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Effect of structural imperfections on luminescence of ZnCdSe/ZnSe quantum wells

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Abstract

The structural and luminescence properties of $Zn_{1-x}Cd_xSe$/ZnSe multi-quantum well (MQW) structures with high molar fraction of cadmium (30–50%) and wide ZnSe barriers (50, 100 and 500 nm) grown by molecular beam epitaxy (MBE) have been investigated by high-resolution X-ray diffraction (HRXRD) and photoluminescence (PL) methods. It is shown that the fluctuations of composition within the quantum well layer determine the full-width at half maximum (FWHM) of the QW photoluminescence peak. The unusual polarization characteristics of this photoluminescence have been observed. The emission peak in the edge geometry is strongly polarized perpendicularly to the QW plane. This effect is ascribed to the localization of the ground-state heavy-hole-like excitons in the regions with increased cadmium content.

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1. Introduction

The deviation from stoichiometry is typical for II–VI compounds. In the crystals of Cd-containing compounds there are many interstitial cadmium atoms in the crystal lattice. These defects are mobile even at room temperature [1]. The Cd_i atoms can form clusters or complexes with other point defects. As a result electric, photoelectric and luminescent material characteristics are changed [1]. Cd segregation influences the processes of nano-island formation in ZnCdSe/ZnSe heterostructures [2] that are promising for the fabrication of visible light-emitting devices. Cd segregation is undesirable for quantum wells (QWs) because it causes the fluctuations in their composition. In the present work the influence of the composition fluctuations on luminescence characteristics of $Zn_{1-x}Cd_xSe$/ZnSe multi-quantum well (MQW) heterostructures has been investigated using high-resolution X-ray diffraction (HRXRD) and photoluminescence (PL).

2. Experimental procedure

The structures were grown on the semi-insulating (1 0 0) GaAs substrates by molecular beam epitaxy (MBE) at VI/II group beam pressure ratio of 2:1. The growth temperature was 280–320 °C. The growth characteristics of ZnSe and $Zn_{1-x}Cd_xSe$ layers were monitored in situ by reflection high-energy electron diffraction. All the structures were grown on a 1 μm thick ZnSe buffer layer and capped by a 30 nm ZnSe layer. The MQW structures included the periodical sequences of 4, 15 or 30 $Zn_{1-x}Cd_xSe$ QWs separated by ZnSe barriers with the thicknesses of 500, 100 or 50 nm, respectively. The QW thickness was varied from 4 to 6 nm and

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the molar fraction x of cadmium in $Zn_{1-x}Cd_xSe$ QWs was changed from 0.3 to 0.5 in different samples. More precise information about the QW thickness and composition was obtained from the simulation of (0 0 4) diffraction profiles.

The X-ray diffraction measurements were carried out using HRXRD (Philips MRD) with the 4× Ge (2 2 0) monochromator and standard Cu anode. The PL spectra were measured at 4.2–300 K under excitation of the 337 nm line of a N_2-laser. The PL emission was detected both from the surface of the structure (surface emission mode) and from the cleaved edge of the sample (edge emission mode).

3. Experimental results and discussion

Fig. 1 shows the (0 0 4) diffraction profiles of the $Zn_{0.51}Cd_{0.49}Se$/ZnSe MQW structure (sample A, Table 1). The signal of the ZnSe layers as well as the broad and modulated peak of QWs are observed on the low angle side of the intense substrate Bragg peak. The measured $\omega/2\theta$-scans are evaluated using simulations based on semi-dynamical diffraction theory. Fig. 1 demonstrates the satisfactory correlation between the measured (solid) and simulated (dotted) curves. The structural parameters of the sample, estimated using the HRXRD curves, are presented in Table 1. It is known that $Zn_{1-x}Cd_xSe$ QW must be compressively stressed. This in-plane stress is observed at any x because the lattice constant of a zinc blende CdSe is larger than that of ZnSe. The simulation of diffraction profiles confirms the presence of the stress. The deformations perpendicular to the epilayer interface are defined as $e_\perp = (d_\perp^L - d_S)/d_S$, where d_S and $d_\perp^L$ are the lattice parameters of the substrate and of the heteroepitaxial layer, respectively. The determined values of deformations in the direction perpendicular to the interface for the QWs and ZnSe barriers are given in Table 1.

The simulation of the $\omega/2\theta$-scans reveals an asymmetry of the first order satellites. It indicates the presence of fluctuations of the QW thickness and/or composition between different QWs or/and within the same QW. The calculations show that the largest possible fluctuations of layer thickness or cadmium molar fraction in QWs, that can cause this asymmetry, are 0.5–0.6 nm or 3–5%, respectively. The broadening of the superlattice satellites in comparison with the simulated ones confirms the presence of point or extended defects within the QW layer.

