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Observations of Nucleation and Growth of Epitaxial ZnO on {11$\bar{2}$0} Sapphire

Paul FONS[1], Ken Nakahara[2], Akimasa YAMADA[1], Kakuya Iwata[1], Shigeru NIKI[*1]
[1]AIST, Photonics Institute, Tsukuba, Ibaraki 305-8568, Japan
[2] Rohm Corporation, 21 Mizosaki-cho Saiin, Kyoto, 615-8585 JAPAN

Introduction

The 3.37 eV room-temperature direct bandgap material ZnO (space group $P6_3mc=C^4_{6v}$) has recently solicited a great deal of interest as an alternative wide-bandgap material. ZnO has the advantage that it is possible to achieve heteroepitaxial growth onto sapphire substrates at substrate temperatures $T_S < 350$°C. [1] In addition, its unusually high exciton binding energy of 60 meV may allow the fabrication of room-temperature devices that utilize excitonic effects.

Elimination of 30° rotation twins observed in epitaxial ZnO films grown by MBE on (0001) sapphire substrates was demonstrated by growing (0001) oriented ZnO on the (1$\bar{1}$20) face of sapphire despite the apparent symmetry mismatch between the (C_6) epilayer and the (C_2) substate. [2]

Experiment

To provide data for further optimization of the growth process, we have investigated the initial growth stages of ZnO on (1$\bar{1}$20) sapphire using a combination of high-resolution x-ray diffraction (HRXRD) and extended x-ray absorption measurements (EXAFS).

Samples of varying thickness 3, 5, 8, 10, 20, 100, and 600 nm, were grown by molecular beam epitaxy using elemental Zn and a RF radical source for sources at a temperature of 350°C. Diffraction measurements indicated that the films were c-oriented with an in-plane epilayer/substrate orientation < 11$\bar{2}$0 > / / [0001]. HRXRD Reciprocal space maps were taken about the (0002) reciprocal lattice points; the lateral coherence length of the optics allowed for probing long-range order over the entire film thickness. Short-range order was probed by EXAFS measurements in fluorescence mode taken using the Zn K_α-edge with an in-plane polarization geometry using beamline 12c.

Results and Discussion

Fig. 1 shows a reciprocal space area map for a ~5 nm thick ZnO epilayer near the ZnO (0002) RLP. In the figure, a resolution limited (~0.003°) streak is visible with no intensity present outside the central streak. The slight tilt observable along the RLP diffraction streak reflects the substrate miscut; the normal to the surface corresponding to the elongation direction of the RLP.

EXAFS analysis of the films indicated a monotonic increase in c-axis lattice constant with decreasing film thickness consistent with HRXRD results. Unlike the HRXRD results, the static disorder parameter was found to strongly increase as film thickness decreased as can be seen in Fig. 2.

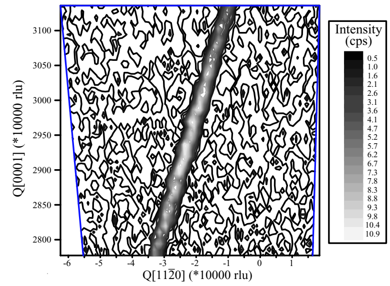

Figure 1: Triple axis x-ray reciprocal space map near the ZnO (0002) reflection for a ZnO film grown on approximately 5 nm thick

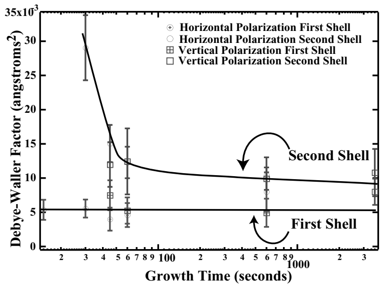

Figure 2: Fitted Debye-Waller disorder parameters for the first and second shells for both vertical and horizontal polarizations

Conclusion

Both HRXRD and EXAFS data were found to be consistent with a relaxation process involving large in-plane bond angle distortion which preserved the long-range order along the c-axis. Concomitant with this, a slight extension in c-lattice constant was observed with decreasing film thickness. For thicker films, the large in-plane bond angle distortion was observed to decrease leading to a columnar like structure which could be observed using glancing incidence HRXRD.

References

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