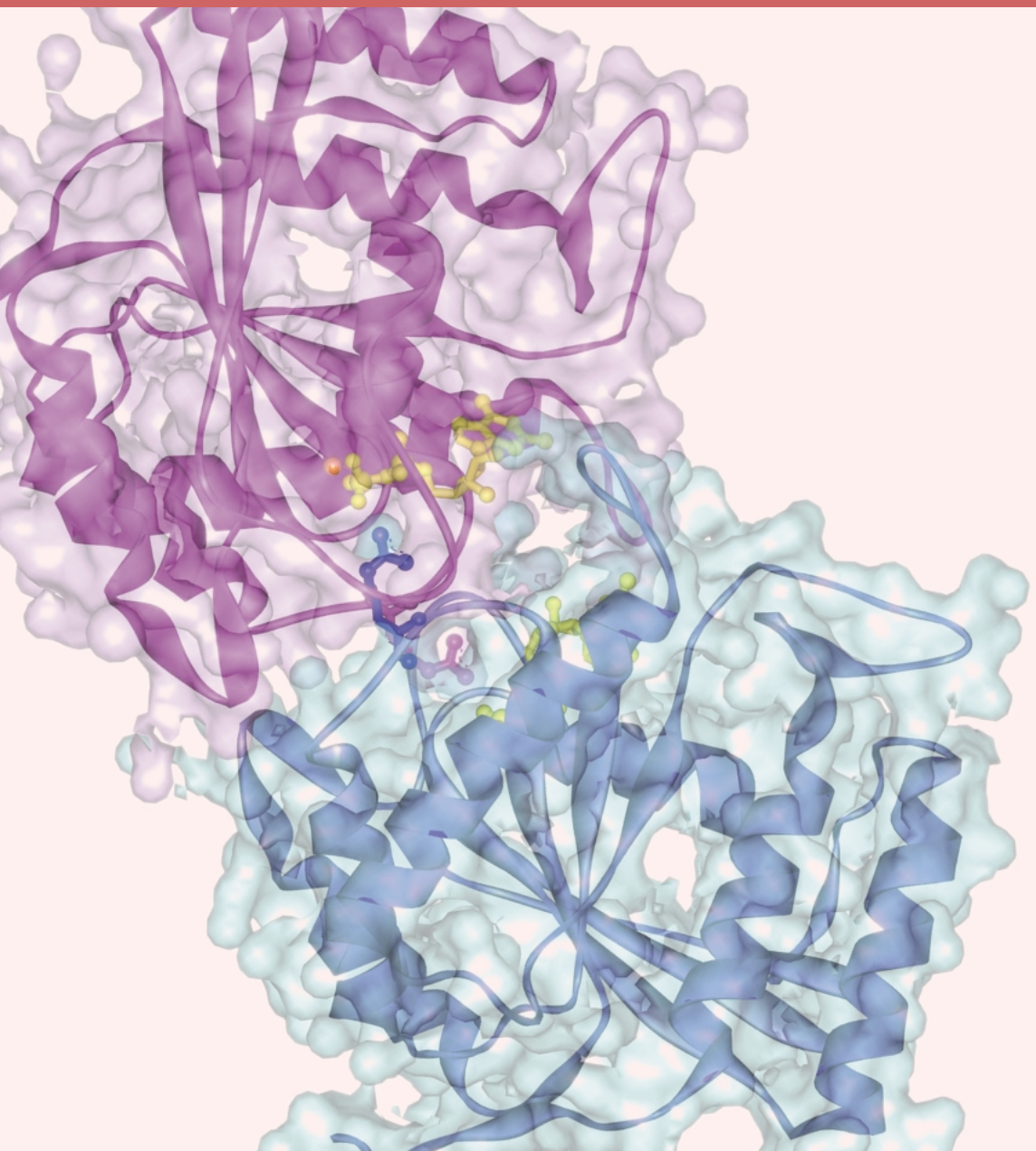
Highlights



4 Electronic Structure of Condensed Matter

4-1 Study of Partial Electronic Density of States of B-2*p* in MgB_2 Compound Using X-ray Fluorescence Measurement

The discovery of MgB_2 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 MgB_2 is to clarify the difference between this material and non-superconductors such as AlB_2.

