Polarized XAFS study of Mg *K*-edge for MgB₂ on ZnO

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Abstract

Polarization-dependent Mg *K*-edge XAFS study was carried out for MgB₂ films epitaxially deposited by MBE method on ZnO single crystal. 50 and 150 nm MgB₂ films were deposited on the O-plane side of the ZnO single crystal. The investigation for the O-plane side of ZnO is interesting because the local structure of MgB₂ should be affected by Mg-O interaction on the ZnO. The results indicate that the structure of 50 nm MgB₂ film was expanded in the *a-b* plane and compressed along the *c*-axis, but that of 150 nm MgB₂ was relaxed on the ZnO surface and should be close to the MgB₂ crystalline phase.

Keywords : polarized XAFS, Mg *K*-edge, MgB₂ film, superconductor

1. Introduction

Superconductor MgB₂ was discovered in 2001 and shows the superconducting transition temperature of 39 K which is the highest for metal compounds. The superconducting mechanism and applications as a device are attracting great interest. An important issue for application to a device is the production of high-quality MgB₂ thin films. For this purpose, various methods of film growth have been investigated. For the heteroepitaxial method, the interface state between MgB₂ and substrate affects the quality of the crystal growth. It is important to study the properties of polarized materials *e.g.* ZnO as buffer substrates. Although the lattice matching and surface/interface structure have been discussed recently for MgB₂ thin films, the amount and quality of the results are insufficient. Sapphire is known as a typical material as a substrate MgB₂ deposition. On the other hand, the lattice distance of ZnO is close to that of MgB₂ (the lattice mismatch is about 5%) and therefore it is expected to be a suitable buffer layer. Although there exists a reactive region at the boundary between MgB₂ and ZnO, it is known that the MgB₂/ZnO system is highly crystallized and shows high performance as a superconductor [1]. This effect is especially prominent on the O-side surface of ZnO because the Mg-O bond may expand the lattice of MgB₂ film, possibly inducing an increase in the DOS and increasing *T_c*. First principle

calculations of the interaction between MgB_2 and ZnO have been done [2]. For studying the local structure of such thin films, EXAFS (Extended X-ray Absorption Fine Structure) is a powerful tool. Using a synchrotron radiation source, polarized EXAFS analyses are available. In this paper, the local structure of 50nm and 150nm MgB_2 deposited on O-side surface of ZnO crystal are investigated by polarized Mg K -edge EXAFS analyses.

2. Experimental and data analyses

The MgB_2 films were prepared by MBE (Molecular Beam Epitaxy) with the co-evaporation method [3]. 50nm and 150nm thick MgB_2 films were deposited on ZnO single crystal. We analyze the MgB_2 sample deposited on the O-side of ZnO crystal to assess the possibility of the existence of Mg-O interaction.

Mg K -edge (1306eV) X-ray absorption spectra were measured on BL11A at Photon Factory, KEK, Tsukuba using fluorescence mode with Silicon Drift Detector (SDD). Polarization-dependent XAFS measurement was applied to two directions:

(1) The horizontal direction of the sample in which the electric vector of X-ray, $\mathbf{E}$, is perpendicular to the c -axis of the MgB_2 film; (2) the vertical direction in which $\mathbf{E}$ is parallel to the c -axis. The EXAFS analyses were performed by XANADU code [4] and FEFF 8.10 code [5]. We applied the non-linear least square fitting (curve-fitting) method to EXAFS data and obtained the structural parameters. Effective coordination number was taken into account in the curve-fitting process, because the grown MgB_2 was c -axis oriented and very anisotropic.

Figure 1 Normalized X-ray absorption spectra for (a) the horizontal direction and (b) the vertical direction for 50 and 150 nm thick MgB_2 on ZnO .

3. Results and discussion

Figure 1 shows the normalized X-ray absorption spectra for (a) the horizontal direction and (b) the vertical direction for 50 and 150 nm thick MgB_2 on ZnO . Fairly good data were obtained up to 1600eV.

Figure 2 shows the EXAFS function, $k\chi(k)$, for (a) the horizontal direction and (b) the vertical direction for 50 and 150 nm thick MgB_2 on ZnO. The EXAFS data were available up to $8.5 \text{ \AA}^{-1}$.

Figure 2 EXAFS functions, $k\chi(k)$, for (a) the horizontal direction and (b) the vertical direction for 50 and 150 nm thick MgB_2 on ZnO.

Figure 3 Fourier transforms of $k\chi(k)$ for (a) the horizontal direction and (b) the vertical direction for 50 and 150 nm thick MgB_2 on ZnO.

Figure 3 shows the Fourier transforms of $k\chi(k)$ for (a) the horizontal direction and (b) the vertical direction for 50 and 150 nm thick MgB_2 on ZnO. In Fig. 3 (a), the first 2 peaks within the range 1-4 Å correspond to 1NN (1st nearest neighbor) Mg-B and 2NN Mg-Mg. On the other hand, in Fig. 3 (b), the first 2 peaks within 1-4 Å correspond to 1NN Mg-B and 3NN Mg-Mg. We applied the non-linear least square-fitting to k -space EXAFS data, back-Fourier transformed with the window 1-4 Å and obtained the structural parameters. We discuss interatomic distances in the present paper.

The following results are obtained:

- (1) Horizontal direction (perpendicular to c -axis): Both of the interatomic distances of 1NN Mg-B (2.521 Å) and 2NN Mg-Mg (3.158 Å) for 50 nm MgB_2 are longer than those for 150 nm MgB_2 (2.513 Å for Mg-B and 3.151 Å for 2NN Mg-Mg).
- (2) Vertical direction (parallel to c -axis): Both of the interatomic distances of 1NN

Mg-B (2.487Å) and 3NN Mg-Mg (3.557Å) for 50 nm MgB₂ are shorter than for 150 nm MgB₂ (2.506Å for Mg-B and 3.568Å for 3NN Mg-Mg).

These results indicate that the structure of 50 nm MgB₂ film was expanded in the *a-b* plane and compressed along the *c*-axis, but that of 150 nm MgB₂ was relaxed apart from the ZnO surface and should be close to the crystalline MgB₂. The fitting quality for 50 nm film using MgB₂ as a model is worse than that for 150 nm. This suggests that the reactive region for Mg and O atoms may exist between the MgB₂ film and the ZnO single crystal.

4. Conclusion

We show the result for the polarization dependent Mg *K*-edge XAFS study for MgB₂ films deposited by MBE method on ZnO single crystal for the first time. The present results suggest that the reactive region by Mg and O atoms may exist between MgB₂ film and ZnO. This mean the interaction between Mg and O atom is effective in the interface of MgB₂ and ZnO layer.

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