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Origin of high-density two-dimensional electron gas in ZnO/ZnMgO heterostructures

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Abstract. Numerical calculations are performed for determining the polarization charge density $\sigma$ and residual donor concentrations in ZnO/ZnMgO heterostructures. The $\sigma$ value is determined to be 10 mC/m$^2$ for explaining the cathodoluminescence (CL) peak positions in narrow ZnO/ZnMgO multiple-quantum-well (MQW) structures ($\leq$ 4 nm), and is consistent to those obtained from the two-dimensional electron gas (2DEG) density formed in single-hetero and single-quantum-well structures. A significantly high residual donor concentration of $9 \times 10^{18}$ cm$^{-3}$ for ZnMgO layers is obtained for explaining the CL energy to level off for wider wells ($\geq$ 4 nm), and is confirmed by predicting the 2DEG density in a thick ZnO layer grown on an MQW buffer layer which is identical to the one of the MQW structures. The calculation also shows that the 2DEG concentrations in the MQW structures are dominated by the high residual donor concentration.

1. Introduction
ZnO is an n-type semiconductor which exhibits a wide band gap (3.37 eV) comparable to other wide gap semiconductors such as SiC or GaN. As one of these wide band gap semiconductors, ZnO is expected to exhibit a superior high-field transport properties[1] suitable for high-temperature applications. In addition, it has a low-temperature synthesis capability which is a great advantage for fabricating thin-film transistors (TFTs) on a flexible substrate. The potential for transparent and flexible electronics has motivated variety of research on ZnO TFTs[2, 3] and related fabrication processes for TFTs[4]. For practical applications, we have demonstrated that the use of a ZnO/ZnMgO heterostructure is critical for obtaining high performance TFTs. It is therefore important to investigate material parameters in ZnO/ZnMgO heterostructures such as polarization charges and related ones that are indispensable for the device design.

2. Sample preparation
The growth was carried out by using an EpiQuest-made radical source molecular beam epitaxy system equipped with Knudsen cells for Zn and Mg, and a plasma cell for oxygen radicals operated at 350 W. An a-plane sapphire substrate was used as the substrate. On top of the substrate, a 10-nm-thick ZnO layer (LT-ZnO) was grown at a low-temperature of 250°C. After the LT-ZnO layer was annealed at 750°C for 10 minutes, a 1-μm-thick ZnO buffer layer was grown at 500°C and a 40-period multiple quantum wells (MQWs) of Zn$_{0.7}$Mg$_{0.3}$O barrier (5 nm) and ZnO well (1-8 nm) layers and a 50-nm-
thick Zn$_{0.7}$Mg$_{0.3}$O cap layer were grown at 400°C. The lower growth temperature of the MQW layers was to suppress the phase separation\cite{5} of the ZnMgO layers while the ZnO layers were grown at 500°C. A 30-s growth interruption was introduced at each interface in order to make abrupt interface. The structure was grown in the O-polarity (c-axis orientation) and was nominally undoped. The cross sectional structure is depicted in Fig. 1.

3. Results and discussion

An X-ray diffraction (XRD) spectrum for the MQW structure with 8-nm-thick ZnO wells is shown in Fig. 2. The primary diffraction peaks are (0002) diffractions from the ZnMgO/ZnO MQW and ZnO buffer layer. The MQW period of 12.7 nm was determined by comparing the XRD satellite peak positions and the calculated spectrum. In the calculation, the thickness of the ZnO and ZnMgO layers were 7.83 nm and 4.85 nm, respectively.

Cathodoluminescence (CL) spectra were measured for investigating the electronic structure in the MQW structures. The CL peak position corresponding to the bound exciton emission was plotted as a function of the ZnO well width in Fig. 3. The solid line is the emission energy calculated using a square potential model. The exciton binding energy $E_b(L_w)$ is subtracted from the calculation by assuming that the well-width dependence is given by

$$E_b(L_w) = E_{bx} + aL_w \exp \left( - \frac{L_w - cL_w^2}{b} \right) \text{[eV]},$$  \hspace{1cm} (1)

where $L_w$ is the well width in nm, $E_{bx}$ is the exciton binding energy for bulk ZnO (0.06), and $a$, $b$, and $c$ are fitting parameters. The parameters $a$, $b$, and $c$ were chosen to reproduce the experimental values reported by Sun et al.\cite{6} and determined to be 0.115, 1.2, and 0.028, respectively.

