Temperature dependence of energy band gap for ZnO thin films

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Abstract *ZnO films on* Al_2O_3 *substrates were grown using a pulsed laser deposition method.* Through photoluminescence (PL) and X-ray diffraction (XRD) measurements, the optimum growth conditions for the ZnO growth were established. The results of the XRD measurements indicate that ZnO films were strongly oriented to the c-axis of the hexagonal structure and epitaxially crystallized under constraints created by the substrate. The full width half maximum for a theta curve of the (0002) peak was 0.201°. Also, from the PL measurements, the grown ZnO films were observed to give free exciton behaviour, which indicates a high quality of the epilayer. The Hall mobility and carrier density of the ZnO films at 293 K were estimated to be 299 cm^2/V s and 8.27×10^{16} cm^{-3}, respectively. The absorption spectra revealed that the temperature dependence of the optical band gap on the ZnO films was $E_g(T) = 3.4393$ eV $- (5.30 \times 10^{-4}$ eV/K$)T^2/(367 + T)$.

Keywords: Zinc Oxide thin films, photoluminescience , optimum growth conditions, absorption spectra , energy band gap

1. Introduction

A II-VI compound semiconductor with a wide direct band gap of 3.37 eV at room temperature [1], Zinc oxide (ZnO) is an attractive material because of its optoelectronic applications such as for light emitting diodes (LED), laser diodes (LD), surface acoustic waves (SAW), and surface elastic-wave filters [2-6]. In particular, ZnO has a higher exciton binding energy of about 60 meV at room temperature than do the materials ZnSe and GaN [1]. In the present study, the ZnO films were grown on sapphire (Al_2O_3) substrates by a PLD method. The grown ZnO was investigated for its structural and optical characteristics by means of X-ray diffraction (XRD), photoluminescence (PL), and absorption spectroscopy. This paper reports on the optimum growth conditions, structural characteristics, and band gap.

2. Experimental procedures

Fig. 1 shows a schematic diagram of the PLD system for ZnO film growth. Prior to PLD growth, the ZnO target disk (3 mm thick and 12 mm in diameter) fabricated by compressing ZnO powder was used as a source of the PLD. In order to grow ZnO films, an ArF pulsed excimer laser (Lambda Physik, LPX110i, $\lambda = 193$ nm) was used as a photon source. In order to get a uniform film thickness, the rotating speed of the target was kept at 40 rpm during the deposition. Also, pure oxygen gas as a background gas was used to create the ambient pressure during ZnO film growth. The laser repetition rate was 10 Hz, and the power per pulse was 100 mJ. Therefore, the energy density on the target was estimated to be 2 J/cm^2. At this time, the gas pressure was 10 Pa. The target-substrate distance was set at 4 cm. The substrate used for ZnO films was (0001) Al_2O_3.

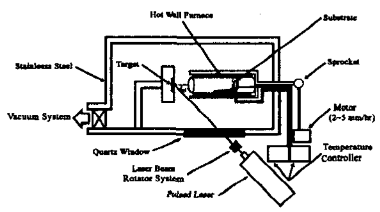

Fig. 1. A schematic diagram of the PLD system for ZnO film growth.

3. Result and discussion

3.1. Optical absorption measurements

Fig. 2 shows the optical absorption spectra obtained in the temperature range of 10 K to 293 K. To identify the energy band gap for ZnO films, we carefully examined the relation between the optical absorption coefficient (α) and the incident photon energy (hv) from the optical absorption measurements in Fig2. The relation for a direct band gap between hv and α is given by:

$$(\alpha h\nu)^2 \sim (h\nu - E_g). \quad (1)$$

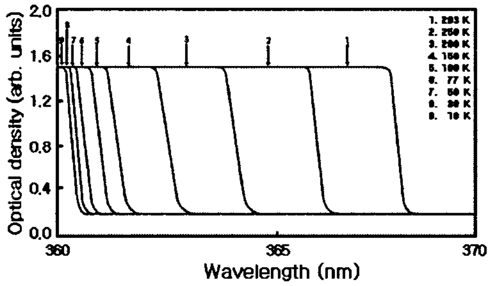

Fig. 1. Optical absorption spectra obtained in the temperature range of 10 K to 293 K.

Fig. 3 displays the band gap energy variation of ZnO film using Eq. (1) as a function of temperature. This figure does not follow the conventional linear relationship. Therefore, the temperature dependence of the optical energy band gap in our experiment is well fitted numerically by the following formula:

$$E_g(T) = E_g(0) - \alpha T^2/(T + \beta) \quad (2)$$

where α is a constant and β is approximately the Debye temperature. Also, $E_g(0)$ is the energy band gap at 0 K, which is estimated to be 3.4393 eV. When α and β are taken to be 5.30×10^{-4} eV/K and 367 K, respectively, the curve plotted by Eq. (2) closely fits the experimental values, as shown in Fig.32. However, $E_g(0)$ and α were nearly consistent to the values obtained by Ray . Also, the Debye temperature of ZnO was found to be 370 K and in a reasonable agreement with our result.

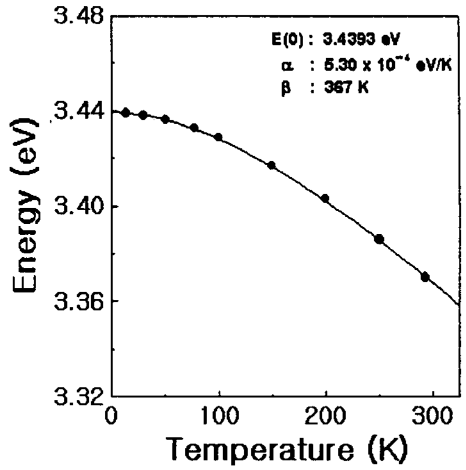

Fig.3. Optical energy band gap of ZnO films plotted as a function of temperature.

4. Conclusions

ZnO films were grown on Al_2O_3 substrates using a PLD method and the optimum growth conditions were described. The results of the PL and the XRD measurements revealed that the grown ZnO films are highly crystalline and good quality. The results of the XRD measurements indicate that ZnO films are strongly oriented to the c-axis of the hexagonal structure and epitaxially crystallized under constraints created by the substrate. The FWHM the (0002) peak turned out to be 0.201°. This value corresponded to that of a film grown using an MBE method. The Hall mobility and the carrier density of the ZnO film at 293 K were estimated to be 299 cm^2/V s and 8.27×10^{16} cm^{-3}, respectively. Finally, the optical band gap obtained from the absorption measurements was well described by the Varshni's relation, $Eg(T) = 3.4393$ eV $-$ $(5.30 \times 10^{-4}$ eV/K$)T^2/(367 + T)$.

References

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