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Year 2023	**Summary of Thesis**

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(Title)

Study of optical band gap and crystal structure of β-$(Ga_{1-x}Al_x)_2O_3$

Introduction

β-Ga_2O_3 is a textbook semiconducting material for power devices with high breakdown voltage and low power consumption owing to its larger band gap energy. In general, β-$(Ga_{1-x}Al_x)_2O_3$, in which the Ga site of β-Ga_2O_3 is replaced by Al, has a larger band gap. It is important to study the changes in band gap and crystal structure due to Al substitution for further low power consumption and high breakdown voltage of devices. Although there are many reports on thin films, there is a few studies in single crystals, especially for compositions with higher Al substitutions. In particular, the effect of Al substitution on the anisotropy of β-Ga_2O_3 remains unclear.

Experimental

In this study, the crystal structure and lattice parameter of β-$(Ga_{1-x}Al_x)_2O_3$ ($x<0.4$) were investigated in single crystals prepared by the Floating Zone (FZ) method by X-ray diffraction (XRD). The change in optical band gap and its anisotropy were measured by optical transmission spectra. Unfortunately, it was not easy to make the single crystal with the composition of $x\geq0.4$, in terms of the FZ method. Thus, the polycrystalline samples were prepared by the combustion synthesis method. Their crystal structures and lattice parameters were also determined by XRD. The optical band gap was measured using diffuse reflection spectra.

Results and discussions

The XRD studies confirm that the monoclinic structure of β-Ga_2O_3 is maintained at least up to an Al concentration of 33.3 at.%. It was also confirmed that the lattice volume, estimated from the lattice parameters, decreases linearly with increasing Al concentration. This attributes to the smaller ionic radius of Al^{3+} relative to that of Ga^{3+}.

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The optical transmission spectra show that the optical band gap increases linearly with increasing Al concentration, as shown in Fig. 1. Regarding anisotropy, the difference between E//b and E//c band gaps tends to decrease slightly, although the effect of Al substitution on anisotropy is small.

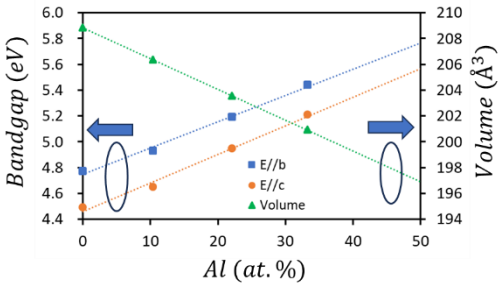

Fig.1 Dependence of optical band gap and lattice volume of on Al concentration. (single crystals)

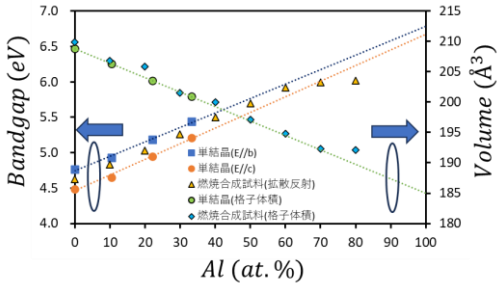

Fig.2 Dependence of optical band gap and lattice volume of on Al concentration. (poly-crystals)

In polycrystalline samples, the XRD patterns showe no α-Al_2O_3 diffraction peaks at least up to 50 at.% Al content, indicating that the samples still form the β-Ga_2O_3 structure. As shown in fig. 2, the lattice volume decreased linearly with increasing Al concentration below 70 at.%. The variation of lattice parameters is very similar to that in single crystals. At least up to 60 at.%, the optical band gap increases linearly with increasing Al concentration. The value agrees basically with the respective one estimated in the single crystals. It is noted that, over 60 at.%, the small diffraction peaks of α-Al_2O_3 appear in the XRD pattern, and, then, the phase separation of β- and α-types manifests itself at 80 at.%. As in the case of the lattice parameter, the β-type structure changed little at compositions above 70 at.%. It is also noted that only the α-Al_2O_3 structure is observed above 87 at.%.

Conclusion

The optical band gap and crystal structure have been studied in single- and poly-crystals of β-$(Ga_{1-x}Al_x)_2O_3$. Up to at least 60 at.%, the optical band gap increases linearly with increasing Al concentration and the lattice volume decreases linearly. It follows from these facts that the optical band gap can be scaled with the lattice volume. The results observed in the single-crystals demonstrate that the anisotropy is still significant for the electronic band structure in β-$(Ga_{1-x}Al_x)_2O_3$.

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