![Figure 1. Cross-sectional view of the MQW structure. The MQW and the cap ZnMgO layers are pseudomorphically grown on the thick ZnO buffer layer.](image1)

![Figure 2. Measured (upper) and calculated (lower) XRD spectra for the MQW structure with 8-nm-thick ZnO wells.](image2)

![Figure 3. Cathodoluminescence peak energy (circles) and the calculated peak energy (solid line) using a square potential model.](image3)
The calculated peak energy agrees only for narrow well width ($L_w \leq 2$ nm). The deviation of the calculation is considered primarily due to the quantum-confined Stark (QCS) effect caused by the interplay between the spontaneous and piezoelectric polarizations\[7\]. A dense two-dimensional electron gas (2DEG) is therefore formed by the polarization charges induced at heterointerfaces in ZnO/ZnMgO heterostructures and can be utilized for applications to heterostructure field-effect transistors\[8, 9\] or further practical devices\[10\]. The 2DEG concentration is the one of crucial parameters for the device design. We thus performed numerical calculations of the emission energy of the MQWs by taking the interface polarization charge $\sigma$ as the fitting parameter. The electric field strength for ZnO $E_1$ and ZnMgO $E_2$ were assumed to be constant and satisfy

$$E_1L_w + E_2L_b = 0,$$
$$\varepsilon_1E_1 - \varepsilon_2E_2 = \sigma. \tag{2}$$

Here $L_b$ denotes the barrier thickness and $\varepsilon_1$ and $\varepsilon_2$ are the dielectric constants for ZnO and ZnMgO, respectively. The emission energies for $\sigma = 5$, 10, and 15 mC/m$^2$ are plotted in Fig. 4. Overall agreement is good for $\sigma = 5$ mC/m$^2$. However, the agreement is better for $\sigma = 10$ mC/m$^2$ when the well width is less than 4 nm, and the $\sigma$ value is consistent to that obtained for both single-hetero (SH) and single-quantum-well (SQW) structures\[11\]. The deviation from the observed emission energy increases for wider wells since no space charge effects are included in the calculation. Monotonic reduction in the calculated emission energy occurs due to the QCS effect. In contrast, the CL peak energy approaches to a constant value, indicating that a space-charge effect which flattens the energy band has to come into play.

![Figure 4. Calculated emission energy values for $\sigma = 5, 10, \text{ and } 15 \text{ mC/m}^2$.](image1)

![Figure 5. Emission energy values obtained for various donor concentrations in the ZnMgO barriers.](image2)

We then performed a self-consistent calculation by solving Schrödinger and Poisson equations simultaneously in order to take the space charges into account. The space charges considered include the 2DEG and donors in the ZnO wells and donors in the ZnMgO barriers in addition to the polarization charge $\sigma$ of 10 mC/m$^2$. The residual donor concentration in the ZnO well $N_{dw}$ is lower than middle $10^{17}$ cm$^{-3}$. It is too low to explain the level off of the CL peak energy for wider well width since the net sheet donor concentration in the well is on the order of $10^{11}$ cm$^{-2}$ for wider wells and is much lower than that of the polarization charge $\sigma (= 6.2 \times 10^{12}$ cm$^{-2}$). A higher donor concentration for the ZnMgO barrier is therefore required to explain the CL peak position. The calculated emission energy for various donor concentrations in the ZnMgO barrier $N_{db}$ of 5, 7, and $9 \times 10^{18}$ cm$^{-3}$ is shown in Fig. 5. The $N_{dw}$ value is $5 \times 10^{17}$ cm$^{-3}$. The experimental result is best explained for $N_{db} = 9 \times 10^{18}$ cm$^{-3}$. The significantly high $N_{db}$ value might be due to the low purity of the Mg source and/or to the lower growth temperature of the MQW.
We previously reported a higher value of $\sigma$ in order to estimate the 2DEG concentration in a thick ZnO channel grown on ZnO (5 nm)/ZnMgO (5 nm) MQW layer[12]. The value of 17 mC/m$^2$ was obtained from the 2DEG concentration by a naive approximation where the space-charge effects were neglected. Note that the 2DEG concentration of $5.2 \times 10^{12}$ cm$^{-2}$ was obtained by assuming the above mentioned parameters for the donor concentrations and polarization charge. Therefore, the high value assumed for $N_{db}$ is considered to be plausible.

We now consider the charge neutrality in one period of the MQW structure. The charges have to satisfy the relation

$$N_s = N_{da} L_{eff} + N_{db} L_b,$$

(3)

where $N_s$ denotes the 2DEG concentration and $L_{eff}$ is the effective well width where the donors are ionized. Note that the positive and negative polarization charges induced at the opposite sides of the ZnO well cancel each other. $L_{eff}$ becomes zero for narrow ZnO well width. The 2DEG concentration is therefore dominated by the donor concentrations in the ZnMgO barrier layer since the $N_{db}$ value is much higher than that of $N_{da}$. This situation is quite different from the case for SH or SQW structures where the polarization charge dominates the 2DEG concentration[13].

4. Summary

Numerical calculations were made for determining the polarization charges $\sigma$ induced at ZnO/ZnMgO heterointerfaces by comparing emission energies between cathodoluminescence and the calculation for ZnO (1-8 nm)/ZnMgO (5 nm) MQW structures. The $\sigma$ value of 10 mC/m$^2$ explains the QCS effects well for the narrow well width. The self-consistent calculation revealed that a significantly high donor concentration of $9 \times 10^{18}$ cm$^{-3}$ for ZnMgO layers was predicted although the layers were nominally undoped. The high $N_{db}$ value dominates the 2DEG concentration in the ZnO/ZnMgO MQW structures.

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