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Theoretical study of the O- and Zn-face polarity effect on the optical properties of the conventional and staggered ZnO/Zn_{1-x}Cd_xO/ZnO quantum wells

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Abstract

In this work we present a comparative study of Zn-face and O-face polarity Zn_{1-x}Cd_xO-based conventional and staggered quantum-well (QW) structures. The calculation of optical properties of QWs was performed by means of self-consistent Schrodinger-Poisson solver with consideration of polarization-induced effects. The conventional Zn-face and O-face QWs possess similar values of transition energy and an overlap of electron and hole wave functions. A change of the polarity from Zn-face to O-face for the conventional QWs influences only a shape of the conduction and valence band edge profile. It is revealed that the utilization of the staggered QWs leads to an improvement of the confinement characteristics. In addition, the O-face staggered QW structure has larger values of transition energy and overlap integral compared to the Zn-face staggered QW structure. O-terminated staggered QW structure is less dependent on a well thickness and has lower sensitivity to Cd content in embedded Zn_{1-x}Cd_xO layer. Controlling the material polarity and designing the staggered QWs provide cost-effective approaches to engineer the QW band structures for enhancing the QW performance, which has great potential to achieve Zn_{1-x}Cd_xO-based light emission diodes with improved radiative efficiency emitting applicable for solid state lighting.

Key words: staggered layer, ZnCdO ternary alloy, quantum well, transition energy

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1. Introduction

Zinc oxide (ZnO) belonging to a class of transparent conducting oxides and its ternary alloys (especially $\text{Zn}_{1-x}\text{Cd}_x\text{O}$) are perspective semiconductor materials that possess intriguing electrical and optical properties, allowing them to be used as transparent electrodes in solar cells and active media in light emitting sources and photovoltaic devices [1-8]. It is due to the direct band-gap of ZnO and a substantial tunability of the band gap leading to a large absorption/emission range covering the nearly entire solar spectrum [9]. High quality optoelectronic and photovoltaic devices require the quantum-well (QW) structure design. For this reason, study of the QW-related effects is very essential for the understanding the radiative recombination processes and carrier confinement in $\text{Zn}_{1-x}\text{Cd}_x\text{O}/\text{ZnO}$ QWs.

Recently, several groups have studied the properties of $\text{Zn}_{1-x}\text{Cd}_x\text{O}/\text{ZnO}$ QWs [10-13]. Liu *et al.* [10] observed the increase of the spontaneous emission rate from $\text{Zn}_{1-x}\text{Cd}_x\text{O}$ QWs by surface plasmon coupling. Yang *et al.* [11] have revealed that the QW is characterized by a very strong photoluminescence from the ZnCdO well layer and extremely weak emission from ZnO barriers. Yamamoto *et al.* [12] obtained the band-edge green electroluminescence (EL) at 500 nm from $\text{Zn}_{0.80}\text{Cd}_{0.20}\text{O}/\text{Zn}_{0.92}\text{Cd}_{0.08}\text{O}$ multiple quantum-well light-emitting diodes (LEDs) on *p*-type 4H-SiC substrates. The change of the emission energy from the green to the violet spectral range (2.5 eV to 3.1 eV) by tuning the quantum well thickness was observed by Lange *et al.* [13]. Thus, the optical performance of ZnO-based devices and heterostructures is strongly governed by the phenomena occurring in the $\text{Zn}_{1-x}\text{Cd}_x\text{O}$ layer. It is also well-known that the hexagonal wurtzite structure exhibits noticeable spontaneous and piezoelectric polarization effects due to the absence of a center of symmetry and the characteristics of the ionic bonds between Zn (Cd) and O atoms. The performance of the LEDs based on $\text{Zn}_{1-x}\text{Cd}_x\text{O}$ ternary alloys may be detrimentally affected by the strong internal field induced by polarization [14, 15]. Kalusniak *et al.* [14] revealed a low-energy shift of the photoluminescence of several 100 meV, caused by the polarization-induced electric fields of $\sim 10^8$ V/m in (Zn,Cd)O/ZnO quantum well structures. Benharrats *et al.* [15] theoretically

predicted that the internal field in $\text{Cd}_x\text{Zn}_{1-x}\text{O}/\text{ZnO}$ ($x \leq 0.2$) QWs increases with x with a linear slope $A=17.83$ MV/cm. The large internal electric field in the $\text{Zn}_{1-x}\text{Cd}_x\text{O}$ well layer induces the low electron and hole wavefunctions overlap and instability in transition energy, especially for QW with high cadmium content and thick QW active layer (well-known quantum confined Stark effect). Therefore, the main efforts of investigations should be focused on a searching the ways of the effective suppression of the carrier separation effect. Utilizing staggered QW is a simple approach to obtain emitting structures with enhanced electron–hole wavefunction overlap and enhanced recombination rate of the active regions [16].

