

Structural and photoluminescence properties of ALD zinc oxide thin films

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In this paper, we report structural and optical properties of ZnO thin films grown on single crystal ZnO substrates by means of Atomic Layer Deposition (ALD). Our x-ray diffraction data and photoluminescence measurements indicate a good crystallinity and low concentration of lattice defects of the ZnO films, which depend on the deposition temperature.

ZnO films were grown at 120 C and 200 C using diethylzinc and water as precursors. The films were grown on oxygen-terminated single crystal ZnO substrates to a thickness of 100nm. The X-ray diffraction data were obtained using a Rigaku Ultima IV XRD. The XRD measurements show that the films are polycrystalline with a strong preferred *c*-axis orientation. The (002) peak, shown in Fig.1, is essentially due to the substrate, since the signal from the film and substrate

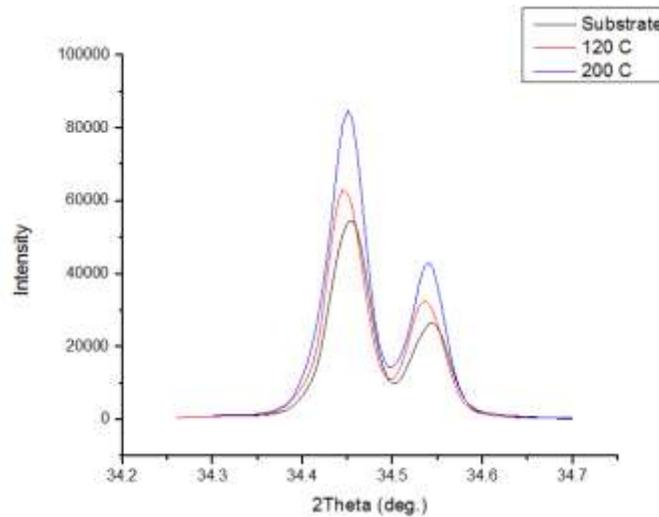


Figure 1: $2\theta/\omega$ scan of the (002) diffraction peak of the ZnO films, as compared to the substrate.

overlap at the (002) peak. The second peak in the (002) diffraction pattern is from the Cu $K\alpha_2$ wavelength. On the other hand, the (001) peak, shown in Fig 2, is due to the film, as it cannot be seen in hexagonal zinc oxide. The (001) peak is due to point defects, such as oxygen vacancies, which produce deformations of the ZnO lattice. The (001) peaks in the films grown at 120 and 200 C have different shapes and are slightly shifted. The *c* lattice constant of the ZnO films

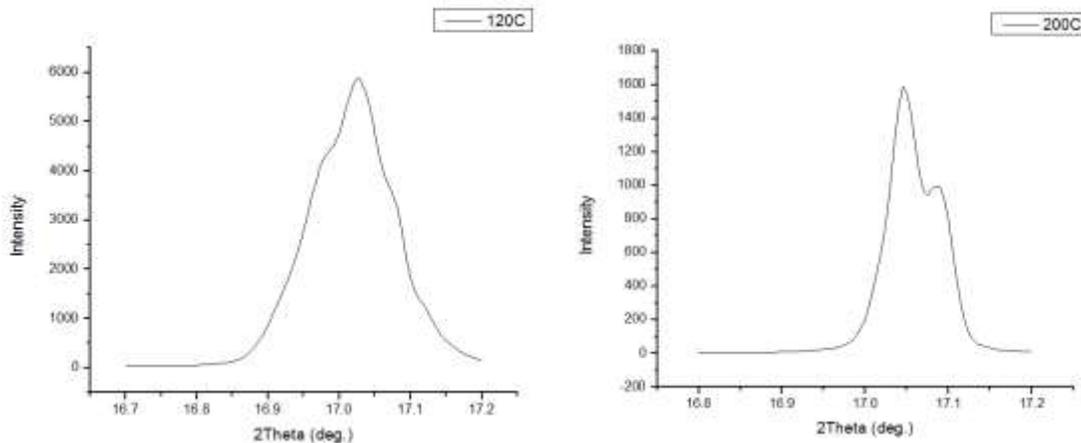


Figure 2: $2\theta/\omega$ scan of the (001) diffraction peak of the ZnO films grown at 120 and 200 C.

were determined from the (001) peak positions (Table 1). The shift in the peak positions of the films grown at 120 and 200 C corresponds to 0.2% difference in the c lattice constant.

