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Effect of c -axis inclination angle on the properties of ZnO/Zn_{1-x}Cd_xO/ZnO quantum wells

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Abstract

The development of optoelectronic devices based on highly-promising Zn_{1-x}Cd_xO semiconductor system demands deep understanding of the properties of the Zn_{1-x}Cd_xO-based quantum wells (QWs). In this regard, we carried out a numerical study of the polarization-related effects in polar, semi-polar and non-polar ZnO/Zn_{1-x}Cd_xO/ZnO QWs with different parameters of the quantum well structure. The effects of well width, barrier thickness, cadmium content in the active layer and c -axis inclination angle on the distribution of the electron and hole wavefunction and transition energy were investigated using the 6×6 $\mathbf{k}\cdot\mathbf{p}$ Hamiltonian and one-dimensional self-consistent solutions of nonlinear Schrödinger–Poisson equations with consideration of spatially varying dielectric constant and effective mass. The strong sensitivity of the internal electric field, transition energy and overlap integral to cadmium content and well thickness in the angle range from 0 to 40° was revealed. An unexpected change of the internal electric field's sign was observed at the angles ranging from 70 to 90°. We also found a difference in the electronic properties between (0001)-, (11 $\bar{2}2$)- and (10 $\bar{1}0$)-oriented QWs.

Key words: inclination angle, quantum well, polarization, ZnCdO alloy, transition energy

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1. Introduction

Zn_{1-x}Cd_xO ternary alloy, composed of zinc and cadmium oxides, at present is a much studied semiconductor system in optoelectronics [1-8]. It possesses many

similar properties to the commercialized $\text{In}_x\text{Ga}_{1-x}\text{N}$ solid solution [9-12] and can have a huge potential for light-emission diodes (LED) applications [13]. Among the most important properties of $\text{Zn}_{1-x}\text{Cd}_x\text{O}$ one can note the tunable band-gap energy (from 3.26 to 2.88 eV) [14], high exciton localization energy (~ 160 meV) [15] and the isoelectronic nature of cadmium for zinc substitution in the cation sublattice [16]. Taking into account the above-mentioned, the strong attempts to grow $\text{Zn}_{1-x}\text{Cd}_x\text{O}$ -based quantum wells – key elements for designing the LEDs – don't seem to be surprising [17-19]. Nevertheless, there are some obstacles blocking the full-scale use of $\text{ZnO}/\text{Zn}_{1-x}\text{Cd}_x\text{O}/\text{ZnO}$ QWs for optoelectronics' needs. Until now, all investigations have been mainly focused on $\text{Zn}_{1-x}\text{Cd}_x\text{O}$ -based QWs with polar c -plane crystal orientation, for which some progress has been obtained [20-22]. However, the $\text{ZnO}/\text{Zn}_{1-x}\text{Cd}_x\text{O}/\text{ZnO}$ QWs grown on polar planes suffer from the quantum confined Stark effect (QCSE), resulting from the polarization-induced built-in internal electric field that restricts the efficiency of devices [15]. This issue can be completely neutralized by means of growing $\text{ZnO}/\text{Zn}_{1-x}\text{Cd}_x\text{O}/\text{ZnO}$ QWs on substrates with non-polar orientations, where the polar c -axis is parallel to the growth plane (for example $(10\bar{1}0)$ m -plane and/or $(11\bar{2}0)$ a -plane) [23]. It is significant to note that the QWs grown on non-polar planes can have non-tilted conduction and valence band edge profiles (CBEP and VBEP, respectively), preventing a spatial separation of electron and hole wave functions [24]. The deposition of $\text{Zn}_{1-x}\text{Cd}_x\text{O}$ layers onto non-polar planes, none the less, can have its own bottleneck, since the film growth on foreign substrates (generally m -sapphire) is accompanied by the appearance of a great number of 2D-defects and surface imperfections. Additionally, the stress relaxation mechanism in the case of a non-polar plane seems to be very complicated for clear understanding. On the other hand, there is an additional possibility to neutralize the polarization-induced field effect. It is related to the use of the semi-polar substrate orientations [23]. It is rather interesting to note that one of the biggest benefits of the semi-polar crystal orientation is that the combined effect of spontaneous and strain-induced polarization significantly suppresses the internal electric field for peculiar

orientations of the growth plane [25]. Furthermore, the semi-polar growth orientations possess a strong advantage over non-polar and polar planes, since the stress relaxation mechanism in semi-polar structures is associated with dislocation glide on a single slip plane [25]. In other words, semi-polar layers are characterized by only one unique (0001) basal plane, and its inclination angle is dependent on the growth orientation.

Despite a lot of papers devoted to the $\text{Zn}_{1-x}\text{Cd}_x\text{O}$ -based QWs study, many fundamental crystal orientation effects on quantum well properties are still not well understood. By virtue of strong dependence of the properties of QWs on the crystal inclination angle (as was already observed for InGaN/GaN QWs [26]), the theoretical study of the crystal orientation effect on the polarization field, transition energy and overlapping of the electron and hole wavefunctions has a tremendous meaning not only from a fundamental point of view, but also for practical applications.

The present work analyzes the impact of the crystal plane angle on the properties of the $\text{Zn}_{1-x}\text{Cd}_x\text{O}$ -based QWs. The study is carried out by self-consistently solving the Schrödinger and Poisson equations with consideration of the spontaneous and piezoelectric polarizations, dielectric mismatch and spatially varying effective electron mass.

