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

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Introduction

Mg$_x$Zn$_{1-x}$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$_x$Zn$_{1-x}$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$_x$Zn$_{1-x}$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.

<table>
<thead>
<tr>
<th>Name</th>
<th>Aspect</th>
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<tr>
<td>Mg0</td>
<td>99.9999%-pure undoped ZnO</td>
</tr>
<tr>
<td>Mg5</td>
<td>Mg$<em>{0.05}$Zn$</em>{0.95}$O mixed crystal</td>
</tr>
<tr>
<td>Mg6</td>
<td>Mg$<em>{0.06}$Zn$</em>{0.94}$O mixed crystal</td>
</tr>
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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$_{0.05}$Zn$_{0.95}$O (x=0.05, 0.06) and ZnO thin films at the 2nd and 3rd peaks.

References


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