In spite of huge interest to $\text{Zn}_{1-x}\text{Cd}_x\text{O}$ solid solution for optoelectronics, a lot of fundamental properties of $\text{Zn}_{1-x}\text{Cd}_x\text{O}$ -based QW structures are not yet well understood. Particularly, there has been lack of studies on the effect of the polar plane (O- or Zn-face) on the optical properties of the staggered $\text{Zn}_{1-x}\text{Cd}_x\text{O}/\text{ZnO}$ QWs. This, however, may have a significant influence on the improvement of the optoelectronic devices performance/efficiency, as it was previously demonstrated for InGaN QWs LEDs [16].

In this paper, we investigate theoretically the optical properties of the conventional and staggered $\text{ZnO}/\text{Zn}_{1-x}\text{Cd}_x\text{O}/\text{ZnO}$ quantum wells with O- and Zn-faces, with taking into account the spontaneous and piezoelectric polarizations.

2. Theoretical approach

Compressively strained $\text{ZnO}/\text{Zn}_{1-x}\text{Cd}_x\text{O}/\text{ZnO}$ quantum wells with Zn-face and O-face polarity were considered in this work. It is a common knowledge that the ZnO has partial ionic nature that causes an appearance of a net dipole moment along the [0001] growth direction (c -axis). ZnO, by virtue of crystal symmetry, has two basal planes: (0001) and (000 $\bar{1}$). The (0001) plane is terminated by Zn, whereas (000 $\bar{1}$) plane terminated by O. If the polarity is changed from Zn-face to O-face, both the piezoelectric and the spontaneous polarization change their signs. Figure 1 depicts the schematic diagrams of the polarizations in conventional $\text{ZnO}/\text{Zn}_{1-x}\text{Cd}_x\text{O}/\text{ZnO}$ structures with Zn-face along the (0001) orientation and O-face along the (000 $\bar{1}$)

orientation. The direction of the spontaneous polarization (P_{SP}) in Zn-face structure is built from the surface to the bulk, but the direction is opposite in the O-face structure. Consequently, the negatively bound charges were induced at the surface of Zn-face structure by the spontaneous polarization and vice versa for O-face structure. The signs of the relevant piezoelectric coefficients in the Zn-face ZnO/Zn_{1-x}Cd_xO/ZnO structure are such that for (0001) ZnCdO films grown under compressive strain, P_{PE} is in the (0001) direction and vice versa for the O-face structure.

Fig. 1. Schematic diagrams of the polarizations in different epitaxial layers of ZnO/Zn_{1-x}Cd_xO/ZnO structure with (a) Zn-face and (b) O-face configurations.

In order to obtain the transition energy and carriers' wavefunctions for the ZnO/Zn_{1-x}Cd_xO/ZnO QWs with O- and Zn-faces we solved self-consistent Schrödinger-Poisson equations using the finite difference method. The term “transition energy” refers to optical interband transition at the Γ point at $k=0$ (according to optical selection rules) between the states in quantum well that are confined in the z -direction but free in the x - y plane. In our case, the transition energy for all quantum well structures was calculated using the band gap energy of active layer (Zn_{1-x}Cd_xO) 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 [14]. Generally, interband transitions in quantum well structures are of considerable