2. Theoretical approach

Our study of the orientation dependence of the polarization-related effects in $\text{ZnO}/\text{Zn}_{1-x}\text{Cd}_x\text{O}/\text{ZnO}$ QWs started from the conversion of the ordinary coordinate system (x, y, z) into a new one (x', y', z') using a rotation matrix $R_y(\theta)$. Figure 1a illustrates both coordinate systems used in our calculations. The basic rotation matrix, which rotates vectors by angle θ – the angle between the growth direction z' in the new coordinate system and the z axis in the old one – can be written as

$$R_y(\theta) = \begin{bmatrix} \cos \theta & 0 & \sin \theta \\ 0 & 1 & 0 \\ -\sin \theta & 0 & \cos \theta \end{bmatrix} \quad (1)$$

Therefore, the conventional coordinates are related to the transformed coordinates via rotation matrix as

$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} = R_y(\theta) \begin{pmatrix} x \\ y \\ z \end{pmatrix} \quad (2)$$

It should be mentioned that the angle $\theta=0^\circ$ corresponds to the polar (0001) growth direction, $\theta=58.057^\circ$ is related the semipolar (11 $\bar{2}2$) plane and $\theta=90^\circ$ is associated with the non-polar (10 $\bar{1}0$) *m*-plane (see Fig. 1b-d).

Fig. 1. (a) Configuration of the converted coordinate system (x' , y' , z'). z' axis is normal to the substrate surface. The coordinate system (x , y , z) denotes the primary

crystallographic axes. Illustration of the (b) polar c -plane, (c) semipolar $(11\bar{2}2)$ plane and (d) non-polar m -plane in $\text{Zn}_{1-x}\text{Cd}_x\text{O}$.

Using the Eq. 1 and 2 one can calculate the dependence of the polarization-induced electric field. In the case of a $\text{Zn}_{1-x}\text{Cd}_x\text{O}$ well layer sandwiched between two barrier layers of zinc oxide having wider band-gap energy, the total polarization in the QW system can be described as the sum of the spontaneous and piezoelectric polarization components:

$$P = P_i^{PE} + P^{SP} \quad (3)$$

Origin of the spontaneous polarization is related to the lack of inversion symmetry of the hexagonal crystal lattice and the characteristics of the ionic bonds between Zn (Cd) and O atoms, leading to a displacement of the electron charge clouds towards one of the atoms. It causes the appearance of net positive charge on one face of the crystal and net negative charge on the other face. Nature of the piezoelectric polarization is attributed to the strain caused by pseudomorphical growth between two lattice mismatched layers. Generally, by virtue of the symmetry of the space group $P6_3mc$ of wurtzitic $\text{Zn}_{1-x}\text{Cd}_x\text{O}$, the piezoelectric polarization in the (x, y, z) coordinates for a general crystal orientation is related to strains as [27]:

$$\begin{pmatrix} P_x^{PE} \\ P_y^{PE} \\ P_z^{PE} \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 & 0 & e_{15} & 0 \\ 0 & 0 & 0 & e_{15} & 0 & 0 \\ e_{31} & e_{31} & e_{33} & 0 & 0 & 0 \end{pmatrix} \cdot \begin{pmatrix} \varepsilon_{xx} \\ \varepsilon_{yy} \\ \varepsilon_{zz} \\ \varepsilon_{yz} \\ \varepsilon_{xz} \\ \varepsilon_{xy} \end{pmatrix} = \begin{pmatrix} e_{15}\varepsilon_{xz} \\ e_{15}\varepsilon_{yz} \\ e_{31}(\varepsilon_{xx} + \varepsilon_{yy}) + e_{33}\varepsilon_{zz} \end{pmatrix} \quad (4)$$

where e_{ij} are elements of piezoelectric tensor and ε_{kl} are strain tensor components. The components of the strain tensor ε_{kl} in the normal coordinate system can be represented as [27]:

$$\begin{cases} \varepsilon_{xx} = \varepsilon_{x'x'} \\ \varepsilon_{yy} = \varepsilon_{y'y'} \cos^2 \theta + \varepsilon_{z'z'} \sin^2 \theta + \varepsilon_{y'z'} \sin 2\theta \\ \varepsilon_{zz} = \varepsilon_{y'y'} \sin^2 \theta + \varepsilon_{z'z'} \cos^2 \theta - \varepsilon_{y'z'} \sin 2\theta \\ \varepsilon_{xz} = \frac{\varepsilon_{z'z'} - \varepsilon_{y'y'}}{2} \sin 2\theta + \varepsilon_{y'z'} \cos 2\theta \end{cases} \quad (5)$$

where $\varepsilon_{k'l'}$ are the components of the strain tensor in the converted coordinate system, which are calculated by using the algorithm presented in [27].

Substitution of (5) into (4) gives the following equation for strain-induced piezoelectric polarization in the new coordinates (x' , y' , z'):

$$\begin{aligned} P_{z'}^{PE} &= e_{31} \cos \theta \varepsilon_{x'x'} + \left(e_{31} \cos^3 \theta + \frac{e_{33} - e_{15}}{2} \sin \theta \sin 2\theta \right) \varepsilon_{y'y'} \\ &+ \left(\frac{e_{33} + e_{15}}{2} \sin \theta \sin 2\theta + e_{33} \cos^3 \theta \right) \varepsilon_{z'z'} \\ &+ [(e_{31} - e_{33}) \cos \theta \sin 2\theta + e_{15} \sin \theta \cos 2\theta] \varepsilon_{y'z'} \end{aligned} \quad (6)$$

The z' components of the total polarizations for the quantum well and the barrier layer are given by:

$$\begin{cases} P_{z'}^{QW} = (P_{sp}^{QW} - P_{sp}^b) \cos \theta + P_{z'}^{PE} \\ P_{z'}^b = P_{sp}^b \cos \theta \end{cases} \quad (7)$$

Electric fields in the well (F_{QW}) and the barrier (F_b) layer can be determined by the following equations [28]:

$$\begin{cases} F_{QW} = \frac{(P_{z'}^b - P_{z'}^{QW}) L_b}{\varepsilon_0 (\varepsilon_b L_{QW} + \varepsilon_{QW} L_b)} \\ F_b = \frac{(P_{z'}^{QW} - P_{z'}^b) L_{QW}}{\varepsilon_0 (\varepsilon_b L_{QW} + \varepsilon_{QW} L_b)} \end{cases} \quad (8)$$

where L_b is the barrier thickness, L_{QW} is the well width, $\varepsilon_{b,QW}$ is a dielectric constant of the material, ε_0 is the permittivity of free space ($\sim 8.854 \cdot 10^{-12}$ F/m)

