from ZnSe, [‡] calculated, [*] at 2 K).

	a_0 [Å][*]	C_{11} [GPa]	C_{12} [GPa]	E_0 [eV][*]	Δ_0 [meV][*]	a [eV]
ZnSe	5.6596 [10]	85.9 [3]	50.6 [3]	2.8234 [2]	432 [2]	−4.9 [2]
CdSe	6.0672	66.7 [11]	46.3 [11]	1.757 [2]	410 [2]	−2.7 [2]

	b [eV]	a_v [eV]	m_c/m	γ_1	γ_2	B_0 [GPa]	B_0'
ZnSe	−1.14 [2]	−1.0 [12]	0.145 [13]	2.45 [13]	0.61 [13]	62.4 [3]	4.77 [3]
CdSe	−0.65[†]	−0.6[†]	0.12[‡][14]	3.33[‡] [14]	1.11[‡] [14]	53 [11]	4.77[†]

For ternary compounds linear interpolations of binary parameters were used; bowing of E_0 was taken into account ($b_{E_0} = 0.35$ [2]). However, the elastic moduli C_{11} and C_{12} show a weak pressure dependence which is known for ZnSe to be $\partial C_{11}/\partial P = 4.44$ and $\partial C_{12}/\partial P = 4.93$ [3]. These values are used for all compositions.

A pressure dependence of b of ZnSe, reported by Rockwell et al. [4] was not taken into account, for this increases the fitting error.

In order to derive the absolute band structure, the band offsets of Zn$_x$Cd$_{1-x}$Se/ZnSe at room pressure must be known. From the observed transitions $n_{cb} = 1 \rightarrow n_{vb} = 1$ it is not possible to obtain band offsets. Therefore we used results of photoreflection measurements on single quantum wells, which yield $\Delta E_{cb}(Zn_xCd_{1-x}Se/ZnSe) = 75, 200$ meV at $x = 0.91, 0.75$, respectively [5].

2.2. Bound states, minibands

Bound energy states E_n in uncoupled type-I single quantum wells are well known [6]. In superlattices these states are broadened to "minibands". Their energies E_n are given by the solutions of the dispersion relation (zero energy at the bottom of the well) [6]

$$\left| -\frac{1}{2}\left(\tilde{\xi} - \frac{1}{\tilde{\xi}}\right)\sin(k_w d_w)\sinh(\kappa_b d_b) + \cos(k_w d_w)\cosh(\kappa_b d_b) \right| \leq 1 \qquad (4)$$

with $\Delta E_{cb/vb}$ — band offset of cb or vb; $m_{eff,b/w}$ effective masses;

$$\tilde{\xi} = \frac{k_w}{\kappa_b}\frac{m_{eff,b}}{m_{eff,w}}; \qquad k_{w,n} = \sqrt{\frac{2m_{eff,w}E_n}{\hbar^2}}, \quad \kappa_{b,n} = \sqrt{\frac{2m_{eff,b}(\Delta E_{cb/vb} - E_n)}{\hbar^2}},$$

where b and w denote barrier and well parameters. Electronic transitions have excitonic character. An increase in the excitonic binding energy R under pressure is caused by a change of the effective masses and the dielectric constant ε_{stat} [7]. Furthermore the confinement changes under pressure. In this work we used an analytical model by Mathieu et al. [8] for confined excitons.

3. Experimental results and discussion

Both samples have been investigated at pressures up to 10 GPa. Absorption spectra at different pressures are shown in Figs. 1a, 2a. The hh- and lh-absorption signals show a large splitting due to biaxial strain. Under the present experimental conditions an additional biaxial strain in the (001)-plane was observed due to freezing of helium in the DAC. Therefore a separation of buffer-hh and -lh is visible, too. This was taken into account in the calculations. Figure 1b shows the measured and calculated pressure shift of all SL absorption peaks. The calculations fit well to both experimental data sets and to a Zn$_{0.82}$Cd$_{0.18}$Se/ZnSe SL, presented in Ref. [9], but it is not very sensitive to variation of the band offset. Some parameters of cubic CdSe were not available and had to be extrapolated (see Table).

In the SQW absorption the lh-signal is vanishing at pressures $P > 6.2$ GPa. At those pressures calculations for the SQW give — in contrast to the SL — a lh band offset, which is zero or negative (Fig. 2b). This is due to additional strain caused by the ZnSSe-layer. Although the calculations are sensitive to the material parameters, they may give an explanation for this effect.

Figure 1a also shows luminescence spectra of the SL. A comparison of the energies of hh-absorption and luminescence gives information on exciton localization at impurities and lattice dislocations. There is a constant energy shift of
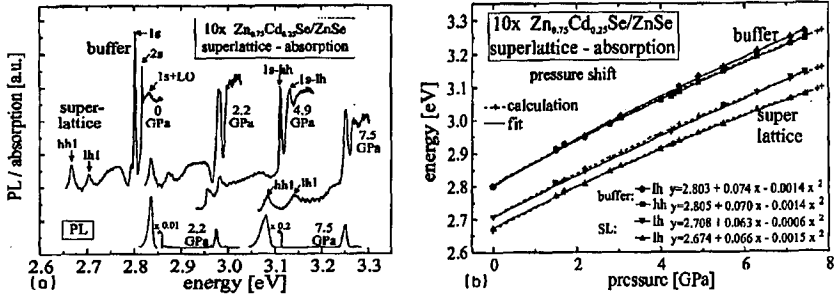
Fig. 1. Absorption and photoluminescence of the superlattice. In absorption hh1- and lh1-transitions are visible up to 9 GPa (a). Experimental and calculated pressure dependence of the hh1- and lh1-absorption of the superlattice (b).
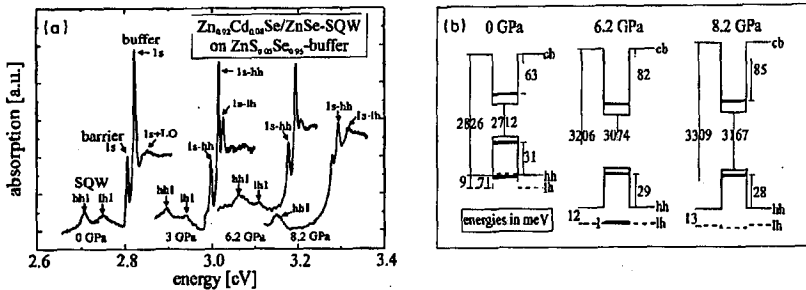

Fig. 2. Absorption spectra of the single quantum well. The lh1-absorption disapears at pressures $P > 6.2$ GPa (a). Calculated band structure, with an additional strain built-up in the ZnSSe-buffer the lh-band offset becomes negative at high pressures (b).

about 5 meV in the buffer, which is due to chlorine donors, whereas in the quantum structures there is a significant shift from about 6 up to 12 meV at pressures $P > 5$ GPa. In the same pressure range there is also an increase in the FWHM of absorption and of the PL-signal, which may be due to lattice defects in the quantum structures.

Acknowledgments

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