Table 1: XRD data of the ZnO films on ZnO substrate.

Sample	2-theta	c lattice constant	FWHM
(002)			
Substrate	34.4532	5.20194	0.0505
120C	34.4461	5.20298	0.0480
200C	34.4527	5.20202	0.0496
(001)			
120C	17.0333	5.2012	0.0372
200C	17.0477	5.1968	0.0479

Our photoluminescence (PL) and surface photovoltage (SPV) spectroscopy results also indicated that the obtained thin films are of high quality. In particular we observed that, on the one hand, “deep” defect signatures in the PL and SPV spectra have low relative intensity. On the other hand the excitonic peaks in the near-band gap range of the low-temperature PL spectra are intense and narrow whereas the super-band gap SPV transitions are sharp and well-defined. In comparison, for ZnO thin films vapor phase-deposited on single-crystalline ZnO substrates [1] the reported excitonic lines were order of magnitude broader in the low-temperature spectra. Also, the XRD results for those films showed a strong mosaicity which limited the structural quality of their film.

Nonetheless, the thin films grown at different temperatures exhibited discrepancies in their optical and structural characteristics. For example, the relative intensity of the ~ 3.33 eV luminescence peak in the 10 K PL spectra, commonly attributed to extended structural defects [2], was significantly greater for the sample grown at 120°C (cf. Fig. 3A). Moreover, the deep level (visible) luminescence in the room temperature PL spectra is also different. For the same

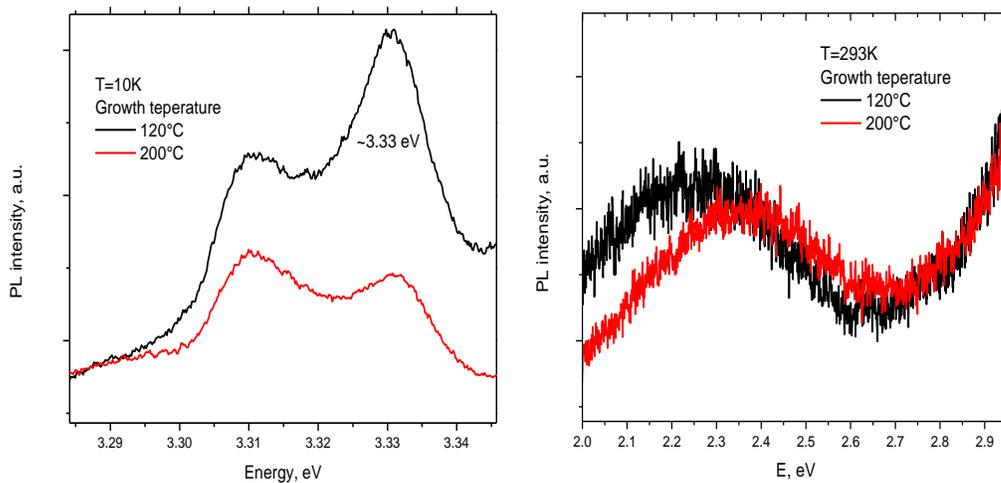


Figure 3: Photoluminescence at 10K (A) and 293K (B) of the ZnO films grown at 120 and 200 C.

sample grown at 120°C the broad emission exhibits a substantial red shift (cf. Fig. 3B). The ~ 2.4 eV emission is most often attributed to oxygen deficiency whereas the observed shift may indicate presence of the second lower-energy luminescent component usually associated with the Zn interstitial defects.

To further elucidate the nature of these differences we analyzed temperature dependences of the relative intensities, spectral positions and widths of the excitonic luminescent features in the PL spectra of the studied specimens. In particular, we obtained activation energies of the bound excitonic states, as well as rough estimates of intensities of the exciton-phonon scattering.

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