# Structural Characterization and Photoluminescent Properties of $Zn_{1-x}Mg_xO$ Films on Silicon *

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*$Zn_{1-x}Mg_xO$ films have been grown on silicon at various substrate temperatures by pulsed laser deposition. The structural and photoluminescent properties of films as a function of substrate temperature have been studied. The optimized substrate temperature is 650°C. The x-ray diffraction spectra indicate that the films are highly C-axis oriented, and no phase separation is observed. The crystal grain size of the films is about 100 nm as examined by atomic force microscopy. The cross-sectional transmission electron microscopy verified the C-axis orientation of the $Zn_{1-x}Mg_xO$. These films showed ultraviolet photoluminescence at room temperature. The near-band-edge emission peak of the $Zn_{1-x}Mg_xO$ film deposited at 600°C has a blueshift (0.40 eV) larger than that of the film deposited at 500°C (0.33 eV). The ratio of the near-band-edge to defect level peak intensity is as large as 159.*

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The intense interest in blue and ultraviolet (UV) light emitters and detectors has promoted great research effort into wide bandgap semiconductors. ZnO, with a direct bandgap of 3.3 eV, has attracted significant attention.[1−4] Its large exciton binding energy (60 meV) has enabled observation of laser action and stimulated emission of excitons at room temperature. Heterostructures, superlattices and quantum wells are key structures for constructing various electronic and optical devices.[5−8] Modulation of the bandgap is essential in order to keep the lattice constant unchanged. ZnMgO has been considered as a promising candidate for optoelectronic devices, because the bandgap energy of $Zn_{1-x}Mg_xO$ can be tuned from 3.3 eV to 4.0 eV by varying the Mg composition. In addition, the replacement of Zn by Mg is not expected to induce a significant change in lattice constant due to the similarity of their ionic radii.[9,10] In recent reports, sapphire or $S_CAlMgO_4$ (SCAM) have been used as substrates for ZnMgO films.[9−11,14,16] There have been no reports yet on using Si as a substrate, though Si substrates will facilitate the device processing. In this Letter, we report on high-quality ZnMgO films on an Si substrate. We discuss the crystalline quality and photoluminescent properties of ZnMgO as a function of substrate temperature.

The pulsed laser deposition (PLD) method was employed to prepare the films by ablating the $Zn_{0.8}Mg_{0.2}O$ ceramic target. We used a p-type Si wafer, with a diameter of 3 inches, as the substrate. The Si wafer was cleaned in $NH_3H_2O$, HCl and HF alternatively before being loaded into the deposition chamber. The base pressure was $4 \times 10^{-5}$ Torr. Oxygen was introduced to reduce the oxygen vacancies in films. A KrF laser (248 nm, 1.5 Hz) was used as the ablation laser. The target and substrate were rotated to maintain the uniformity of the films. In order to study the effects of substrate temperature, we prepared the $Zn_{1-x}Mg_xO$ films at various substrate temperatures. Other growth parameters were kept constant. The crystal structure of the films was analysed by x-ray diffraction (XRD) (Philip, Cu $K_\alpha = 0.15409$ nm). The surface morphology was examined using atomic force microscopy (AFM). The cross-section microstructure of the film was observed by transmission electron microscopy (TEM). The optical properties were characterized by photoluminescence (PL) spectra at room temperature. A continuous He–Cd laser (325 nm) was used for the PL measurements.

The substrate temperature is significant for the crystalline quality of $Zn_{1-x}Mg_xO$ films. Five samples were deposited at five substrate temperatures, 500, 550, 600, 650 and 700°C, respectively. Figure 1 shows the XRD spectra of $Zn_{1-x}Mg_xO$ films deposited at 550, 600 and 650°C. In Fig. 1(a), three peaks, (002), (101) and (102), can be observed. In Fig. 1(b), the (102) peak disappears. The intensity of the (002) peak is much higher than that of the (101) peak. In Fig. 1(c), only the (002) peak is observed. Compared with Figs. 1(a) and 1(b), the intensity of the (002) peak in Fig. 1(c) is higher, and the full width at half maximum (FWHM) is much narrower. This indicates that the film is of better crystalline quality. In the XRD spectra, the dominance of the (002) peaks shows that the films are of *c*-axis orientation. No peak of MgO is observed in the XRD spectra, demonstrating single-phase $Zn_{1-x}Mg_xO$ without a separate MgO phase. Figure 2 shows the FWHM as a function of substrate temperature. When the substrate tempera-

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ture is 650°C, the FWHM is minimum (0.192°), and the crystalline quality is the best. The following can be interpreted. When the substrate temperature is very low, atoms cannot obtain enough energy to diffuse to appropriate positions for nucleation; when the substrate temperature is very high, the desorption of oxygen atoms is enhanced, increasing oxygen vacancies in $Zn_{1-x}Mg_xO$ films, while oxygen vacancies will destroy the crystalline quality and photoluminescent properties of films. From this study, we conclude that the optimized substrate temperature is about 650°C.