interest because of their potential applications in light-emitting diodes. In fact, the interband transition energy in most cases matches very well with energy of emission peak observed on photoluminescence spectra of real quantum wells. The numerical model takes into account the spontaneous and piezoelectric polarizations, which were calculated by means of formalism proposed in Ref. [17]. It should be mentioned that a linear interpolation between the physical parameters of ZnO [18, 19] and CdO [18-20] has been performed to calculate those of $\text{Zn}_{1-x}\text{Cd}_x\text{O}$, to obtain the lattice constants a and c , elastic constants (C_{13} , C_{33} , C_{12} , C_{11} , C_{44}), 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 $0.79m_0$ [15]), the band-gap energy E_g , the dielectric constant ϵ , piezoelectric constants (e_{31} , e_{15} , e_{33}), piezoelectric and spontaneous polarization P_{PE} and P_{SP} of the $\text{Zn}_{1-x}\text{Cd}_x\text{O}$ well and ZnO barrier layers. In order to determine the conduction and 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. [21]. Because of lack information in the literature concerning the dependences of the elastic constants and effective masses on the Cd content we assume that these parameters of $\text{Zn}_{1-x}\text{Cd}_x\text{O}$ ternary alloy follow the Vegard's law. This is a reasonable assumption because solid solutions usually contain compounds with nearly identical parameters ($m_{e\text{ZnO}}=0.21m_0$ vs. $m_{e\text{CdO}}=0.24m_0$). On the other hand, real solid solutions always demonstrate slight nonlinearity in the parameters due to alloy disorder and native defects. In an ideal case, more precise calculations require using the semiempirical approximation.

3. Results and discussions

Figure 2 illustrates the band edge profiles and the wave functions of the 1st conduction subband and the 1st valence subband at the zone center for the ground state of (a) Zn- and (b) O-face conventional 2 nm-ZnO/1 nm- $\text{Zn}_{0.85}\text{Cd}_{0.15}\text{O}$ /2 nm-ZnO QW structures. Due to polarization discontinuity at the interface between the ZnO barrier layer and $\text{Zn}_{0.85}\text{Cd}_{0.15}\text{O}$ well layer, the internal built-in electric field is present in QW (-2.19 MV/cm for Zn-face and +2.19 MV/cm for O-face). This

internal field results in the transformation of the band edge profiles of a conventional 2 nm-ZnO/1 nm-Zn_{0.85}Cd_{0.15}O/2 nm-ZnO QW structures from flat lineups to tilted ones. It leads to observable spatial separation between electron and hole wavefunctions (see Fig. 2c and 2d).

Fig. 2. Conduction and valence band edge profiles together with electron and hole wavefunctions for the (a) Zn- and (b) O-face conventional 2 nm-ZnO/1 nm-Zn_{0.85}Cd_{0.15}O/2 nm-ZnO QW. Color visualization of the electron and hole probability distributions is depicted for (c) Zn- and (d) O-face QW.

In addition, we observe that the potential lineup and the spatial separation between carriers' wavefunctions for conventional QW structures depend on the face polarity. We revealed that the electron wavefunction shifts towards left corner in the case of O-face QW, whereas the hole wavefunction displacements towards right corner. In the case of Zn-face polarity QW structure the situation is observed to be opposite.

This is because the alignment of the piezoelectric and spontaneous polarizations is antiparallel in the case of compressive strain for the O-face. If the polarity changes from the O-face to the Zn-face, the piezoelectric, as well as the spontaneous polarization changes its sign. We revealed that the polar face in the case of conventional QWs slightly effects on the well width dependence of the transition energy (these dependences will be presented further). Similar trend was earlier reported for InGaN/GaN QWs [22]. It was shown that in the case of the single InGaN/GaN QW structure, the spatial separation between electron and hole wave functions is independent of the polar face [22]. Nevertheless, in real case the structural quality of the cation-face and anion-face polarity QWs differs from each other [23]. Generally, optical properties of realistic quantum wells may be strongly affected by (i) charged adsorbates at the free surface and charged defects located close to the heterointerface, which can screen polarization-induced internal electric field [24], (ii) diffusion of Cd atoms from the well to the barrier that can change the composition and confinement potential profiles [25] and (iii) Cd fluctuations [12]. In addition, a presence of the surface dipole perpendicular to bulk surface can give rise to modification of unstable surfaces of O-face and Zn-face ZnO [26] via competing stabilization mechanisms, such as metallization of the surface layer, adsorption of OH groups or O adatoms, the formation of Zn vacancies, and large scale triangular reconstructions [27]. Generally, it can cause surface band bending that significantly affects the optical properties of QWs [28]. Since the optical performance of QWs is strongly governed by the quality of heterointerface (by virtue of dependence of polarization field on the lattice mismatch-induced strain), then the material polarity can affect the transition energy and overlap integral even in the case conventional QWs.

