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Theoretical study of 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}CdxO-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 the well thickness and has lower sensitivity to Cd content in embedded Zn_{1-x}CdxO layer. Control of the material polarity and design of the staggered QWs provide cost-effective approach for engineering the QW band structures with enhanced QW performance. This enables constructing of the Zn_{1-x}CdxO-based light emission diodes with improved radiative efficiency emitting, applicable for solid state lighting.

1. Introduction

Ternary alloys of zinc oxide (ZnO), particularly $Zn_{1-x}Cd_xO$, are prospective 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]. Due to the direct band-gap of ZnO and possibility to tune its band gap, its absorption/emission range is large and covers virtually the entire solar spectrum [9]. High quality optoelectronic and photovoltaic devices require the quantum-well (QW) structure to be embedded inside. Therefore study of the QW-related effects is very essential for the understanding the radiative recombination processes and carrier confinement in $Zn_{1-x}Cd_xO$/ZnO QWs.

Recently, several groups have studied the properties of $Zn_{1-x}Cd_xO$/ZnO QWs [10–13]. Liu et al. [10] observed the increase of the spontaneous emission rate from $Zn_{1-x}Cd_xO$ 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 $Zn_{0.80}Cd_{0.20}O$/$Zn_{0.92}Cd_{0.08}O$ 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 $Zn_{1-x}Cd_xO$ layer.

It is also well-known that the hexagonal wurtzite structure exhibits noticeable spontaneous and piezoelectric polarization 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 $Zn_{1-x}Cd_xO$ 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 ~10^8 V/m in (Zn,Cd)O/ZnO quantum well structures. Benharrats et al. [15] theoretically predicted that the internal field in $Cd_xZn_{1-x}O$/ZnO ($x \le 0.2$) QWs increases with x with a linear slope A = 17.83 MV/cm. The large internal electric field in the $Zn_{1-x}Cd_xO$ 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 (so called "Quantum Confined Stark Effect"). Therefore, the main efforts should be focused on a searching the ways for the effective suppression of the carrier separation. Staggered QW is a simple

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approach to obtain emitting structures with enhanced electron–hole wavefunction overlap and enhanced recombination rate of the active regions [16].

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

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

2. Theoretical approach

Compressively strained ZnO/$Zn_{1-x}Cd_xO$/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. Fig. 1 depicts the schematic diagrams of the polarizations in conventional ZnO/$Zn_{1-x}Cd_xO$/ZnO structures with Zn-face along the (0001) orientation and O-face along the (000$\bar{1}$) orientation. The spontaneous polarization (P_{SP}) in Zn-face structure is directed 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 as for (0001) ZnCdO films grown under compressive strain, P_{PE} is in the (0001) direction and vice versa for the O-face structure.

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 $Zn_{1-x}Cd_xO$, 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 0.79 m_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 $Zn_{1-x}Cd_xO$ 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]. Due to the lack information in the literature, we assume that dependences of the elastic constants and effective masses on the Cd content of $Zn_{1-x}Cd_xO$ ternary alloy follow the Vegard's law. This is a reasonable assumption since solid solutions usually contain compounds with nearly identical parameters ($m_{eZnO} = 0.21\ m_0$ vs. $m_{eCdO} = 0.24\ m_0$). 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

Fig. 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-$Zn_{0.85}Cd_{0.15}O$/2 nm-ZnO QW structures. Due to polarization discontinuity at the interface between the ZnO barrier layer and $Zn_{0.85}Cd_{0.15}O$ 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 d).

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,

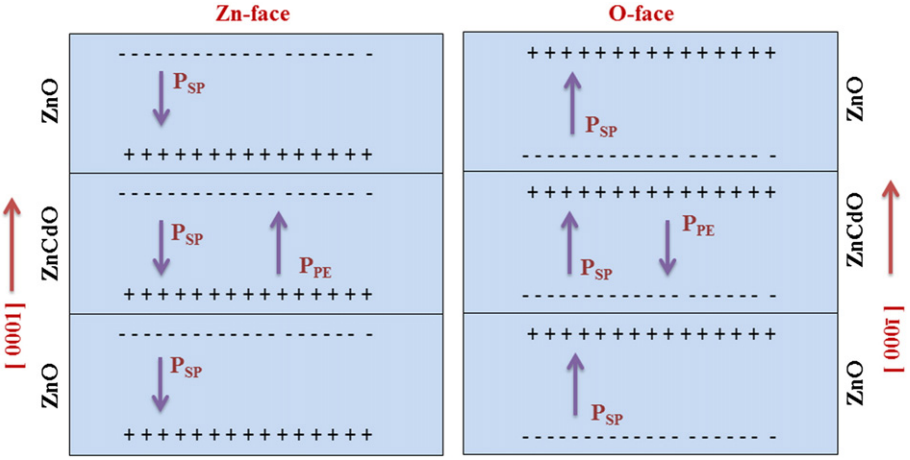

Fig. 1. Schematic diagrams of the polarizations in different epitaxial layers of ZnO/$Zn_{1-x}Cd_xO$/ZnO structure with (left) Zn-face and (right) O-face configurations.