Materials Science

7C, 12C/2005G197

Local structure around Zn atoms in $Mg_xZn_{1-x}O$ thin film studied by XAFS

Shinya SASAKI[1], Takafumi MIYANAGA*[1], Takashi AZUHATA[1], Takahiro KOYAMA[2], Shigefusa F. CHICHIBU[2]
[1]Hirosaki Univ., Hirosaki, Aomori 036-8561, Japan
[2]Univ. of Tsukuba, Tsukuba, Ibaraki 305-8573, Japan

Introduction

$Mg_xZn_{1-x}O$ mixed crystals that were made by mixing Mg with ZnO have large band-gap energies (Eg) covering from 3.3eV for ZnO to 4.5eV for $Mg_{0.5}Zn_{0.5}O$[1]. Besides, the bond energies of the self-trapped excitons are large, therefore it is expected that the $Mg_xZn_{1-x}O$ mixed crystals could be the alternative materials for GaN based semiconductors. However, the crystal structures of ZnO are wurtzite-type and that of MgO are NaCl-type so it is difficult to mix them. In $Mg_xZn_{1-x}O$ thin films on sapphire (0001) substrates, it was reported that the crystal structure is wurtzite-type for $x<0.33$ and NaCl-type for $0.44<x$, on the other hand the phase is separated for $0.33<x<0.44$. In this work, Zn *K*-edge EXAFS measurements were carried out to study local structures around Zn atoms in $Mg_{0.05}Zn_{0.95}O$, $Mg_{0.06}Zn_{0.94}O$ and ZnO thin films.

Experiment and Analysis

The samples were grown by helicon-wave-excited-plasma sputtering epitaxy (HWPSE) on sapphire (0001) substrates[2]. The sample thickness is about 800nm. X-ray absorption measurements were carried out at BL-7C and 12C. The Zn K_α-fluorescence emission was measured using a Lytle detector. The samples were set in horizontal directions to the electric field of incident X-ray. In order to analyze the experimental EXAFS data, XANADU code[3] and FEFF6.01 code[4] were used. The sample species are listed in Table 1.

Table1: Sample species

Name	Aspect
Mg0	99.999%-pure undoped ZnO
Mg5	$Mg_{0.05}Zn_{0.95}O$ mixed crystal
Mg6	$Mg_{0.06}Zn_{0.94}O$ mixed crystal

Results and Discussion

Figures 1 and 2 show the Zn *K*-edge XANES and the Zn *K*-edge EXAFS $k\chi(k)$. For Fig.1, any spectral differences of these samples are not found. In Fig.2, the difference in the spectra can be almost neglected. Figure 3 shows the Fourier transforms for these samples. The 1st peak at 1.5Å corresponds to Zn-O bond, the 2nd peak at 2.8Å corresponds to Zn-Zn and/or Zn-Mg bonds and the 3rd peak at 4.2Å corresponds to Zn-O and Zn-Zn bonds. We found clear difference between $Mg_xZn_{1-x}O$ (x=0.05, 0.06) and ZnO thin films at the 2nd and 3rd peaks.

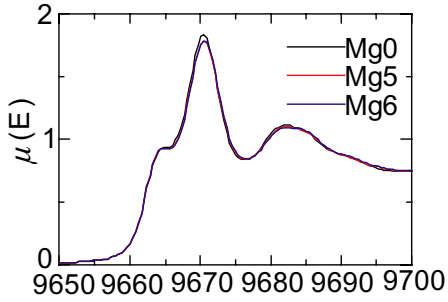

Fig. 1 Zn *K*-edge XANES for $Mg_xZn_{1-x}O$ and ZnO thin film

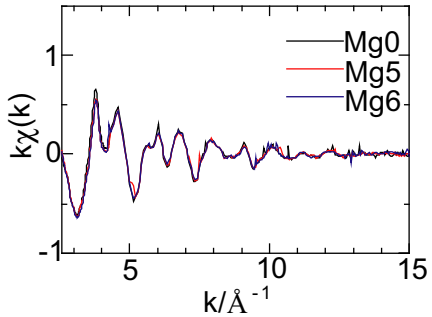

Fig. 2 Zn *K*-edge $k\chi(k)$ for $Mg_xZn_{1-x}O$ and ZnO thin film

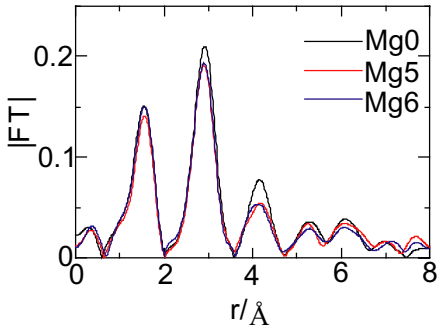

Fig. 3 Fourier transforms of Zn *K*-edge EXAFS for $Mg_xZn_{1-x}O$ and ZnO thin film

References

[1] T. Takagi, H. Tanaka, Sz. Fujita, Jpn. J. Appl. Phys., Part 2 **42** L401 (2003).
[2] S. F.Chichibu, T. Yoshida, T. Onuma, and H. Nakanishi, J. Appl. Phys. **91**, 874 (2002).
[3] H. Sakane, T. Miyanaga, I. Watanabe, N. Matsubayashi, S. Ikeda, and Y. Yokoyama, Jpn. J. Appl. Phys. **32** 4641 (2001).
[4] S. I. Zabinski, J. J. Rehr, A. Ankudinov, R. C. Albers, and M. J. Eller, Phys. Rev. B, **52** 2995 (1995).

*takaf@cc.hirosaki-u.ac.jp