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Rapid Research Note

Temperature dependence of the energy gap of $Mg_xZn_yCd_{1-x-y}Se$ alloy

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The temperature dependence of the energy gap of $Mg_xZn_yCd_{1-x-y}Se$ ($x \sim 0.5$) and $Zn_{0.5}Cd_{0.5}Se$ alloys was determined from reflectivity measurements at temperatures between 4.2 and 300 K. The data were fitted to a Bose–Einstein type relationship and temperature dependence of band gaps was compared. A similar temperature dependence of band gap was observed indicating that quantum confinement in the $Mg_xZn_yCd_{1-x-y}Se/Zn_{0.5}Cd_{0.5}Se$ quantum wells did not depend on temperature.

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1 Introduction The quaternary $Mg_xZn_yCd_{1-x-y}Se$ alloy is a promising material for the fabrication of full color light emitting and laser diodes (LEDs and LDs). $Mg_xZn_yCd_{1-x-y}Se$ based red, green, and blue LEDs [1, 2], current injected LDs (operating at liquid nitrogen temperature) [3], and optically pumped lasers [4] were demonstrated. These light emitting devices are usually grown by molecular beam epitaxy (MBE) on InP substrates (metal organic vapor-phase epitaxy of $Mg_xZn_yCd_{1-x-y}Se$ was also reported [5]) and consist of a $Zn_{0.5}Cd_{0.5}Se$ quantum well (QW) layer ($E_g \sim 2.15$ eV) and $Mg_xZn_yCd_{1-x-y}Se$ barrier layers ($E_g \sim 3.0$ eV, $x \sim 0.5$). However, in spite of a significant progress achieved, no current injected LDs operating at room temperature were reported so far. Also, a significant increase in the threshold pumping intensity with the rise in temperature was observed for the optically pumped lasers due to the leakage of electrons from the well to the barriers, indicating insufficient quantum confinement [6]. It was suggested that the quantum confinement can be improved either by increasing the band gap of the barrier layers or by using artificial "multi-quantum barriers". To optimize the electronic structure of the active area, it is important to know the dependence of band gap energy on temperature. Temperature band gap variation of $Zn_{0.5}Cd_{0.5}Se$ was studied by photoluminescence (PL) spectroscopy [7]. Studies of $Mg_xZn_yCd_{1-x-y}Se$ showed that the PL emission was dominated by the localized excitons and did not follow the band gap [8]. Thus, the temperature band gap variation of $Mg_xZn_yCd_{1-x-y}Se$ is unknown.

We report the use of PL and reflectivity spectroscopies to study the temperature band gap variation of $Mg_xZn_yCd_{1-x-y}Se$ ($x \sim 0.5$). The temperature dependence of the band gap energy is determined from reflectivity spectra and modelled by a Bose–Einstein type Eq. [9]. It is observed that temperature dependence of the $Mg_xZn_yCd_{1-x-y}Se$ band gap is similar to that of $Zn_{0.5}Cd_{0.5}Se$. Thus, quantum confinement does not significantly change as a function of temperature in the $Mg_xZn_yCd_{1-x-y}Se/Zn_{0.5}Cd_{0.5}Se$ QWs, simplifying the design of the active region of the light emitting devices.

2 Experimental details All of the samples were grown by MBE on semi-insulating InP (100) substrates under the growth conditions described elsewhere [1]. The composition of the ternary $Zn_xCd_{1-x}Se$

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alloy was calculated from the lattice constant measured by X-ray diffraction, assuming a linear dependence of lattice constant on the alloy composition (Vegard's law). The composition of the quaternary $Mg_xZn_yCd_{1-x-y}Se$ alloy was determined by the combination of lattice constant and band gap energy data [10]. PL measurements were performed in a liquid He continuous flow cryostat in the temperature range from 4.2 K to 300 K. Excitation was provided by the 325 nm line of a He–Cd laser. The collected PL was spectrally resolved by a monochromator and detected by a cooled charge coupled device array detector. Reflectivity measurements were performed in the same cryostat using a 200 W Hg lamp.

3 Results and discussion PL and reflectivity spectra at 4.2 K for the samples grown are shown in Fig. 1 by the solid and dotted lines, respectively. In order to elucidate the origin of the emission lines, the dependence of the emission on the excitation laser intensity was studied (not shown). The excitation laser intensity was varied over three orders of magnitude and a linear dependence of the PL emission with a slope near unity was obtained. Also, no shift of the emission energy as a function of the excitation laser density was observed. This behavior is consistent with the excitonic origin of the $Mg_xZn_yCd_{1-x-y}Se$ emission [11]. The quenching of Fabry–Perot oscillations in the reflectivity spectrum corresponds to the onset of interband absorption and is used to identify position of the $\Gamma \rightarrow \Gamma$ direct band gap with an uncertainty of ~6 meV. An increase in the Stokes shift, given by the difference in the energies of absorption edge and emission line, from ~10 meV for $Zn_{0.5}Cd_{0.5}Se$ to ~90 meV for $Mg_{0.54}Zn_{0.26}Cd_{0.2}Se$ is evident.

A significant Stokes shift observed for $Mg_xZn_yCd_{1-x-y}Se$ indicates that localized exciton emission dominates the spectra. When studied as a function of temperature, the emission energy did not follow the band gap and exhibited a characteristic 'S-shaped' behavior (decrease–increase–decrease) due to the ionization of localized excitons to free excitons [8].

