Highlights
4-1 Study of Partial Electronic Density of States of B-2p in MgB₂ Compound Using X-ray Fluorescence Measurement

The discovery of MgB₂ to be a superconductor with the transition temperature of 39 K by the Akimitsu group [1] stimulated a large number of research studies from experimental and theoretical points of view, because of the higher transition temperature as a conventional BCS type of superconductor. An efficient step towards understanding the mechanism of superconductivity in MgB₂ is to clarify the difference between this material and non-superconductors such as AlB₂.

First principle band calculations reveal that a large difference between MgB₂ and AlB₂ is that the Fermi level intersects the 2p-α band in the former, while it does not in the latter, suggesting that the α band plays an important role in the occurrence of superconductivity in MgB₂ [2]. To clarify this point, we directly observed the partial density of states (PDOS) of B-2pα and 2pπ bands in MgB₂ and AlB₂ by performing polarization-dependent X-ray emission spectroscopy (XES) and X-ray absorption spectroscopy (XAS) measurements on single crystalline MgB₂ and AlB₂ compounds [3]. Experiments on XES and XAS were carried out at BL-2C and BL-19B, respectively. By measuring the dipole transition between 2p and 1s core levels of boron, we can specifically probe the partial density of states of B 2p states. Then, by measuring the polarization dependence of XES and XAS for single crystalline specimens using linear polarization of synchrotron radiation, we could successfully derive the partial density of states (PDOS) of B-2pα and 2pπ bands in MgB₂ and AlB₂ [3].

Figure 1 shows the PDOS of B-2pα and 2pπ in MgB₂ derived from observed fluorescence data. In the figure the theoretical PDOS of B-2pα and 2pπ are shown by the solid line (α) and the broken line (π), respectively [2]. It was found that there are significant amounts of state density at the Fermi energy in both B-2pα and 2pπ states for MgB₂ as shown in the figure. However, for AlB₂, there was almost no density of states at the Fermi energy in B-2pα and a considerable amount of density of states at the Fermi energy in B-2pπ, as reported in ref. [3]. The importance of the B-2pα state for superconductivity in MgB₂ was confirmed.

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References

4-2 Fabrication and Electronic Structures of Zinc-Blende Type Ferromagnet Grown by Molecular-Beam Epitaxy

Quite recently “spintronics”, that positively uses the electron spin in electronics, has attracted much attention and a search for new spintronic materials such as a half-metallic ferromagnet and a magnetic semiconductor becomes very active. We propose a new scheme for the search of spintronic materials, which is a combination of a materials design, a materials fabrication by molecular-beam epitaxy (MBE), and an in situ electronic structure characterization using photoemission.

We have succeeded in the growth of zinc-blende (zb) type ferromagnets MnAs and CrAs that have been predicted to be a half-metallic characteristics based on the first principles band calculation using FLAPW (Full Potential Linearized Augmented Plane Wave) method. MnAs dots and CrAs epitaxial films were grown by MBE.

Figure 1
Partial density of states (PDOS) of B-2pα (↑) and 2pπ (↓) in MgB₂, derived from fluorescence spectroscopy. Solid and broken lines represent the theoretical partial density of states of B-2pα and 2pπ given by Oguchi, respectively.
and their electronic properties were measured by in situ synchrotron radiation photoemission spectroscopy (SRPES), respectively. Zb-type CrAs epitaxial films grown on GaAs (001) by MBE show a ferromagnetic property at room temperature with the magnetic moment of about 3 $\mu_B$, suggesting the possibility of the half-metallic characteristics. The electronic structure of zb-CrAs obtained by SRPES (Fig. 2) agrees well with the first principles band calculation (Fig. 3). Furthermore, sulfur termination of GaAs surfaces enabled the formation of zb-type MnAs dots, which was confirmed by cross-sectional transmission electron microscope and selected area electron diffraction. SRPES analysis shown in Fig. 4 reveals that the zb-MnAs dots show a distinctive valence band electronic structure with Mn 3$d$-related peak at about 4 eV of binding energy which is quite similar to that of (Ga,Mn)As, but different from the NiAs-type MnAs thin film.

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**Figure 2**
In situ photoemission spectra of MBE-grown zinc-blende CrAs thin film.

**Figure 3**
Band mapping of zinc-blende CrAs.

**Figure 4**
In situ photoemission spectra of (Ga,Mn)As, zinc-blende MnAs dots, and NiAs-type MnAs film.