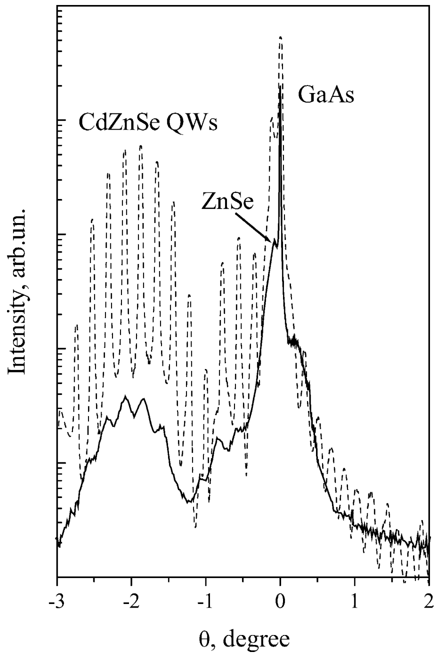

Fig. 1. Experimental (solid) and simulated (dashed) (0 0 4) $\omega/2\theta$-scans of the $Zn_{0.51}Cd_{0.49}Ze$/ZnSe MQW structure A.

Fig. 2 shows the PL spectra of the MQW structures measured in the surface emission mode at 4.2 K. Only the bands related to the QWs are present in all spectra. For all samples the intensity of MQW-related peak is practically the same and the full-width at half maximum (FWHM) varies from 20 to 30 meV. Such values of the FWHM can be caused by the presence of fluctuations of QW thickness and/or of QW composition. A simple calculation [3] indicates that to explain the observed broadening of MQW-related peak either the molar fraction of Cd in the QW should change by $\Delta x = 0.03$ or the QW thickness should vary within 1.5–3.5 nm. But X-ray diffraction data show that the fluctuations of thickness do not exceed 0.5–0.6 nm. Therefore, the broadening of the PL peak is explained by the fluctuations of Cd molar fraction in different QWs or/and within the same QW. Since the PL spectrum of the sample C (Table 1) exhibits only the emission from the upper QW (due to the large thickness of ZnSe barriers), at least for this sample, the fluctuations of Cd within the same QW in fact take place. It agrees with the tendency of Cd segregation observed in Cd-containing II–VI compounds [4].

Table 1
Some parameters and characteristics of the samples obtained by HRXRD and PL measurements of $Zn_{1-x}Cd_xZe$/ZnSe MQW structures

Sample	A	B	C
Number of QWs	30	15	4
Thickness of ZnSe barriers, (nm)	50	100	500
Thickness of $Zn_{1-x}Cd_xSe$ QWs, (nm)	4	5	6
Molar fraction x of Cd in $Zn_{1-x}Cd_xSe$ QWs	0.49	0.31	0.41
Deformations in ZnSe layers, perpendicular to the QW plane	3.87×10^{-3}	2.177×10^{-3}	2.7×10^{-3}
Deformations in $Zn_{1-x}Cd_xSe$ layers, perpendicular to the QW plane	4.918×10^{-2}	3.31×10^{-2}	4.1×10^{-2}
PL maximum position at 4.2 K, (eV)	2.258	2.538	2.366

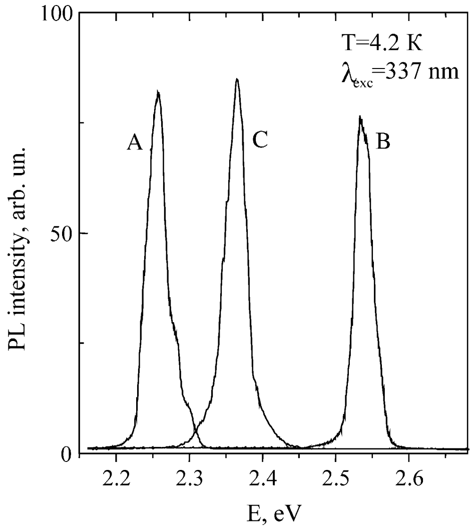

Fig. 2. Photoluminescence spectra of $Zn_{1-x}Cd_xSe$/ZnSe MQW structures A, B and C ($T = 4.2$ K, $\lambda_{exc} = 337$ nm).