We calculated the conduction and valence band structures of the quantum wells using a $k \cdot p$ approach. In order to know the electron (or hole) wavefunctions and confined energy levels in a quantum well one needs to solve the one-dimensional (1-D) Schrodinger equation for envelope wavefunction with consideration of the

fact that the effective electron (hole) mass is a function of the coordinate z . The Schrodinger equations can be written in the following form [26, 29]:

$$\begin{aligned} \left[\mathbf{H}_c \left(k_x, k_y, k_z = -i \frac{\partial}{\partial z} \right) + V_E^{eff}(z) \right] \Psi_E^i &= E_E^i \Psi_E^i \\ \left[\mathbf{H}_v \left(k_x, k_y, k_z = -i \frac{\partial}{\partial z} \right) + V_H^{eff}(z) \right] \Psi_H^i &= E_H^i \Psi_H^i \end{aligned} \quad (9)$$

where $\hbar$ is the reduced Planck constant ($1.054 \cdot 10^{-34}$ J·s), $V_{E,H}^{eff}(z)$ is the effective potential, $E_{E,H}^i(z)$ and $\Psi_{E,H}^i(z)$ are energy eigenvalues and their corresponding wave functions, respectively. Let us consider only bound quantum states. The conduction band Hamiltonian can be written as

$$\begin{cases} \mathbf{H}_c \left(k_x, k_y, k_z = -i \frac{\partial}{\partial z} \right) = E_c + a_{c1} e_{zz} + a_{c1} (e_{xx} + e_{yy}) + \frac{\hbar^2 (k_x^2 + k_y^2)}{2m_{||}} - \frac{\hbar^2}{2m_{\perp}(z)} \frac{\partial^2}{\partial z^2} \\ E_c = E_g + \Delta_{cr} + \Delta_{SO}/3 \\ a_{c1} = a_1 + D_1 \\ a_{c2} = a_2 + D_2 \end{cases} \quad (10)$$

Important to note is that effective electron mass mismatch between a barrier (ZnO) and an active layer (ZnCdO) can be considered by applying finite difference method to solve the Schrodinger equation for electrons in a quantum well. In other words, the Schrodinger equation for the case of variable effective mass can be written as follows [28]:

$$\frac{\Psi_E(z + \delta z)}{m_{e\perp}^*(z + \delta z/2)} = \left[\frac{2(\delta z)^2}{\hbar^2} [V_E^{eff}(z) - E] + \frac{1}{m_{e\perp}^*(z + \delta z/2)} - \frac{1}{m_{e\perp}^*(z - \delta z/2)} \right] \Psi_E(z) - \frac{\Psi_E(z - \delta z)}{m_{e\perp}^*(z - \delta z/2)} \quad (11)$$

The valence band Hamiltonian can be represented in the following form:

$$\mathbf{H}_v \left(k_x, k_y, k_z = -i \frac{\partial}{\partial z} \right) = \begin{pmatrix} F & -K^* & -H^* & 0 & 0 & 0 \\ -K & G & H & 0 & 0 & \Delta \\ -H & H^* & \Lambda & 0 & \Delta & 0 \\ 0 & 0 & 0 & F & -K & H \\ 0 & 0 & \Delta & -K^* & G & -H^* \\ 0 & \Delta & 0 & H^* & -H & \Lambda \end{pmatrix} \quad (12)$$

where

$$\left\{ \begin{array}{l} F = \Delta_{cr} + \frac{\Delta_{so}}{3} + \Lambda + \Theta, \\ G = \Delta_{cr} - \frac{\Delta_{so}}{3} + \Lambda + \Theta, \\ \Lambda = \frac{\hbar^2}{2m_0} [A_1 k_z^2 + A_2 (k_x^2 + k_y^2)] + \Lambda_e, \\ \Theta = \frac{\hbar^2}{2m_0} [A_3 k_z^2 + A_4 (k_x^2 + k_y^2)] + \Theta_e, \\ K = \frac{\hbar^2}{2m_0} A_5 (k_x + ik_y)^2 + D_5 (e_{xx} - e_{yy}), \\ H = \frac{\hbar^2}{2m_0} A_6 (k_x + ik_y) k_z + D_6 e_{xz}, \\ \Lambda_e = D_1 e_{zz} + D_2 (e_{xx} + e_{yy}), \\ \Theta_e = D_3 e_{zz} + D_4 (e_{xx} + e_{yy}), \\ \Delta = \frac{\sqrt{2}}{3} \Delta_{so}. \end{array} \right. \quad (13)$$

In order to write down the correct (hermitian) form of the Hamiltonian matrix for holes in QW it is necessary to apply the finite difference formulas to describe the differential operators, $A_i(z) \frac{\partial^2}{\partial z^2}$ and $A_i(z) \frac{\partial}{\partial z}$ (where A_i is coordinate-dependent Luttinger parameter), which are included into the expressions for the components of the k.p six-by-six Hamiltonian matrix after substitution of k_z in (13) by $-i \frac{\partial}{\partial z}$.

Generally, these operators can be represented in the following form:

$$\begin{aligned} A_i(z) \frac{\partial^2 \Psi}{\partial z^2} &= \frac{A_i(z_{j+1}) + A_i(z_j)}{2(\delta z)^2} \Psi_i(z_{j+1}) - \frac{A_i(z_{j-1}) + 2A_i(z_j) + A_i(z_{j+1})}{2(\delta z)^2} \Psi_i(z_j) + \frac{A_i(z_j) + A_i(z_{j-1})}{2(\delta z)^2} \Psi_i(z_{j-1}) \\ A_i(z) \frac{\partial \Psi}{\partial z} &= \frac{A_i(z_{j+1}) + A_i(z_j)}{4\delta z} \Psi_i(z_{j+1}) - \frac{A_i(z_j) + A_i(z_{j-1})}{4\delta z} \Psi_i(z_{j-1}) \end{aligned} \quad (14)$$

After mathematical transformations one can obtain the banded matrix for valence-band Hamiltonian, as was shown in Ref. [30].

