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Local structure analysis of Ga_2O_3 polymorphs by XAFS

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1 Introduction

Gallium oxide (Ga_2O_3) has many of functionalities, such as wide-gap semiconductor for transparent conductive thin film and catalysis for dehydrogenation of paraffin to olefin. Ga_2O_3 appears a polymorphism similar to aluminum oxide. Roy *et al.* reported five polymorphs of Ga_2O_3[1]. Among them, β phase which has a monoclinic structure is commonly formed under ordinary conditions. We have already reported the stability of these five phases by first principles lattice dynamics calculations[2]. Recently, many works related to metastable phases of Ga_2O_3 were reported through chemical or physical deposition and sol-gel routes. In this study, we prepare Ga_2O_3 polymorphs by sol-gel method and investigate the local structure of them by XAFS.

2 Experiment

A total amount of 1 g gallium nitrate hydrate was solved in 50 ml water. A aqueous ammonia solution which was diluted in water (50 vol.%), was slowly added to this solution until no further precipitate was observed. The resulting gels were separated from the solutions with filter papers and were immediately washed with water. The obtained solids were calcined on a platinum foil in electric furnace at each temperature, 500, 600 and 700 ºC for 1 hour. Ceramic specimens were powdered before structure analysis.

Ga *K*-edge XAFS spectra were obtained at BL-7C of Photon Factory (PF) in High Energy Accelerator Research Organization (KEK). All of the spectra were recorded in transmission mode at room temperature with Si(111) double crystal monochromator. Specimens are diluted by high purity hexagonal type boron nitride powder before measurement.

3 Results and Discussion

The XRD measurements of samples were performed with versatile Cu-tube type instruments. The diffraction patterns of the sample calcined at 500 ºC and 700 ºC are indexed as α-Ga_2O_3 with corundum structure and β-Ga_2O_3, respectively. The profile of the sample calcined at 600 ºC is mixed with α-Ga_2O_3 and β-Ga_2O_3. Ga *K*-edge XANES spectra of these samples are showed in Fig. 1, together with standard sample of β-Ga_2O_3. The spectrum of α-Ga_2O_3 (calcined at 500 ºC) shows single peak at 10376 eV. Alpha phase of Ga_2O_3 has only one Ga site, which is octahedral. On the other hands, β-Ga_2O_3 spectrum has a peak with a shoulder at which is located at 10372 eV (indicated with an arrow in Fig. 1). Beta phase has equal numbers of two kind Ga sites, tetrahedral and octahedral ones. Theoretical XANES spectrum of β-Ga_2O_3 performed by first principles calculation shows that the rising edge of spectra is mainly composed by tetrahedral site and strong main peak is composed by octahedral site[3]. In comparison to the standard sample β-Ga_2O_3, the ration of intensity between the main peak and shoulder in the spectra of the sample calcinated at 700 ºC which is assigned as β phase by XRD, is slightly different. It shows that atom arrangement in long range is composed, but local structure is not conclusively laid out as β-Ga_2O_3.

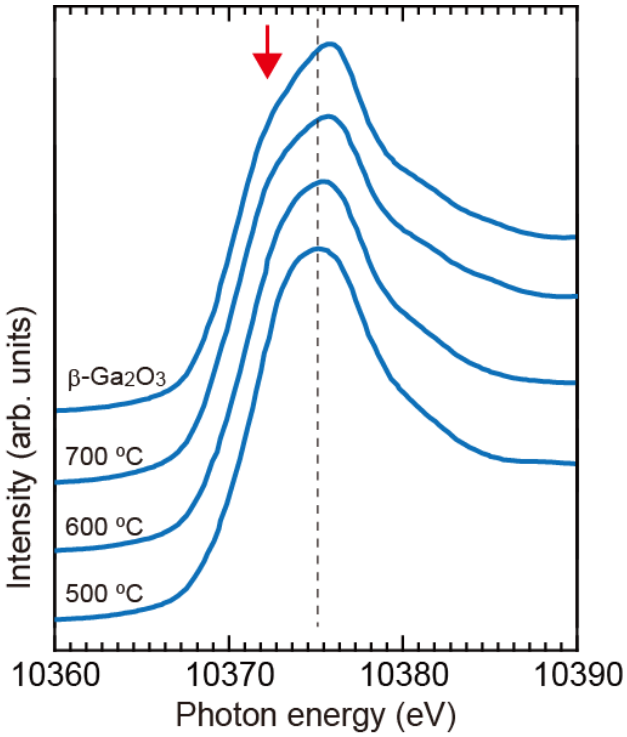

Fig. 1: Ga *K*-edge XANES spectra of samples prepared with water and calcined at each temperature for 1 h, together with that of β-Ga_2O_3 as a reference.

References
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