

# Structural Investigation of MBE Grown Yttrium-Doped HfO<sub>2</sub> Heterostructure

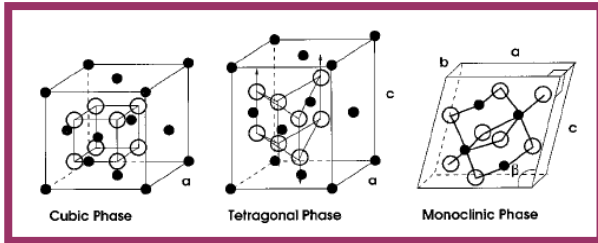
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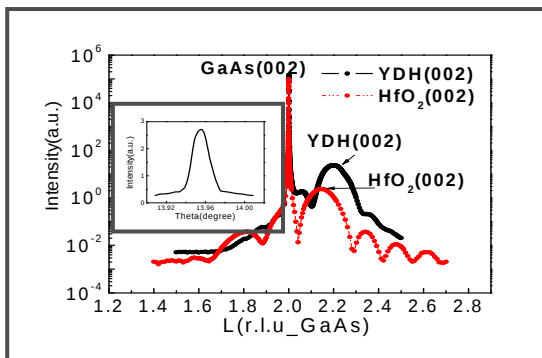
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Cubic phase yttrium-doped HfO<sub>2</sub> (YDH) ultra-thin films were grown on n-type (100) GaAs substrates by molecular beam epitaxy (MBE) deposition at 550 °C substrate temperature. Systematically structural and morphological investigations by x-ray scattering reveal the YDH thin films are epitaxial to the semiconductor substrates with their <100> axes parallel to each other. The structure transformation of HfO<sub>2</sub> induced by yttrium doping significantly increases its dielectric constant.



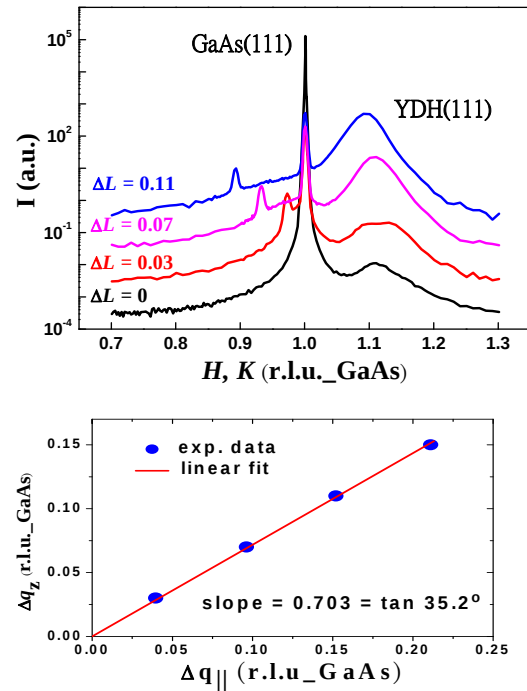
**Figure 1.** Three known structures of HfO<sub>2</sub> and their dielectric constants.

The intensity profile of x-rays scattered by the YDH film grown on GaAs(001) along the (002) crystal truncation rod (CTR) is shown by the solid curve in Fig. 2. As a comparison, the same scan of a pure HfO<sub>2</sub> film, which has the monoclinic crystal structure with four domains rotated 90° against each other coexisting, is also depicted by the dash line and exhibits a drastically different profile. With careful analysis of the crystal structure, all the observed reflections can be indexed by the Bragg peaks belonging to a cubic crystal structure. The best fit of measured atomic planar distances yields a lattice constant  $a = 5.12$  Å. The full width at half maximum (FWHM) of the HfO<sub>2</sub> (0 0 2) reflection 0.076 nm<sup>-1</sup> gives a coherent length  $\sim 7.6$  nm along the growth direction, which is very close to film thickness. This indicates that the YDH layer epitaxially grown on GaAs by our MBE approach is of high crystalline quality, even with a lattice mismatch as large as -10.37 %.



**Figure 2.** Intensity profile of the (0 0 2) CTR. The black curve is the scan of YDH; the red one is pure HfO<sub>2</sub>. The inset shows the rocking curve at YDH (002) which has a FWHM of 0.022°. (As a comparison, the FWHM of GaAs (0 0 2) reflection is 0.006°).

Sharp satellite peaks were observed in [110] scans across (11L) with various  $L$  values. The traces of the satellite peaks make an angle of  $\sim 35.3^\circ$  with the (001) surface plane. This can be attributed to the lowest surface energy of {111} planes for oxides with a fluorite type structure.



YDH, one of the most promising oxide candidates for high  $\kappa$  epitaxial thin film transistors, has been successfully grown on GaAs substrates. We have demonstrated that the epitaxial YDH films is cubic phase with their <100> axes parallel to those of the underneath GaAs substrates.

(111) and (1-11) facets formed at YDH surface decrease the total energy of the system.