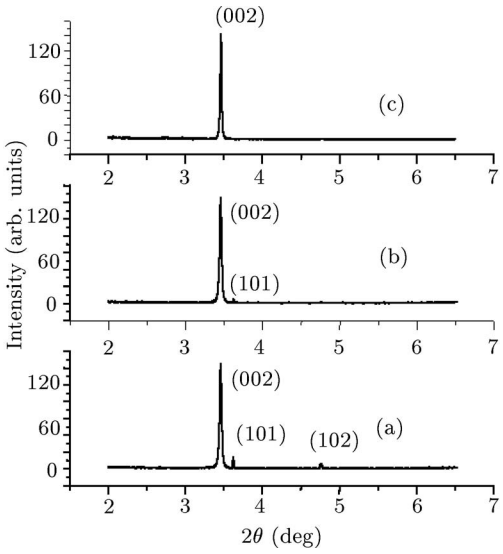



**Fig. 1.** XRD spectra of films prepared at (a) 550°C, (b) 600°C and (c) 650°C.

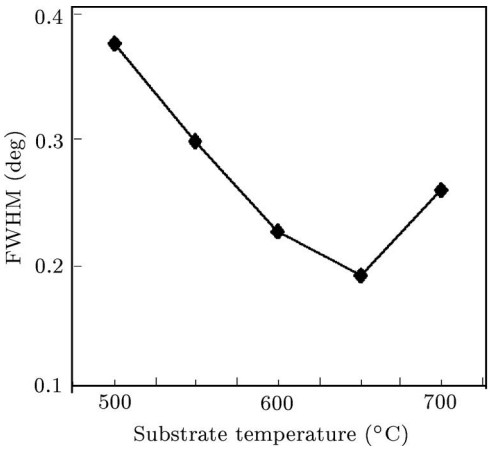



**Fig. 2.** FWHM versus substrate temperature.

In the XRD spectra, the (002) peaks were found to shift to higher angles from those of ZnO. The *c*-axis lattice constant of the films is calculated to be only 0.50% smaller than that of ZnO, which is much better than many recent results.[10,11,13,14]

Figure 3 shows the surface morphology of the $Zn_{1-x}Mg_xO$ film prepared at 600°C. The grain size is about 100 nm. The surface roughness is about 20 nm.

The cross-sectional TEM image of the film deposited at 600°C is showed in Fig. 4. Columnar grains are perpendicular to the silicon substrate. This indicates the *c*-axis orientation of the $Zn_{1-x}Mg_xO$ film, in good agreement with the results of the XRD spectra.