The effective potential $V_{E,H}^{eff}(z)$ reflects the effect of the conduction (valence) band discontinuity, formation of the two-dimensional electron (hole) gas 2DEG (2DHG) at the heterointerface and the influence of the potential related to the built-in electric field (induced by spontaneous and piezoelectric polarization). Furthermore, the potential associated with the dielectric mismatch was also taken into account. In many cases, the role of dielectric mismatch between well and barrier region in describing the behavior of the carriers in the quantum well structure is frequently ignored. At the same time, to obtain the exact value of the interband transition energy it is important to take into account all types of interactions involved in carrier dynamics and possibly influencing the interband transitions occurring in QWs. In particular, due to the compositional dependence of the dielectric constant of $\text{Zn}_{1-x}\text{Cd}_x\text{O}$ we deal with a high value of dielectric mismatch in the QW structure (approximately ~16%) even at Cd content as low as 10 at. %. Generally accepted is that a difference between the dielectric constant in well and barrier regions causes so-called image charges [31]. Therefore, the self-consistent potentials for electron and holes as well as corresponding transition energies should be corrected by the self-energy image charge potential. Solving the Poisson's equation for the case of interaction between carriers confined in a QW and their image charges as well as the consideration of the coordinate-dependent spatially varying dielectric constant give us a possibility to write down the expressions for the self-energy potentials [32]:

$$\left\{ \begin{array}{l} \sum_i^{Left Bar}(z_i) = \frac{\varepsilon_{QW} \lambda q^2}{2\pi(\varepsilon_{QW} + \varepsilon_{Left Bar})} \int_0^\infty \frac{e^{k(2z_i - L_{QW})}}{1 + \lambda^2 e^{-2kL_{QW}}} dk + \frac{\lambda q^2}{16\pi\varepsilon_{Left Bar}(z_i + L_{QW}/2)} \\ \sum_i^{QW}(z_i) = \frac{\lambda q^2}{8\pi\varepsilon_{QW}} \int_0^\infty \frac{e^{k(2z_i - L_{QW})} + 2\lambda e^{-2kL_{QW}} + e^{-k(2z_i + L_{QW})}}{1 + \lambda^2 e^{-2kL_{QW}}} dk \\ \sum_i^{Right Bar}(z_i) = \frac{\varepsilon_{QW} \lambda q^2}{2\pi(\varepsilon_{QW} + \varepsilon_{Right Bar})} \int_0^\infty \frac{e^{k(2z_i + L_{QW})}}{1 + \lambda^2 e^{-2kL_{QW}}} dk + \frac{\lambda q^2}{16\pi\varepsilon_{Right Bar}(z_i - L_{QW}/2)} \end{array} \right. \quad (15)$$

Immediately after the total effective potential can be calculated using the following formula:

$$V_{E,H}^{eff}(z) = V_p(z) + V_{2D}(z) + \Sigma(z) \quad (16)$$

where $V_p(z)$ is the potential induced by polarization charge and $V_{2D}(z)$ is the electronic potential which is related to 2DEG (2DHG) distribution by Poisson's equation,

$$\frac{d}{dz} \left(\varepsilon(z) \varepsilon_0 \frac{d}{dz} V_{2D}(z) \right) = -q N_{2D}(z) \quad (17)$$

where ε is a dielectric constant of material, ε_0 is the permittivity of free space ($\sim 8.854 \cdot 10^{-12}$ F/m), q is the elementary charge ($\sim 1.602 \cdot 10^{-19}$ C), N_{2D} is the distribution of the two-dimensional electron (hole) gas [33]. Under equilibrium conditions, the distribution of the 2DEG (2DHG) in each subband obeys Fermi statistics, and the distribution of the 2DEG (2DHG) is determined by

$$N_{2D}(z) = \sum_i \frac{m^* k_b T}{\pi \hbar^2} \ln \left[1 + \exp \left(\frac{E_F - E_i}{k_b T} \right) \right] |\Psi_i(z)|^2 \quad (18)$$

where k_b is the Boltzmann constant and T is the temperature, which is set at 300 K in our calculation, E_F is the Fermi level. The coupled Schrodinger and Poisson equation is solved self-consistently.

The polarization-induced field alters the quantum well band profile, which can be represented as a step-linear potential [28]:

$$V_p(z) = \begin{cases} eF_b z + \Delta E_{c,v}, & \text{for } -\frac{2L_b + L_{QW}}{2} \leq z \leq -\frac{L_{QW}}{2} \\ eF_{QW} z, & \text{for } -\frac{L_{QW}}{2} \leq z \leq \frac{L_{QW}}{2} \\ eF_b z + F_{QW} L_{QW} + \Delta E_v, & \frac{L_{QW}}{2} \leq z \leq \frac{2L_b + L_{QW}}{2} \end{cases} \quad (19)$$

where e is the elementary charge $\Delta E_{c,v}$ is the conduction (valence) band discontinuity.

A linear interpolation between the physical parameters of the ZnO and the CdO has been performed to calculate those of the $\text{Zn}_{1-x}\text{Cd}_x\text{O}$: the lattice constants a and c , the valence-band effective-mass parameters A_i ($i=1-6$), the deformation potentials D_i ($i=1-6$), the splitting energies Δ_{cr} and Δ_{so} , the effective electron mass m_e (whereas the effective hole mass m_h didn't depend on the cadmium content in our study and was chosen as $0.79m_0$ [34]), piezoelectric stress coefficients (e_{31} , e_{33} , e_{15}), the band-gap energy E_g , the dielectric constant ε , elastic constants (C_{13} , C_{33} , C_{12} , C_{11} , C_{44}), the

piezoelectric and the spontaneous polarization P_{PE} and P_{SP} of the top $Zn_{1-x}Cd_xO$ and the bottom ZnO layers. Table 1 represents the results of the interpolation. In order to determine the valence band offset we used a relative band-edge offset of $\Delta E_C/\Delta E_V=36/64$ for a composition of $x=0.05$, which was reported in Ref. [35].