The temperature dependence of the direct band gap was studied by reflectivity measurements. The data are shown by symbols in Fig. 2. As the temperature increases, the critical point exhibits a red shift due to the decrease in the band gap energy caused by the electron–phonon interactions and lattice dilation. The data are fitted to the equation proposed by Viña et al. (solid lines) [9]:

$$E_{BE}(T) = E(0) - 2a_B/(\exp(\theta/T) - 1)\,, \tag{1}$$

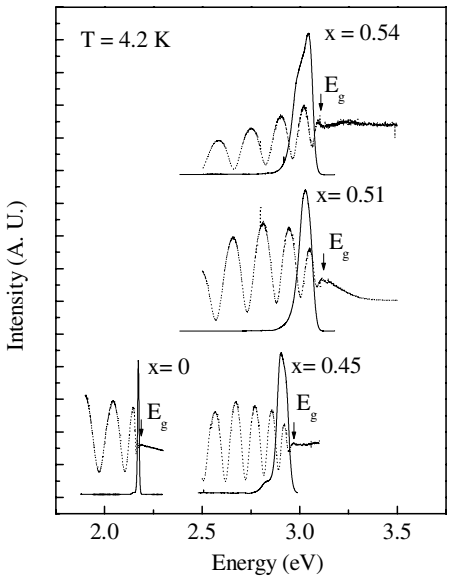

Fig. 1 Photoluminescence (solid lines) and reflectivity (dotted lines) spectra for $Mg_xZn_yCd_{1-x-y}Se$ epilayers.

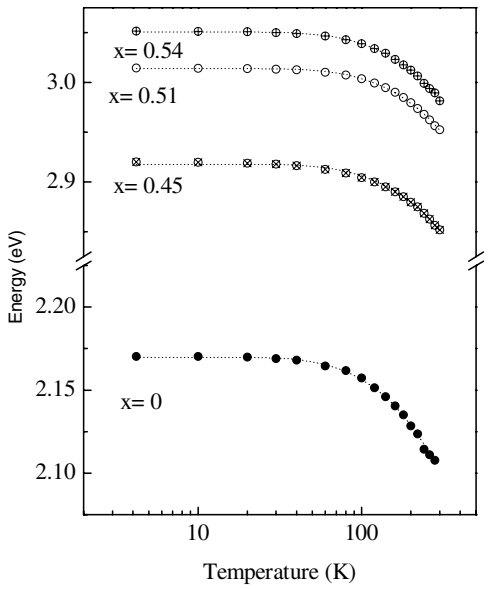

Fig. 2 Temperature dependence of the $Mg_xZn_yCd_{1-x-y}Se$ band gap energy. Symbols are experimental data. The dotted lines are theoretical fits to the Bose–Einstein type equation.

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Table 1 Parameters obtained by modelling the temperature dependence of band gap energy to the Bose–Einstein type equation.

alloy	$E(0)$ (eV)	a_B (meV)	θ (K)	dE/dT (meV/K)
$Zn_{0.5}Cd_{0.5}Se$	2.170	22 ± 2	146 ± 13	0.30
$Mg_{0.45}Zn_{0.3}Cd_{0.25}Se$	2.918	25 ± 2	167 ± 5	0.30
$Mg_{0.51}Zn_{0.28}Cd_{0.21}Se$	3.014	26 ± 2	184 ± 8	0.28
$Mg_{0.54}Zn_{0.27}Cd_{0.19}Se$	3.051	25 ± 2	169 ± 8	0.31

where $E(0)$ is the energy of the transition at 0 K, a_B represents the strength of the electron–average phonon interaction, and θ corresponds to the average phonon temperature. The band gap shift is proportional to the sum of the Bose–Einstein statistical factors for phonon emission and absorption. Fitting parameters are summarized in Table 1. From comparison, it is evident that electron–phonon interaction constant and average phonon temperatures of $Mg_xZn_yCd_{1-x-y}Se$ are either very similar or slightly higher than that of $Zn_{0.5}Cd_{0.5}Se$. (The difference is close to the experimental error.)

At the high temperature limit, Eq. (1) reduces to

$$E_{BE}(T) = E(0) - 2a_BT/\theta \tag{2}$$

and the temperature band gap variation (dE/dT) is proportional to $-2a_B/\theta$ (Table 1). The temperature dependence of the $Mg_xZn_yCd_{1-x-y}Se$ band gap is similar to that of $Zn_{0.5}Cd_{0.5}Se$. This is unlike to a more widely studied ZnS_xSe_{1-x}–$Zn_yCd_{1-y}Se$ material system, where the band gap of ZnS_xSe_{1-x} reduces faster than that of $Zn_yCd_{1-y}Se$. Study of $ZnS_xSe_{1-x}/Zn_yCd_{1-y}Se$ QW structures demonstrated a decrease of the quantum confinement at higher temperatures that induced a leakage of carriers from the well to the barriers quenching the emission [12]. The thermal effect is expected to be smaller for $Mg_xZn_yCd_{1-x-y}Se/Zn_{0.5}Cd_{0.5}Se$ QW structures due to the stability of quantum confinement.

4 Conclusion In conclusion, $Mg_xZn_yCd_{1-x-y}Se$ alloys ($0 < x < 0.5$) were grown and their band gap was studied as a function of temperature. The temperature dependence of the band gap was measured and the data were fitted to the Bose–Einstein type equation. The band gap variation of $Mg_xZn_yCd_{1-x-y}Se$ ($x \sim 0.5$) was similar to that of $Zn_{0.5}Cd_{0.5}Se$. Therefore, temperature-independent quantum confinement is expected in $Mg_xZn_yCd_{1-x-y}Se/Zn_{0.5}Cd_{0.5}Se$ QW structures.

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