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Crystallization Process of $SrZrO_3$ Thin Films by Pulsed Laser Deposition

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Introduction

Pulsed Laser Deposition (PLD) is well known to provide highly epitaxial thin films of perovskite type oxides when they are grown on single crystal substrates at high temperatures. We have reported that room-temperature PLD and the following post-annealing process can be another route for epitaxial crystallization, however, their properties may be different due to different routes of crystallization [1]. *In-situ* XRD analyses of crystallization process have revealed that the as-deposited amorphous phase can easily be rearranged into a periodical structure above 520°C along with the ionic arrangements of the single crystal substrate, while polycrystalline phases of a few hundred-nm sized grains are obtained on amorphous substrates at the same temperature. Furthermore, a zirconia phase is obtained above 620°C on the amorphous substrate.

In this report, the results of XANES analyses of $SrZr_{0.95}Y_{0.05}O_3$ (SZY) and $Zr_{0.84}Y_{0.16}O_{2-\delta}$ (YSZ) thin films are presented to observe the change in the local structures around Zr ions in amorphous and the crystalline phases.

Experimental

Thin films have been deposited on optically-polished fused silica wafers (15×15×0.5 mm^3) by PLD at room temperature using ceramic targets. As-deposited and post-annealed thin films have been investigated by XRD and XANES measurements. Fluorescence XANES spectra of the Zr K-edges have been obtained by a Lytle-type ionization chamber at PF-AR NW10A.

Results and discussion

It is found that the zirconia secondary phase, in the form of nano-sized crystals around the a few hundred nm-sized SZY grains, precipitates only on amorphous substrates and the volume ratio of zirconia phase depends on the PLD condition. In our previous reports [1], it has been shown that configuration (CN, bond length) of the oxygen ions around Sr in as-deposited thin film is clearly different from that of the crystalline phase both in powder and the post-annealed SZO thin films, while almost no difference is found around Zr. It is found that YSZ thin films prepared by the same process crystalize easily below 500°C. These facts suggest that very similar local environment around Zr ion is formed already in the as-deposited amorphous phase as in the perovskite structure, that is, the coordination number of Zr cation in the SZY thin films is 6 to form ZrO_6 molecule both in as-deposited and post-annealed specimens. The formation of ZrO_6 in the as-deposited amorphous phase by PLD from SZY target might enable easy crystallization at relatively low temperatures.

As reported in zirconium oxides with different structures [2], XANES spectrum reflects the coordinating environment of the absorbing atom. Difference in the peak profiles in Zr K XANES spectra observed between YSZ and SZY thin films both in as-deposited and post-annealed thin films in the figure suggests the formation of the similar short range order by PLD at room temperature with each target material.

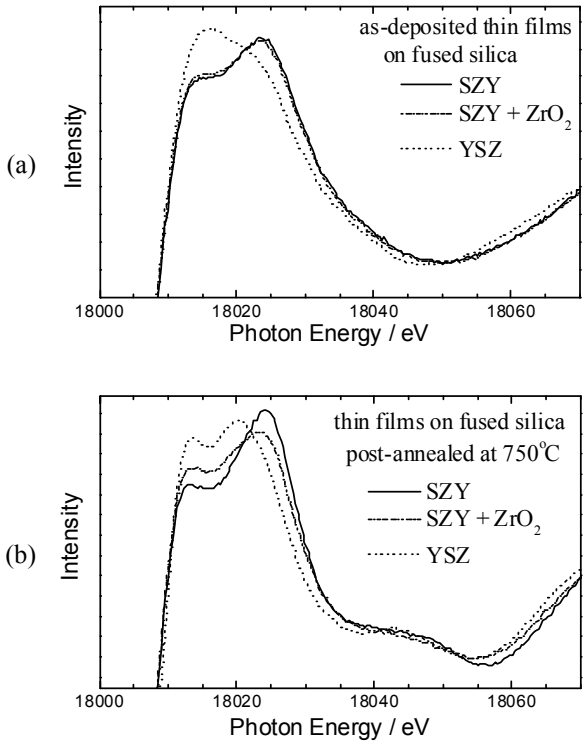

Fig. Zr-K XANES spectra of SZY and YSZ thin films. (a) as-deposited, (b) post-annealed (750C, 10 hrs). ($SZY+ZrO_2$: with higher volume ratio of zirconia phase).

References

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