Table 1. Some physical Parameters of $Zn_{1-x}Cd_xO$ ternary alloy

Parameters	Symbol	Unit	Linear interpolation	References
Elastic constant	C_{13}	GPa	$121-60x$	[36] ^{theory}
Elastic constant	C_{33}	GPa	$225-120x$	[36] ^{theory}
Elastic constant	C_{12}	GPa	$117-9x$	[36] ^{theory}
Elastic constant	C_{44}	GPa	$50-3x$	[36] ^{theory}
Elastic constant	C_{11}	GPa	$217-67x$	[36] ^{theory}
Lattice parameter	a	Å	$3.25+0.296x$	[37] ^{experiment} [38] ^{theory}
Lattice parameter	c	nm	$0.5207+0.056x-0.029x^2$	[39] ^{experiment}
Spontaneous polarization	P_{SP}	C/m ²	$-0.022-0.084x$	[36] ^{theory}
Piezoelectric stress coefficient	e_{31}	C/m ²	$-0.51-0.28x$	[40] ^{theory}
Piezoelectric stress coefficient	e_{33}	C/m ²	$0.89+1.584x$	[40] ^{theory}
Piezoelectric stress coefficient	e_{15}	C/m ²	$-0.45-0.381x$	[40] ^{theory}
Band-gap energy	E_g	eV	$3.28(1-x)+2.3x-3.04x(1-x)$	[39] ^{experiment}
Dielectric constant	ϵ	-	$6.8+11.3x$	[35] ^{theory}
Conduction band deformation potentials	a_1 a_2	eV	$-3.90+1.09x$; $-4.13+3.84x$;	[41] ^{experiment}
Conduction band offset	ΔE_c	eV	$0.8(E_g(x)-E_g(0))$	[35] ^{theory}
Valence-band effective-mass parameters	A_1 A_2 A_3 A_4 A_5 A_6	-	$-2.747-0.551x$ $-0.386+0.006x$ $2.386+0.55x$ $-2.089-1.694x$ $-2.059-1.626x$ $-2.103-1.54x$	[41] ^{theory}
Deformation potentials	D_1 D_2 D_3 D_4 D_5 D_6	eV	$-3.80+0.99x$ $-3.80+3.51x$ $0.80-2.66x$ $-1.40+1.10x$ $-1.20+0.29x$ $-2-0.79x$	[38]
Conduction-band effective masses	$m_{ }$ $m_{\perp}$	m_0	$0.239-0.071x$ $0.244-0.09x$	[41] ^{theory} [42] ^{theory}
Splitting energies and	Δ_{cr} Δ_{so}	eV	0.0042 $0.043+0.074x$	[41] ^{theory}

It should be mentioned that both the Schrödinger and the Poisson equations were discretized using the finite difference method. It is noteworthy that the radiative recombination energy for all cases was calculated using the band gap energy of the active layer and subtracting from the calculated ground-state transition energy $E_{1e1h}=E_{1e}+E_{1h}$ a constant value of 160 meV comprising both localization and exciton binding energy [15]. The spontaneous emission spectra were obtained in the similar manner as in Ref. [4].

3. Results and discussion

In Fig. 2 we plot the strain tensor elements as a function of the crystal orientation θ for the $\text{Zn}_{0.9}\text{Cd}_{0.1}\text{O}/\text{ZnO}$ structures. The component ε_{xx} is constant and doesn't depend of the inclination angle, whereas the component ε_{yz} is zero for the (0001) growth orientation ($\theta=0^\circ$) and non-polar m -plane ($\theta=90^\circ$). The strain components ε_{yy} and ε_{zz} demonstrate opposite behaviors. With increasing the inclination angle the absolute value of ε_{yy} also increments and reaches a maximum at $\theta=90^\circ$, while the ε_{zz} component has a maximum at $\theta=0^\circ$ and then decreases.

Fig. 2. Dependences of the components of the strain tensor on the inclination angle for strained $\text{Zn}_{0.9}\text{Cd}_{0.1}\text{O}/\text{ZnO}$ structures.

It should be mentioned that the growth of the $\text{Zn}_{1-x}\text{Cd}_x\text{O}$ layers on the non-polar substrates (*a*- or *r*-sapphire) with $\theta=90^\circ$ may provide more favorable conditions for

Cd incorporation in $\text{Zn}_{1-x}\text{Cd}_x\text{O}$ [43, 44]. A. Fouzri *et al.* [43] reported that the Cd incorporation in the case of $\text{Zn}_{1-x}\text{Cd}_x\text{O}$ grown on the non-polar r - and a -plane sapphire was higher than that in the case of layer deposited on a (0001)-orientated substrate. This observation was confirmed by the highest redshift of the PL peak ($\sim 340\text{meV}$) [40]. Furthermore, A. Zubiaga *et al.* [44] demonstrated that the non-polar $\text{Zn}_{1-x}\text{Cd}_x\text{O}$ films with Cd concentration ranging between 0.8% and 5% were characterized by a homogeneous distribution of cadmium atoms in the film. Let us speculate that these non-trivial experimental findings can be associated with the behavior of the strain tensor components for non-polar planes with $\theta=90^\circ$. M. V. Durnev *et al.* [45] studied the strain effects on indium incorporation and optical transitions in green-light InGaN heterostructures of different orientations. These authors revealed the strong dependence of the InN molar fraction on c -axis inclination angle and the enhanced indium incorporation on nonpolar ($\theta = 90^\circ$) and, especially, on semipolar ($\theta = 45\text{-}60^\circ$) planes [45]. It was shown that the non-monotonous variation of the InGaN composition with the inclination angle correlated with the angle dependence of the strain energy accumulated in the InGaN alloy. Minimal values of the strain energy at the high inclination angles correspond to the maximal values of indium content at the same angles. In Ref. [11] it was also demonstrated that the strain energy stored in the $\text{Zn}_{0.75}\text{Cd}_{0.25}\text{O}$ lattice matched to ZnO had the lowest values for $\theta = 90^\circ$. Interestingly the strain energy density W is related to strain tensor components ε_{xx} , ε_{zz} , ε_{yy} and ε_{yz} via the following expression [25]:

$$W = \frac{1}{2}C_{11}(\varepsilon_{xx}^2 + \varepsilon_{yy}^2) + \frac{1}{2}C_{33}\varepsilon_{zz}^2 + C_{12}\varepsilon_{xx}\varepsilon_{yy} + C_{13}(\varepsilon_{xx}\varepsilon_{zz} + \varepsilon_{yy}\varepsilon_{zz}) + 2C_{44}\varepsilon_{yz}^2 \quad (16)$$

Thus, taking into account Figure 2 and Eq. 16 we can expect a strong dependence of the Cd content in $\text{Zn}_{1-x}\text{Cd}_x\text{O}$ quantum well layer on the crystal angle θ . In this regard, the enhancement of the cadmium content with increasing the inclination angle may be responsible for shrinking the band-gap energy of the well layer and red-shift of the transition energy.

