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XAFS study of the local lattice distortion in the PLD-fabricated $SrZrO_3$ thin films

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Introduction

Pulsed laser deposition (PLD) is widely used as a powerful tool to fabricate epitaxial oxide thin films on single crystal substrates. To obtain epitaxial thin films of perovskite-type oxides, it is known that the substrate heating is necessary at deposition[1]. Recently, we have found that epitaxial $SrZrO_3$ thin films are successfully obtained on MgO single crystal substrates by PLD without heating at deposition. As-deposited thin films are polycrystalline and are epitaxially crystallized by post-annealing in air. Epitaxial crystallization in post-annealing is very rapid and the epitaxial crystallization temperature in this LT-PLD process is below 600 C, which is much lower than that of HT-PLD. Furthermore, it is found that the epitaxial $SrZrO_3$ thin films on MgO(001) substrates fabricated by the LT-PLD have different structural properties from those by the conventional PLD (HT-PLD): different lattice strain and columnar structure is not very obvious compared to HT-PLD. It is also notable that the lattice strain changes by post-annealing temperature. Large strain is retained below 670C, while the strain becomes smaller at higher temperatures.

In this study, EXAFS spectra of the $SrZrO_3$(SZO) thin films are analyzed to investigate the change in the local structure before and after the epitaxial crystallization.

Experimental

Fluorescence EXAFS spectra of the Sr and Zr K-edges have been obtained by a Lytle type ionization chamber at BL-9C. The thin film specimens were rotated during the measurements and the substrate was fixed at a certain angle to exclude diffractions of the MgO substrate. In order to investigate the influence of substrates, SZO thin films fabricated on fused silica wafers are also studied.

EXAFS data have been analyzed by REX2000 combined with FEFF 8.

Results and discussion

It is observed that Sr K absorption edge of as-deposited thin film is about 3 eV higher than that of HT-PLD. The absorption edge is closer to that of the HT-PLD thin film in the post-annealed thin films but is still higher than that. On the contrary, no peak shift of the Zr absorption edge is observed. Those facts indicate that configuration (CN, bond length) of the oxygen atoms around Sr is different not only in as-deposited thin film but also in post-annealed SZO thin films of LT-PLD process compared to the crystalline SZO fabricated by HT-PLD.

EXAFS analysis shows that the as-deposited SZO thin films have no long-range order, which is consistent with the results of HREM observation. Zr-O inter-atomic distances obtained by one shell fitting of the first peak are not very different among all specimens. On the contrary, Sr-O inter-atomic distances are different from each other. St-O distances are obtained by one-shell fitting (N=12) for as-deposited thin films, and by two-shell fitting (N=8 and 4) for other specimens. The obtained R values of around 2.5Å are almost comparable, however, those around 3.2Å becomes smaller only in the thin films prepared by LT-PLD on MgO(001) substrates. This result indicates that the tilt angle of the ZrO_6 octahedron is smaller in LT-PLD thin films on MgO substrates than the other crystalline SZO specimens.

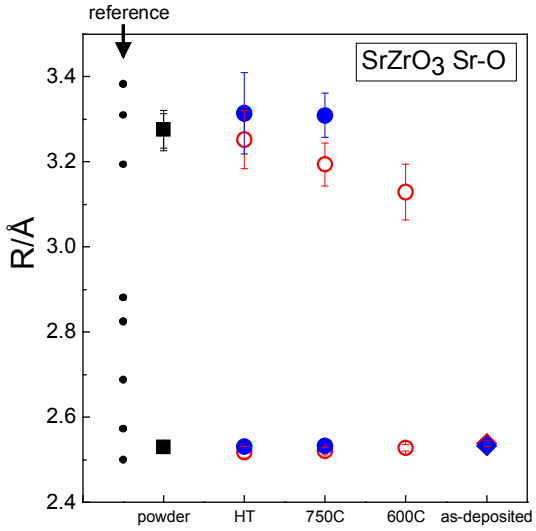

Fig. 1: Results of Sr-O distances in epitaxial (open circle) and polycrystalline (closed circle) $SrZrO_3$ thin films, and as-deposited thin films (open and closed diamond). For comparison, obtained distances in powder specimen (closed square) and the referential data (small dots) of Sr-O distances are given.

References

[1] D.Hondo et al., Solid State Ionics 178 (2007) 685-690.

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