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Local structural study of $Mg_{0.06}Zn_{0.94}O$ film by polarized XAFS

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Introduction

$Mg_xZn_{1-x}O$ has attracted a lot of attention as a useful semiconducting material, because the band gap can be controlled by Mg composition. This is expected to be a new LED or LD materials in place of InGaN.

It is known that, after annealing, $Mg_xZn_{1-x}O$ films with $x \geq 0.18$ decompose into a rocksalt-type and a wurtzite-type phase, while the sample with $x = 0.12$ remain as wurtzite-type single phase. In the wurtzite-type structure the *c*-parameter approximately follows Vegard's law [1]. We have investigated the local structure of around Zn atoms in $x = 0.05$ and 0.06 $Mg_xZn_{1-x}O$ by Zn-*K* EXAFS method [2]. On the other hand, in mixed crystal semiconductor, the structure with low concentration of Mg atoms is more attractive, since the interatomic distance does not simply correspond to Vegard's law. In this report we have examined the local structure around Mg atoms in $Mg_{0.06}Zn_{0.94}$ by Mg-*K* XAFS.

Experimental and Calculation

Those samples were fabricated by HWPSE (Hericon Wave Excited Plasma Sputtering Epitaxy) method. The Mg *K*-edge X-ray absorption spectra have been obtained in BL11A at Photon Factory (KEK) using SDD (Silicon Drift Detector). For the wurtzite anisotropy, we used polarized X-ray and set up the sample as Fig.1. We measured Fluorescent X-ray at $\theta = 90°$ for ***E*//*ab*-**plane and at 6° for ***E*//*c*-**axis. We performed the Mg-*K* XANES simulation calculation by FEFF8.01. In the FEFF calculations, SCF (Self Consistent Field) and FMS (Full Multiple Scattering) were considered.

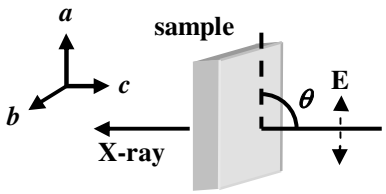

Fig.1 Experimental arrangement

Results and Discussion

Figure 2 and 3 show that measured and calculated Mg-*K* XANES spectra for ***E*//*ab***-plane and ***E*//*c***-axis. For the calculated spectra, the numbers of Mg 0, 3, 6, are corresponding to the number of converted Mg atoms into six Zn atoms for each direction. In Fig. 2, the peaks at 1313eV and 1323eV are decreased and shifted to high energy with increasing the number of Mg atoms. On the other hand, in Fig. 3, the peak at 1317eV is sensitive to substitution of Mg atoms and slightly shift to high energy.

In the ***E*//*ab***-plane spectra (Fig.2), the spectra for Mg 0 and 3 are well reproduced measured spectra. On the other hand, in the ***E*//*c***-axis spectra (Fig.3), the spectra for Mg 3 or 6 are slightly better. These results suggest that Mg atoms are located discretely in the ***E*//*ab***-plane, but still ambiguous for ***E*//*c***-axis. The curve-fitting analyses for Mg *K*-edge EXAFS are interesting future works.

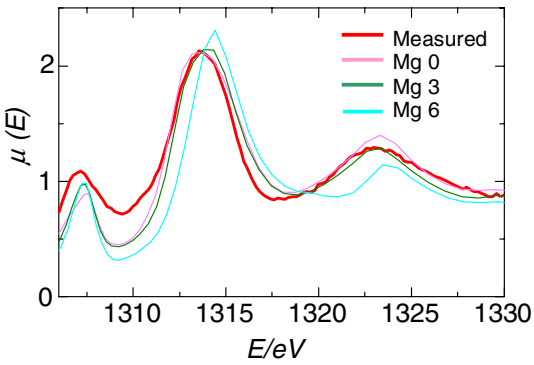

Fig.2 Mg-*K* XANES Spectra for ***E*//*ab***-plane

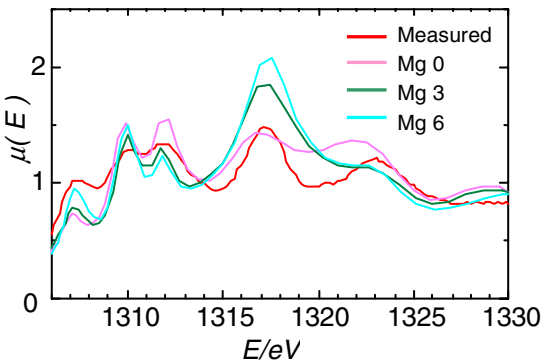

Fig.3 Mg-*K* XANES Spectra for ***E*//*c***-axis.

References

[1]H.Ryoken *et al.*, J. Crystal Growth **287,** 134 (2006).
[2] T.Yamada *et al*, in preparation for publication.

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