The potential band edge profiles and carriers wavefunctions for staggered QW structures composing of O-face and Zn-face 1 nm-Zn_{0.85}Cd_{0.15}O/1 nm-Zn_{0.75}Cd_{0.25}O layers surrounded by ZnO barriers are depicted in Fig. 3. It is significant to note that the electric fields in the well and the barrier layers must be of opposite sign as the

overall potential drop across the staggered quantum well structure has to be zero. This condition can be governed by following expression [29]:

$$F_{B1}L_{B1} + F_W L_W + F_{SL}L_{SL} + F_{B2}L_{B2} = 0 \quad (1)$$

whereas the $F_{B1,2}$, F_W and F_{SL} are the electric fields in the barrier (with thickness $L_{B1,2}$), the well (L_W) and staggered (L_{SL}) layers, respectively.

The use of staggered $\text{Zn}_{0.75}\text{Cd}_{0.25}\text{O}$ layer gives rise to the pulling of electron wave function from the right to the center of the QW (Figure 3a). The hole wave function is relatively unchanged because of the heavier hole effective mass ($0.78m_0$). As a result, the overlap integral for the staggered QWs is increased in comparison to conventional QWs. It can be explained by the weakening the internal field effect with the inclusion of a staggered layer [22]. An improvement of the overlap leads to the improvement of radiative recombination rate and higher optical gain of the active region.

Fig. 3. Potential lineups and corresponding wavefunctions for the staggered Zn-face (a) and O-face (b) staggered 2 nm-ZnO/1 nm- $\text{Zn}_{0.85}\text{Cd}_{0.15}\text{O}$ /1 nm- $\text{Zn}_{0.75}\text{Cd}_{0.25}\text{O}$ /2 nm-ZnO

Figure 4a shows the dependence of the transition energy on the well thickness for the O- and Zn-face staggered 2 nm-ZnO/ 1 nm- $\text{Zn}_{0.93}\text{Cd}_{0.07}\text{O}$ / $\text{Zn}_{0.9}\text{Cd}_{0.1}\text{O}$ /2 nm-ZnO QWs in comparison to same dependence for conventional QWs. For conventional structure, the transition energy is shown to drop down rapidly with increasing well thickness. This is common trend, which is associated with quantum confined Stark

effect. However, in the case of a staggered QW structure, we notice that the well thickness dependence of the transition energy is greatly reduced owing to better carrier confinement in the staggered QWs. Also, in the case of the O-face staggered 2 nm-ZnO/1 nm-Zn_{0.93}Cd_{0.07}O/Zn_{0.9}Cd_{0.1}O/2 nm-ZnO structure, its reduction effect is observed to be slightly smaller than that of the Zn-face staggered QW structure. Difference in transition energy between O-face staggered structure and Zn-face one can be explained by the polarity effect on the conduction and valence band structures of staggered QWs. We note that the 1st subband energies of the O-face staggered QW structure was shifted upward in comparison to those of Zn-face structures. Thus, an increase in subband energies will lead to enhancement of the transition energy (that was observed in the case of O-face staggered well). Even for large values of well width the subband energies of O-face staggered QWs are higher than those of Zn-face ones. Consequently, we expect that the O-face staggered 2 nm-ZnO/1 nm-Zn_{0.93}Cd_{0.07}O/Zn_{0.9}Cd_{0.1}O/2 nm-ZnO QW structure will have improved characteristics compared to the Zn-face staggered QW structure. This assumption is supported by the results in Fig. 3b, that presents the normalized overlap of wavefunctions as function of well thickness. We observed the expected reduction of the overlap integral with increasing the well width. It is observed that the O-face structure possess the larger value of the overlap integral in the whole well thickness range than that of Zn-face structure.

Fig. 4. Dependence of the transition energy (a) and overlapping the electron and hole wavefunctions (b) on the well width for the Zn- and O-face staggered 2 nm-

ZnO/1 nm-Zn_{0.93}Cd_{0.07}O/Zn_{0.9}Cd_{0.1}O/2 nm-ZnO. This figure also represents the results for conventional 2 nm-ZnO/Zn_{0.9}Cd_{0.1}O/2 nm-ZnO QWs.

