Threading Dislocations in Domain-Matching Epitaxial Films of ZnO

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The structures of high quality ZnO epitaxial films grown by pulsed-laser deposition on sapphire (0001) without an oxygen gas flow were investigated by X-ray diffraction. In addition to sapphire (0006) reflection, only ZnO (0002) and (0004) refelctions were observed in radial scan along surface normoal, indicating the ZnO layer is (001) oriented. Azimuthal scan across sapphire $\{20\bar{2}2\}$ and ZnO $\{20\bar{2}2\}$ off normal reflections shown in Fig. 1, exhibit 3 and 6 evenly spaced peaks, respectively. The 30° offset between the two sets of {20-22} refelctions reveals the in-plnae epitaxial relationship of $[10\bar{1}0]_{\text{sapphire}} \parallel [11\bar{2}0]_{\text{ZnO}}$ and $[11\bar{2}0]_{\text{sapphire}} \parallel [01\bar{1}0]_{\text{ZnO}}$.

The radial scans across ZnO (0002) and $(10\bar{1}0)$ reflections are illustrated in Fig. 2 and the symmetry w-rocking curves of the same reflections are shown in Fig. 3.

The great disparity of X-ray diffraction line widths between the normal and in-plane reflections reveals the specific threading dislocation (TD) geometry of ZnO. Using Williamson and Hall plot, we derived the tilt and twist angles and coherence length of the ZnO layer. It is known that the Buregers vectiors for ZnO with the wurtzite structure are $b_E = \langle 11\bar{2}0 \rangle / 3$ for edge type TDs and bc = <0001> for screw type TDs, respectively. With the obtained data, we calculated the density are respectively ~ 2×10^{10} and 2×10^{8} cm^{-1} for edge and screw type TDs. The pure edge TDs is the dominant type. From a combination of scattering and microscopic results, it is found that threading dislocations are not uniformly distributed in the ZnO films, but the films consist of columnar epitaxial cores surrounded by annular regions of edge threading dislocations at a large density. The local surface morphology and capacitance signal obtained from atomic force and scanning capacitance microscopes indicate the aggregation of threading dislocations leads to the high interface traps at the annular regions.

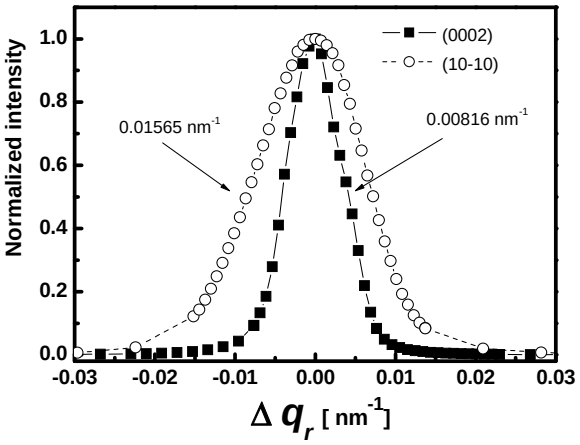

Figure 2. Superimposed radial scans of ZnO (0002) and $(10\bar{1}0)$ reflections. The abscissa, q_r, is the deviation of the scattering vector, $q = 4 \quad \sin(\ .\ )/\ .$ away from the corresponding reflection in the radial direction. (All values denote FWHM.)

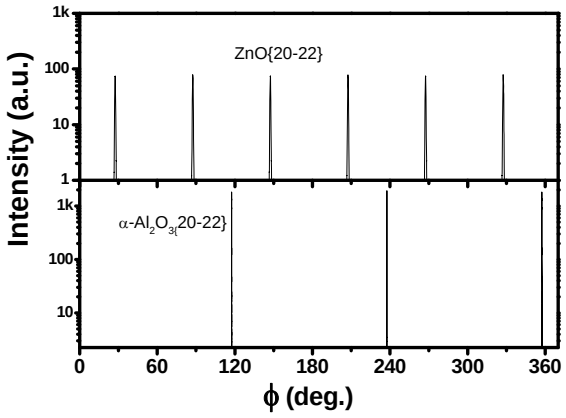

Figure 1. Azimuthal scans of ZnO $\{20\bar{2}2\}$ and sapphire $\{20\bar{2}2\}$ reflections.

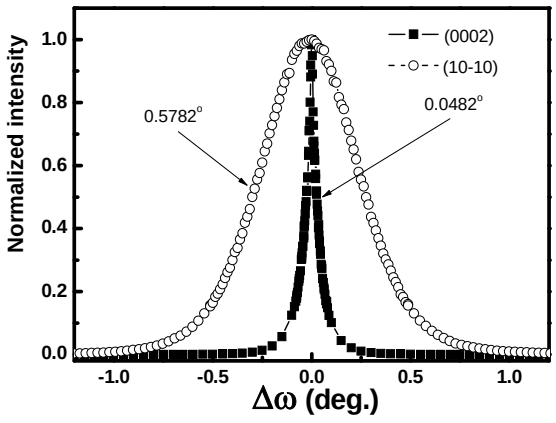

Figure 3. Symmetric ω scans of ZnO (0002) and $(10\bar{1}0)$ reflections.