Materials Science

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XAFS study on epitaxial crystallization of $SrZrO_3$ thin films fabricated by room temperature PLD and post-annealing process

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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. In a conventional PLD process, substrates must be heated at high temperature to grow the thin film epitaxially on deposition. On the other hand, we have found a novel PLD process to obtain epitaxial perovskite-type oxides on MgO single crystal substrates. In this process, thin films are deposited by PLD at room temperature and are epitaxially crystallized by post-annealing in air. As-deposited thin films of about 100nm thick are rearranged into epitaxial structure very rapidly and the epitaxial crystallization temperature in this LT-PLD process is much lower than that of HT-PLD, which is above 700C[1]. Furthermore, it is found that the epitaxial $SrZrO_3$ thin films on MgO(001) substrates fabricated by the novel process (LT-PLD) have different structural properties from those by the conventional PLD (HT-PLD): different lattice strain (Fig.1) and columnar structure is not very obvious compared to HT-PLD.

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.

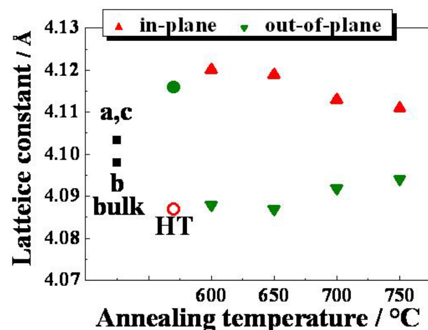

Fig. 1: In-plane and out-of-plane lattice constants of $SrZrO_3$ thin films fabricated on MgO(001) substrates as a function of post-annealing temperature. Referential values of the bulk crystal (orthorhombic) and those of thin films fabricated by the conventional high temperature PLD process are also given.

Experimental

Fluorescence EXAFS spectra of the Sr and Zr K-edges were 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.

Results and discussion

Sr K-edge fluorescence spectra of SZO thin films are given in Fig.2. XAFS analysis of those data showed that the as-deposited SZO thin film has no long-range order, which is consistent with the results of HREM observation. On the other hand, Sr K absorption edge energy of as-deposited thin film is about 3 eV higher than that of HT-PLD. The edge energy becomes closer to that of the HT-PLD thin film by post-annealing but is still higher than that. On the contrary, no peak shift of the Zr absorption edge is observed. This fact indicates 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. Such local structural difference might explain the difference in electrical conductivity of those thin films by different PLD processes.

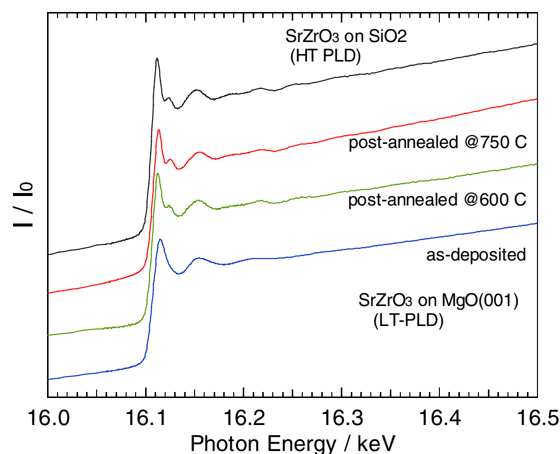

Fig. 2: EXAFS spectra of Sr K-edge in $SrZrO_3$ thin films on MgO(001) (low temperature PLD) and SiO_2 glass (high temperature PLD) for comparison.

References

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

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