It is known that in the strained zinc blende QW the valence band splits and the heavy hole (HH) and light hole (LH) sub bands are formed. Because of the in-plane compressive stress in $Zn_{1-x}Cd_xSe$/ZnSe QWs the lowest energy PL peak should correspond to the radiative recombination of the ground-state HH exciton. Different linear polarization dependencies should be observed for the HH- and LH-related transitions in the edge emission spectra. The HH-related transition is allowed only for the polarization in the QW plane ($E_{\parallel}$ polarization), while the LH related transition is allowed both in the QW plane and in the perpendicular direction ($E_{\perp}$ polarization). Fig. 3 shows the PL spectra of the sample C measured in the surface (curve 1) and the edge (curve 2) emission modes at 77 K at low excitation densities. It has been found that for all structures the edge emission peak is strongly $E_{\perp}$ polarized. The ratio of the intensity of the edge emission peak in the $E_{\perp}$ to the $E_{\parallel}$ polarization varies from 1.1:1 to 2:1 for different samples.

Strong $E_{\perp}$ polarization of the peak dominant in the surface emission spectra is very unusual because it contradicts the selection rules for the HH-related transitions in QW. A similar situation has been observed in GaAs/AlAs short-period superlattices [5], where the dominating PL peak demonstrates the mixed hole sub band polarization in the edge geometry. The polarization properties of this emission were explained [5] by the mixing of the HH and LH states belonging to the wells of different sizes when the HH state of the narrower well is mixed with the LH state of the wider well. In our case such a situation can be realized only if the energy splitting of the HH and LH bands in all samples is of the order of the PL peak FWHM, which is impossible due to the high stress in the QW layer.

The possible reason of the change of polarization characteristics can be the presence of defects (fluctuations of QW composition and thickness, extended defects, etc.) in the QW [6,7]. These defects can produce additional electrical and deformation fields or confinement. We suppose that in our structures the fluctuations of QW composition are responsible for the observed effect. Localization of excitons in QW regions with higher Cd content would reduce k-quantization effect in the growth direction. These regions can be considered as the precursors of quantum dots embedded in the QW [8]. The specific feature of our samples is the high Cd molar fraction in QWs (from 30 to 50%). It can result in a noticeable disorder, stress and increase of non stoichiometric cadmium in QWs that can stimulate the processes of formation of Cd-enriched regions.

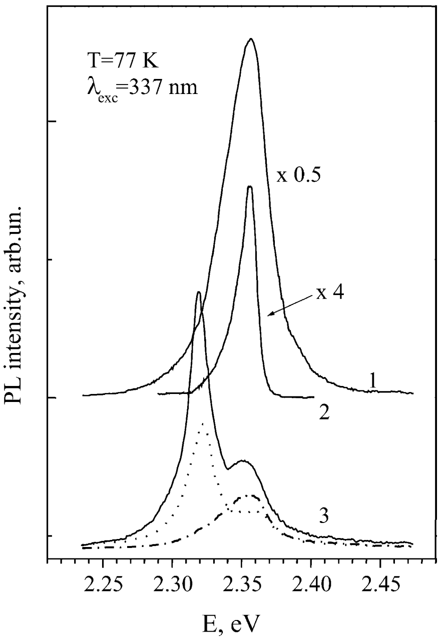

Fig. 3. Surface (curve 1) and edge (curves 2, 3) photoluminescence spectra of the $Zn_{0.59}Cd_{0.41}Ze$/ZnSe MQW structure C at low (curve 2) and high (curves 1, 3) excitation power ($T = 77$ K, $\lambda_{exc} = 337$ nm). Dashed and dashed–dotted curves correspond to the emission band presented in curve 3 polarized in the QW plane and in perpendicular direction, respectively.

It should be noted that at higher excitation power a new additional intense peak shifted by 10–30 meV towards the low energies appears in the edge emission spectra (Fig. 3, curve 3). It is strongly polarized in $E_{\parallel}$ direction. The intensity of this peak increases superlinearly with the rise of the excitation power. At high excitation level this peak predominates in the edge emission spectra and its intensity exceeds the intensity of the surface PL. These facts indicate that this peak corresponds to superluminescence. Its strong $E_{\parallel}$ polarization can be understood in view of the stronger amplification of the $E_{\parallel}$ mode by the waveguide.

4. Conclusions

The structural and luminescence properties of $Zn_{1-x}Cd_xSe$/ZnSe MQW structures with high molar fraction of cadmium (30–50%) have been investigated by HRXRD and photoluminescence methods. Some parameters of the structures studied have been obtained from the simulations of the (0 0 4) diffraction profiles. It is found that the fluctuations of cadmium up to 3% take place within the QW layers. Localization of the ground-state heavy-hole-like excitons in such regions is suggested as the reason for strong $E_\perp$ polarization of the edge emission spectra.

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