MS43-P11 Structure characterization of lattice-matched rutile and TiO_2-II phases grown by atomic layer deposition on α-Al_2O_3(0 0 1)

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Atomic layer deposition of TiO_2 from $TiCl_4$ and ozone on single crystal α-Al_2O_3(0 0 1) substrates was investigated. The structure of films was characterized using X-ray reflection (XRR) and X-ray diffraction (XRD) in high resolution (HR), in-plane (IP) and reciprocal space mapping (RSM) modes.

HR-XRD θ–2θ diffraction patterns of the films deposited on c-sapphire at 400–600°C, showed two reflections together with their Pendellsösung fringes, which implied that (1 0 0)-oriented high-pressure TiO_2-II or strained rutile was formed. X-ray crystallite sizes in direction of surface normal, determined from boardening analysis of the reflections were comparable to the film thicknesses (XRR) at $T_G \geq 400$°C.

IP-XRD analysis revealed that at 400–600°C both rutile and TiO_2-II were epitaxially grown in the films with epitaxial relationships of $[0\ 1\ 0]_R//[1\ 0\ 0]_S$ and $[0\ 0\ 1]_R//[1\ 2\ 0]_S$ for rutile and sapphire, and $[0\ 0\ 1]_{II}//[1\ 0\ 0]_S$ and $[0\ {-1}\ 0]_{II}//[1\ 2\ 0]_S$ for TiO_2-II and sapphire. It is worth noting that the $(0\ 0\ 1)_{II}//(0\ 1\ 0)_R$ in-plane relationship for rutile and TiO_2-II in our films differed from the $(0\ 0\ 1)_{II}//\{0\ 1\ 1\}_R$ relationship reported earlier for TiO_2-II and rutile in a natural form of TiO_2 [1].

Lattice parameters were determined by IP-XRD analysis of reflections 0 2 0, 0 0 2 of TiO_2-II and 0 1 1 of rutile and by RSM of reflection 3 1 1 of TiO_2-II and reflections 3 1 0 and 3 0 1 of rutile. The parameters of TiO_2-II were $a_{II} = 0.4531 \pm 0.0002$ nm, $b_{II} = 0.546 \pm 0.003$ nm and $c_{II} = 0.482 \pm 0.006$ nm while those of rutile equaled to $a_R = 0.4531 \pm 0.0002$ nm, $b_R = 0.475 \pm 0.006$ nm and $c_R = 0.29 \pm 0.01$ nm. According to these results the crystallites with TiO_2-II and highly strained rutile structures were evidently lattice-matched to each other in the films. Comparison of the in-plane atomic arrangements in 2D unit cells of α-Al_2O_3(0 0 1), rutile (1 0 0) and TiO_2-II (1 0 0) (Fig. 1) demonstrated relatively good lattice match explaining the epitaxial growth observed in our experiments.

From boardening analysis of reflections 1 1 0 and 1 1 1 for TiO_2-II and 1 1 0, 1 0 1, 3 0 1 for rutile the in-plane X-ray crystallite sizes were estimated to be 4.0 nm for TiO_2-II and 3.6 nm for rutile.

[1] D.W. Meng, X.L. Wu, F. Sun, L.W. Huang, F. Liu, Y.J. Han, J.P. Zheng, X. Meng, R. Mason, High-pressure polymorphic transformation of rutile to α-PbO_2-type TiO_2 at $\{0\ 1\ 1\}_R$ twin boundaries, Micron 39 (2008) 280–286.

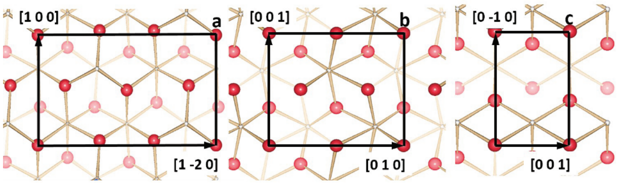

Figure 1. Structure models of in-plane unit cells and atomic arrangements for (a) α-Al_2O_3(0 0 1), (b) TiO_2-II(1 0 0) and (c) rutile(1 0 0) atomic planes. Large spheres designate positions of oxygen and small spheres show location of Al or Ti. Labels at arrows show crystallographic directions.

Keywords: Titanium Dioxide, Thin Films, Atomic Layer Deposition, Crystal Structure, Epitaxy, TiO2-II, Rutile