In Fig. 3, the amount of the spontaneous and piezoelectric polarizations in a barrier layer and well layer is shown versus θ . The spontaneous polarizations in the ZnO and $\text{Zn}_{0.9}\text{Cd}_{0.1}\text{O}$ layers are negative and change nearly linearly (only slight deviation from linear behavior is observed) with the crystal plane angle, whereas the piezoelectric polarization in $\text{Zn}_{0.9}\text{Cd}_{0.1}\text{O}$ is characterized by the well-defined non-linear dependence on the crystal inclination angle. It should be also mentioned that the values of all components of polarization are equal to zero for non-polar $(10\bar{1}0)$ orientation ($\theta=90^\circ$). It is caused by the asymmetry of the polarization induced by the change of the atomic plane type with respect to the $(10\bar{1}0)$ orientation [46]. In fact, the growth of the QWs with $(10\bar{1}0)$ orientation can hinder the large piezoelectric field and block a spatial separation of the electron and hole wave functions, thereby increasing the transition probability between the conduction and valence subbands [47].

Fig. 4a demonstrates the dependence of the polarization-induced internal electric field on the inclination angle. It is clearly seen that the increase of θ leads to decreasing the magnitude of the internal electric field in the well layer. The internal field for QW becomes zero at $\theta=90^\circ$ because the spontaneous and piezoelectric polarization are zero for the $(10\bar{1}0)$ orientation. Additionally, we have revealed that the electric field changes the sign at angles between 70° and 90° and reaches a zero value at 90° . This finding coincides with the results reported by Park [24], who also observed the change of the sign of the internal electric field with crystal angle further increasing for InGaN/GaN quantum wells. At the same time, W. G. Scheibenzuber *et al.* [26] reported that the electric field does not change sign at an angle between 0° and 90° . We also calculated the distribution of the internal electric field depending on both cadmium content in $\text{Zn}_{1-x}\text{Cd}_x\text{O}$ quantum well layer and crystal angle (see Fig. 4b). From the analysis of Fig. 4b it is reasonable to assume that the internal electric field in the $\text{Zn}_{1-x}\text{Cd}_x\text{O}$ well layer at the fixed crystal angle θ is very sensitive to the cadmium content in the angle range from 0° to $\sim 40^\circ$, whereas the magnitude of the electric field at the larger angles is less affected by the cadmium content.

Fig. 3. Dependence of the spontaneous and piezoelectric polarizations in ZnO barrier and $\text{Zn}_{0.9}\text{Cd}_{0.1}\text{O}$ quantum well on crystal angle θ .

Fig. 4. (a) Polarization-induced internal field in the $\text{Zn}_{0.9}\text{Cd}_{0.1}\text{O}$ well layer depending on the crystal angle. (b) Visualization of the dependence of the internal electric field on cadmium content and crystal angle.

Figure 5 shows calculated valence band structures for the valence subbands for a 3 nm- $\text{Zn}_{0.9}\text{Cd}_{0.1}\text{O}$ quantum well grown on c -orientated, semipolar, and m -plane nonpolar substrates.

Fig. 5. The in-plane valence band dispersion of the QWs grown towards different crystallographic orientations: (a) $\theta = 0^\circ$, (b) $\theta = 58^\circ$, (c) $\theta = 90^\circ$ (m-plane)

When $\theta = 0^\circ$ the QCSE is maximal and the self-consistent energy profile of the quantum well is triangle-shaped. The huge existing build-in electric field will push the valence subbands upwards, as shown on Figure 5a. It was revealed that the dispersion of HH1 subband was quite parabolic in shape. It was also found that there is a strong coupling of all heavy-hole (HH1, HH2) and light-hole (LH1, LH2) valence subbands at region k_t smaller than 0.3 nm^{-1} and coupling of HH2 and LH2 in regions where k_t greater than 1.4 nm^{-1} . It is interesting to note that an increase in the inclination angle significantly modifies the valence band structure of the $\text{ZnO}/\text{Zn}_{1-x}\text{Cd}_x\text{O}/\text{ZnO}$ quantum well. The drop in the electric field strength will lead

to flattening the potential energy profile in the quantum well. In this regard, all valence subbands shift downwards and the energetic distance between these subbands is reduced (Fig. 5 b-c). Nevertheless, the HH1 subband remains parabolic both at $\theta = 58^\circ$ and $\theta = 90^\circ$ (*m*-plane). Another observable feature is decoupling of HH2 and LH2 subbands at the region k_t greater than 1.4 nm^{-1} (Fig. 1 b, c). On the other hand, increase in the angle θ results in a strong coupling of the HH2 and LH2 subbands in the range of k_t from 0.5 to 0.7 nm^{-1} . It means that the density of states (DOS) increases with increment of angle θ .