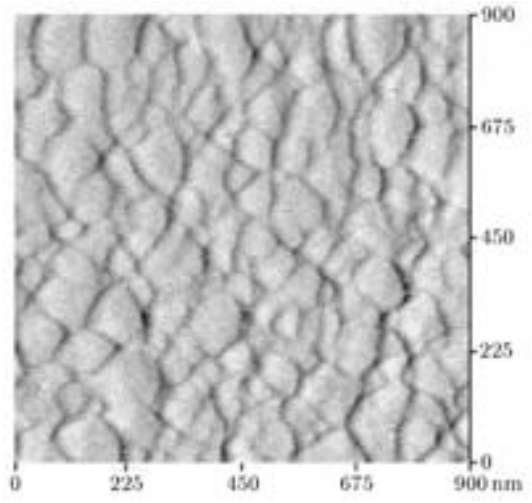



**Fig. 3.** AFM image of the $Zn_{1-x}Mg_xO$ film deposited at 600°C.

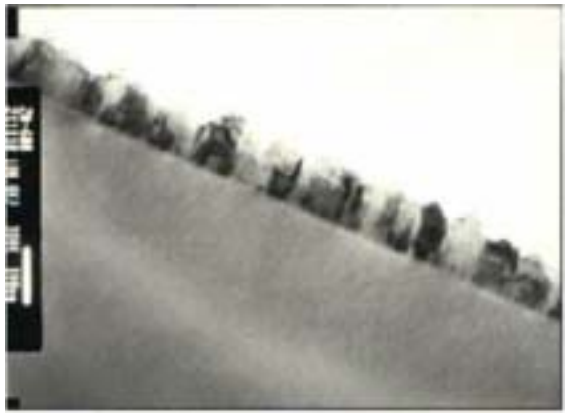


**Fig. 4.** Cross-sectional TEM image of the $Zn_{1-x}Mg_xO$ film deposited at 600°C.

Figure 5 shows the PL spectra of the $Zn_{1-x}Mg_xO$ films measured at room temperature. In Fig. 5(a), the near-band-energy (NBE) emission is located at 337 nm (3.63 eV). It has a blueshift of 0.33 eV from that of ZnO (3.3 eV). The green emission peak (500 nm) associated with the oxygen vacancy is well suppressed. This demonstrates that there are few oxygen vacancy defects in the $Zn_{1-x}Mg_xO$ film. Another emission peak at 408 nm is also observed. This may result from the Zn interstice in the $Zn_{1-x}Mg_xO$ film, according to the literature.[15]

However, in Fig. 5(b), the near-band-energy emission of the film is observed at 330 nm (3.70 eV). It has a larger blueshift (0.4 eV) compared with that of the $Zn_{1-x}Mg_xO$ film (0.33 eV) prepared at 500°C. Moreover, the emission peak at 400 nm associated with the

Zn interstice becomes weaker. This indicates the increase of Mg composition in the film, which is interpreted to be due to an increase of the vapour pressure of ZnO and Zn as the substrate temperature increases, enhancing the desorption of Zn-related species from the substrate.[16] Consequently, the near-band-energy emission of the film deposited at a higher temperature has a larger blueshift, and the Zn interstice related emission becomes weaker. The oxygen vacancy emission at 500 nm is very weak compared with the near-band-energy emission. To evaluate the defect level of the $Zn_{1-x}Mg_xO$ film prepared at 600°C, we employed the ratio of intensity of near-band-energy emission to that of defect level emission ($R = I_{NBE}/I_{DL}$). The ratio is as large as 159, which is much better that the usual ratio, 20, of ZnO films grown by molecular beam epitaxy (MBE).[11,12]

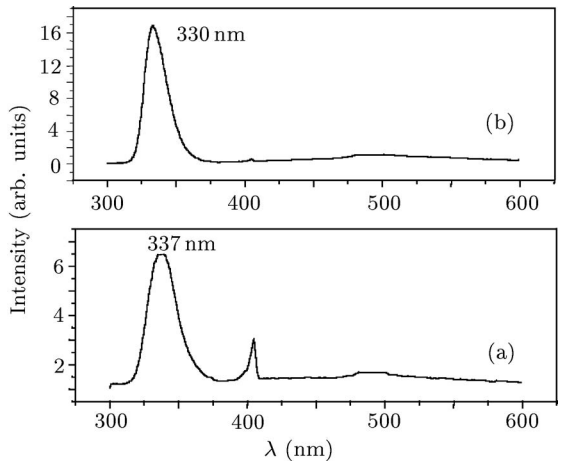



**Fig. 5.** Photoluminescence spectra of $Zn_{1-x}Mg_xO$ films deposited at (a) 500°C and (b) 600°C.

In conclusion, $Zn_{1-x}Mg_xO$ films have been deposited on Si by PLD. The optimized substrate temperature is 650 °C. The XRD spectra show that $Zn_{1-x}Mg_xO$ films are highly *c*-axis oriented and no phase separation is observed. The UV emission peaks of $Zn_{1-x}Mg_xO$ films have a blueshift from those of ZnO. The UV emission peak of the $Zn_{1-x}Mg_xO$ film deposited at 600°C has a larger blueshift compared with that of the $Zn_{1-x}Mg_xO$ film deposited at 500°C. The ratio $R$ ($I_{NBE}/I_{DL}$) of the film deposited at 600°C is as large as 159. Consequently, $Zn_{1-x}Mg_xO$ films are of a high quality for exciton emission at room temperature. These results indicate that $Zn_{1-x}Mg_xO$ films have potential applications in optoelectronic devices.

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