In Fig. 5, the transition energy for Zn-face and O-face staggered 2 nm-ZnO/1 nm-Zn_{1-x}Cd_xO/1 nm-Zn_{0.75}Cd_{0.25}O/2nm-ZnO QWs is plotted as a function of cadmium content in the embedded Zn_{1-x}Cd_xO layer. We revealed that transition energy monotonically decreases with increasing the cadmium content within the range 6-20 at.%. It can be explained as follows. It is known that the energy position of subband levels in QW is mainly determined by the total potential profile which is shaped dominantly by the built-in electric field [30]. Therefore, the subband energies are strongly affected by polarization inside the QW. Enhancement of the Cd content in the embedded layer leads to strengthening of the built-in electric field over the same width, thereby lowering the bottom of the right (embedded) quantum well with respect to the ZnO barrier [30]. In this case, the prevailing effect of the left well (1 nm-Zn_{0.75}Cd_{0.25}O) with higher built-in electric field on the position of subband levels weakens. At the same time, staggered quantum well having nearly triangular single-wide-well can reduce the ground state energy level [23]. As a result, the transition energy is decreased for the higher Cd content. It is interesting to note that the transition energy of the O-face staggered QWs demonstrates less sensitivity to the changing of the Cd content than that of the Zn-face staggered QWs. Lower sensitivity of the transition energy of the O-terminated staggered QWs to the Cd content in embedded layer in comparison to Zn-terminated structure is a result of weaker dependence of the 1st subband energy on the Cd content for O-face staggered structures in comparison with Zn face QWs. It can be explained by the difference in orientation of the polarization-induced build-in electric field, which influence in a different manner on the conduction and valence band structure of the staggered QWs. On one hand, an enhancement of the Cd content lowers the bottom of the embedded well and reduces the transition energy. On the other hand, the configuration of the staggered QW with O-face polarity is less prone to lowering of

transition energy than that of structure with Zn-face polarity. Nevertheless, a detailed study of the electronic structure (density of states, consideration of spin-orbit coupling effect) of staggered QWs and adequate experimental investigation are necessary in order to receive more precise picture.

Fig. 5. Dependence of the interband transition energies on the cadmium content in embedded $\text{Zn}_{1-x}\text{Cd}_x\text{O}$ layer in 2 nm-ZnO/1 nm- $\text{Zn}_{1-x}\text{Cd}_x\text{O}$ /1 nm- $\text{Zn}_{0.75}\text{Cd}_{0.25}\text{O}$ /2 nm-ZnO structure.

It should be mentioned that real surfaces of O-face and/or Zn-face ZnO are unstable and have different peculiarities. In most cases, the Zn face is more appropriate for epitaxial growth of films and quantum well structures, whereas the O face is susceptible to the adsorption of chemical species [31]. In addition, Zn-terminated surface demonstrate higher ability to form surface reconstruction in comparison to O-terminated one [31]. In this context, Zn-face QWs seem to be more realizable from the technological point of view. At the same time, theoretical calculations demonstrate improved optical properties of O-face QWs. Therefore, further experimental work is required for clear understanding of mechanisms of stabilization of the O-face surface and development of the technology of O-face QWs.

4. Conclusions

The optical properties of Zn- and O-face $\text{Zn}_{1-x}\text{Cd}_x\text{O}/\text{ZnO}$ conventional and staggered quantum-well structures were comparatively studied by using the self-consistent Schrödinger-Poisson solver. We have revealed that the polar face affects only the band edge profiles (in the virtue of dependence of the sign of spontaneous and piezoelectric polarization on the type of polar plane) and doesn't influence the optical characteristics of the conventional QWs. For the staggered QWs a better carriers' confinement is expected. The behavior of curves of the well thickness dependences of transition energy and overlap of the electron and hole wavefunctions for staggered QW structures indicates that the O-face staggered QWs possess improved optical characteristics. It is also revealed that the O-face staggered QWs have the weaker dependence of the transition energy on the Cd content in embedded layer in contrast to Zn-face structure. Therefore, using the embedded layer in conventional QW structure may be useful for the neutralization of the quantum confined Stark effect induced by polarization fields. Our calculations suggest that polarization engineering via control of material polarity and parameters of staggered QWs can be used to tune emission wavelength (and/or wavelength of light absorbed) of $\text{Zn}_{1-x}\text{Cd}_x\text{O}$ -based QWs for many optoelectronic applications and to realize high performance LEDs and solar cells.

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