In Fig. 6a the spontaneous emission spectra for a couple of inclination angles are given. They are essentially determined by the behavior of the overlapping the electron and hole wavefunctions with *c*-axis inclination angle, together with the shape of the potential profile. With increasing θ , the intensity of the emission peak is enhanced and blue-shifted due to changing the confinement profile from triangle-shaped (at $\theta=0$) to nearly rectangle-liked (at $\theta=90^\circ$). At the same time, the electron (hole) wavefunction moves from the right (left) corner of the tilted potential profile for *c*-plane structure to the center of the quantum well for the *m*-plane structure. Contour plots in the *x-z* plane of the electron and hole wave functions for the first conduction and heavy hole subbands are shown for three different values of θ in Figure 7(a-c). Figure 6a shows clearly that when $\theta=0$, the overlapping electron and hole wavefunctions is very low due to the spatial separation induced by QCSE. Considering semipolar planes, one can conclude that a decrease in the internal electric field tends to reduce the role of QCSE, which means that the carrier' wavefunctions come to meet each other (Fig. 7b). Finally when the inclination angle is very large (non-polar plane) the specific electron (hole) probability distribution in the *z* direction spreads only inside the QW due to a full neutralization of the QCSE. In this case, the highest probabilities for carriers are at the center of the quantum well (Fig. 7c).

Fig.6. Spontaneous emission spectra of 4 nm-ZnO-1 nm-Zn_{0.9}Cd_{0.1}O/4 nm-ZnO QWs depending on the *c*-axis inclination angle

Fig. 7. *x-z* contour plots of the electron and hole wavefunctions for 4 nm-ZnO-1 nm-Zn_{0.9}Cd_{0.1}O/4 nm-ZnO quantum wells grown towards different crystallographic orientations: (a) $\theta = 0^\circ$, (b) $\theta = 58^\circ$, (c) $\theta = 90^\circ$ (*m*-plane).

Figure. 8 (a) Dependence of the transition energy on the crystal angle for QWs with different values of well widths. (b) The overlap integral vs. the crystal angle. Barrier thickness and Cd content are fixed at 4 nm and 10 at. %, respectively.

Figure 8a shows the dependence of the excitonic transition energy (C1-HH1) on the angle θ between the growth direction and crystallographic direction [0001]. Calculations are made for different values of the width of the quantum well. As might be expected, with increasing the angle θ the transition energy also increases. This is due to a decrease in the built-in electric field due to polarization effects and mitigation of the negative quantum-confined Stark effect (QCSE). There are two critical points for which there is a maximum blue shift of the transition energy: $\theta = 45^\circ$ and $\theta = 90^\circ$. When $\theta=45^\circ$ the electric field tends to a minimum value 0.0301 MV/cm, while for $\theta=90^\circ$ the internal electric field is completely absent. In these two cases, the self-consistent energy profile of the ZnO/Zn_{1-x}Cd_xO/ZnO quantum well is characterized by a lack of tilt of the conduction band bottom and the valence band top. Characteristically, the increase in the well width leads to a red shift of the exciton transition energy due to QCSE, since the wider well corresponds to the higher value of built-in electric field. For the investigated structures the overlap integral of the wave functions of electrons and holes was also calculated. This integral allows estimating the probability of electron-hole transitions and comparing the performance of light-emitting structures oriented in different crystallographic directions. Figure 8b shows a plot of the probability of interband transitions on the angle θ and the width of the quantum well. Obviously, the most probable band-to-band transitions are observed in the absence of polarization ($\theta=90^\circ$) or at its minimum value ($\theta=45^\circ$). At the same time, the observed decrease in transition energy and the overlap integral in the range of angles between $\theta=45^\circ$ and $\theta=90^\circ$ is correlated with the dependence of the piezoelectric polarization on the angle θ . Strictly speaking, this is an region of change of sign of the piezoelectric polarization. In other words, the change in the sign means a change in the direction of the slope

of the potential of the quantum well grown in semi-polar directions. It is clearly seen that the quantum wells grown even on the semi-polar planes have a lower field strength than the quantum wells grown on the polar plane. Figure 8b clearly demonstrates the dependence of an exciton transition probability on the width of the quantum well (in the range of angles $20^\circ < \theta < 40^\circ$ and $50^\circ < \theta < 80^\circ$) for structures with strong polarization fields. On the other hand, in the angular ranges $35^\circ < \theta < 40^\circ$, $50^\circ < \theta < 60^\circ$ and $75^\circ < \theta < 80^\circ$ the influence of the well width on the transition energy and the overlap integral is minimal. The graph shows that using certain semi-polar and non-polar orientations one may increase the width of the quantum well in more than 2 times, without reduction in the probability of interband transitions (even with slight enhancement of the overlap integral due to improve quantum confinement characteristics). That is, near the critical points $\theta = 45^\circ$ and $\theta = 90^\circ$ transition probability hardly depends on the quantum well width.

Figure 9. (a) Dependence of the transition energy on the barrier thickness for QW structures growth in different directions. (b) The overlap integral vs. the barrier thickness. Well width and Cd content are fixed at 1 nm and 10 at. %, respectively.

Figure 9a illustrates the dependence of the transition energy on the angle θ and the thickness of the barrier. It is clearly shown that the increase in the barrier thickness leads to a decrease in the transition energy between the first subband in the conduction band and the first sub-band in the valence band. This is explained by the

point that energy profile tilt is dependent not only on the quantum well width, but also on the barrier width. In general, the slope of the energy profile in the quantum well is an indicator of the electric field in the quantum well and the barrier. With decreasing barrier thickness, the electric field in the quantum well is reduced, whereas the electric field in the barrier is increased. For example, when the barrier thickness (for QW structure grown on polar substrate) is increased from 2 to 4 nm, the electric field strength in the well and barrier varies from -1.1493 MV/cm and 0.57463 MV/cm to -1.3521 MV/cm and 0.33804 MV/cm, respectively. As we can see from the Fig. 9a, semipolar and nonpolar QWs exhibit similar behavior with increasing the barrier thickness. The dependence of the overlap integral on the barrier thickness is characterized by several features (Fig. 9b): (i) quantum wells grown in a non-polar and semipolar crystallographic directions exhibit larger probability of excitonic transitions at all values of barrier thickness and (ii) the region of weak sensitivity of transition probability to a change in the barrier thickness is only observed for QWs with $\theta=58^\circ$, (iii) nonpolar (10-10) and semipolar (10-12) QWs demonstrate a slight increase in the overlap integral with increasing the barrier thickness. Obviously, it is due to the vanishing polarization field in the narrow neighborhood of the critical points $\theta=45^\circ$ and $\theta=90^\circ$.

Figure 10. (a) Dependence of the transition energy on the cadmium content in the active well layer for QW structures grown in different orientations. (b) The overlap integral vs. cadmium content. Well width and barrier thickness are fixed at 1 nm and 4 nm, respectively.

The dependences of the optical transition energy and the overlap integral on the angle θ and cadmium content in the active layer of the quantum well are depicted in Fig. 10. It is worth noting that increasing the cadmium content leads to a significant reduction in the transition energy (in the whole range of angles). Such a dependence is due to the change in the band gap of the active layer of the quantum well (and hence the band-offset ratio, which determines the depth of the quantum well and quantization energies) and the influence of the spontaneous and piezoelectric polarization at the heterointerface. $\text{Zn}_{1-x}\text{Cd}_x\text{O}$ layer grown on a ZnO substrate is subject to strain, which is increasing with increasing the cadmium content. The strain will change the values of the spontaneous and piezoelectric polarization, and accordingly to an increase of the built-in electric field. At such conditions the role of the QCSE in the optical processes is enhanced, which leads to a stronger spatial separation of the charge carriers and the redshift of the optical transition energy. Crystallographic orientation changes the magnitude and the direction of the polarization field relative to the direction of growth. With the increase of the c -axis angle inclination the polarization field strength in the growth direction and hence the QCSE decrease. It is worth noting that at the critical points $\theta = 42^\circ$, $\theta = 58^\circ$ and $\theta = 90^\circ$ (which correspond to (10-12), (11-22) and (10-10) planes) the overlap integral increases with increasing cadmium content in the active layer. This is due to the fact that the effect of Cd content on the band-offset ratio is dominating under the conditions of suppressing electrical field. Deeper quantum well and, consequently, stronger quantum confinement will be observed in the case of a structure with a high Cd content in the active layer. It will result in a change in the quantization energies, the overlap of the wave functions of electrons and holes, as well as transition energy.

It was significant to note that the overlapping of the electron and hole wave functions is a measure of probability of the excitonic radiative recombination. The latter can directly affect the effective carrier lifetime in QW. In other words, increasing the probability of recombination will lead to an increase of the lifetime. In a case of

polar (0001) QW, a high value of the lifetime is expected, whereas non-polar QW should be characterized by the reduced carrier lifetime. This assumption is confirmed by the experimental results of V. Venkatachalapathy *et al.* [48]. These authors observed that carrier lifetime in the non-polar $\text{Zn}_{0.75}\text{Cd}_{0.25}\text{O}$ MQWs was almost insensitive to the well layer thickness and had smaller values compared to the polar structure. Therefore, the growth of the $\text{Zn}_{0.9}\text{Cd}_{0.1}\text{O}$ -based QWs with semi-polar orientation, for example $(11\bar{2}2)$, or with non-polar $(10\bar{1}0)$ orientation can improve the stability of the transition energy and effective carrier time at the different values of the quantum well thickness.

4. Conclusions

In summary, we have studied the effect of the crystal angle between the growth direction and c -axis on the properties of $\text{ZnO}/\text{Zn}_{0.9}\text{Cd}_{0.1}\text{O}/\text{ZnO}$ quantum wells, using the self-consistent Schrodinger–Poisson solver accounting for the spontaneous and piezoelectric polarization. The behavior of the strain tensor components, polarization-induced electric field and transition energy with increasing the crystal angle are comparable to those observed in III-V materials. It was revealed that at the angles ranging from 70° to 90° the electric field in the quantum well changes its sign. It was also found that the internal electric field in the $\text{Zn}_{1-x}\text{Cd}_x\text{O}$ well layer at the fixed crystal angle θ is very susceptible to cadmium content and well thickness in the angle range from 0° to $\sim 40^\circ$, whereas the magnitude of the electric field at the larger angles is less affected by the cadmium content and thickness of the well layer. Finally we compare conduction and valence band edge profiles as well as carrier wave functions for polar (0001), semi-polar $(11\bar{2}2)$ and non-polar $(10\bar{1}0)$ QWs and clearly demonstrate the diminishing of the QCSE, which manifests itself in flattening the potentials profiles, red-shift in transition energy and increasing the overlapping of the electron and hole wavefunctions. The crystal angle engineering approach is therefore very promising for $\text{Zn}_{1-x}\text{Cd}_x\text{O}$ -based LEDs and lasers operating at high injection levels.

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Fig. 1. (a) Configuration of the converted coordinate system (x' , y' , z'). z' axis is normal to the substrate surface. The coordinate system (x , y , z) denotes the primary crystallographic axes. Illustration of the (b) polar c -plane, (c) semipolar ($11\bar{2}2$) plane and (d) non-polar m -plane in $\text{Zn}_{1-x}\text{Cd}_x\text{O}$.

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Figure. 8 (a) Dependence of the transition energy on the crystal angle for QWs with different values of well width. (b) The overlap integral vs. the crystal angle. Barrier thickness and Cd content are fixed at 4 nm and 10 at. %, respectively.

Fig. 8. (a) Dependence of the transition energy on the crystal angle for QW structures with different values of barrier thickness. (b) The overlap integral vs. the crystal angle. Well width and Cd content are fixed at 2 nm and 15 at. %, respectively.

Figure 9. (a) Dependence of the transition energy on the barrier thickness for QW structures growth on different directions. (b) The overlap integral vs. the barrier thickness. Well width and Cd content are fixed at 1 nm and 10 at. %, respectively.

Figure 10. (a) Dependence of the transition energy on the cadmium in active well layer for QW structures grown in different orientations. (b) The overlap integral vs. the cadmium. Well width and barrier thickness are fixed at 1 nm and 4 nm, respectively.

List of tables:

Table 1. Some physical parameters of $\text{Zn}_{1-x}\text{Cd}_x\text{O}$ ternary alloy