First principle band calculations reveal that a large difference between MgB_2 and AlB_2 is that the Fermi level intersects the 2*p*-σ band in the former, while it does not in the latter, suggesting that the σ band plays an important role in the occurrence of superconductivity in MgB_2 [2]. To clarify this point, we directly observed the partial density of states (PDOS) of B-2*p*σ and 2*p*π bands in MgB_2 and AlB_2 by performing polarization-dependent X-ray emission spectroscopy (XES) and X-ray absorption spectroscopy (XAS) measurements on single crystalline MgB_2 and AlB_2 compounds [3]. Experiments on XES and XAS were carried out at BL-2C and BL-19B, respectively. By measuring the dipole transition between 2*p* and 1*s* core levels of boron, we can specifically probe the partial density of states of B 2*p* 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-2*p*σ and 2*p*π bands in MgB_2 and AlB_2 [3].

Figure 1 shows the PDOS of B-2*p*σ and 2*p*π in MgB_2 derived from observed fluorescence data. In the figure the theoretical PDOS of B-2*p*σ and 2*p*π are shown by the solid line (σ) 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-2*p*σ and 2*p*π states for MgB_2 as shown in the figure. However, for AlB_2, there was almost no density of states at the Fermi energy in B-2*p*σ and a considerable amount of density of states at the Fermi energy in B-2*p*π, as reported in ref. [3]. The importance of the B-2*p*σ state for superconductivity in MgB_2 was confirmed.

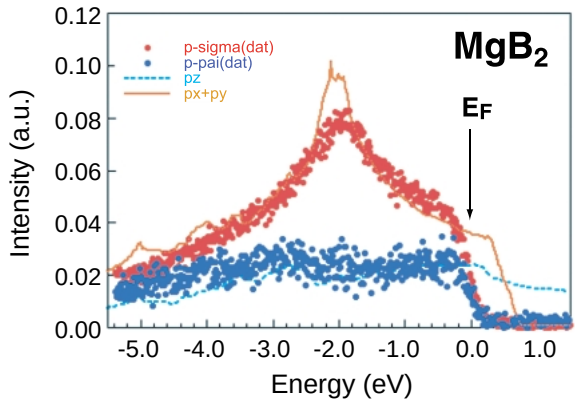


Figure 1
Partial density of states (PDOS) of B-2*p*σ(●) and 2*p*π(●) in MgB_2, derived from fluorescence spectroscopy. Solid and broken lines represent the theoretical partial density of states of B-2*p*σ and 2*p*π given by Oguchi, respectively.

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References

[1] J. Nagamatsu, N. Nakagawa, T. Muranaka, Y. Zenitani and J. Akimitsu, *Nature* **410** (2001) 63.
[2] T. Oguchi, *J. Phys. Soc. Jpn.* **71** (2002) 1495.
[3] J. Nakamura, M. Watanabe, T. Oguchi, S. Nasubida, E. Kabasawa, N. Yamada, K. Kuroki, H. Yamazaki, S. Shin, Y. Umeda, S. Minakawa, N. Kimura and H. Aoki, *J. Phys. Soc. Jpn.* **71** (2002) 408.

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

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 μ_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 *3d*-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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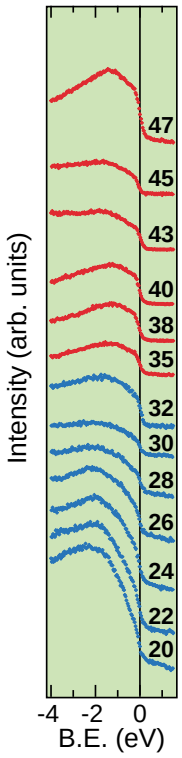

Figure 2
In situ photoemission spectra of MBE-grown zinc-blende CrAs thin film.

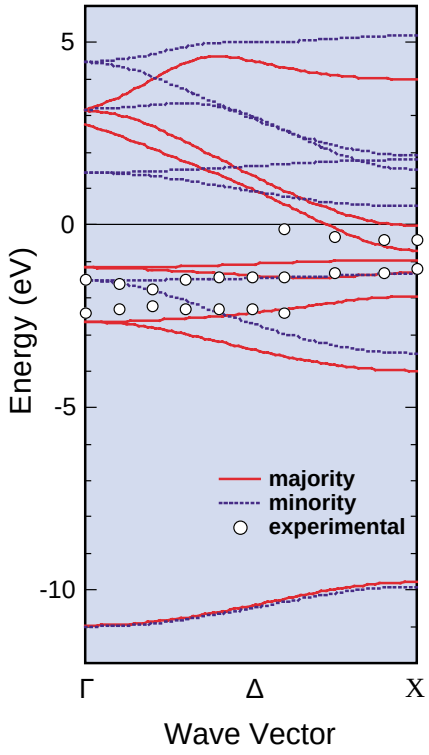

Figure 3
Band mapping of zinc-blende CrAs.

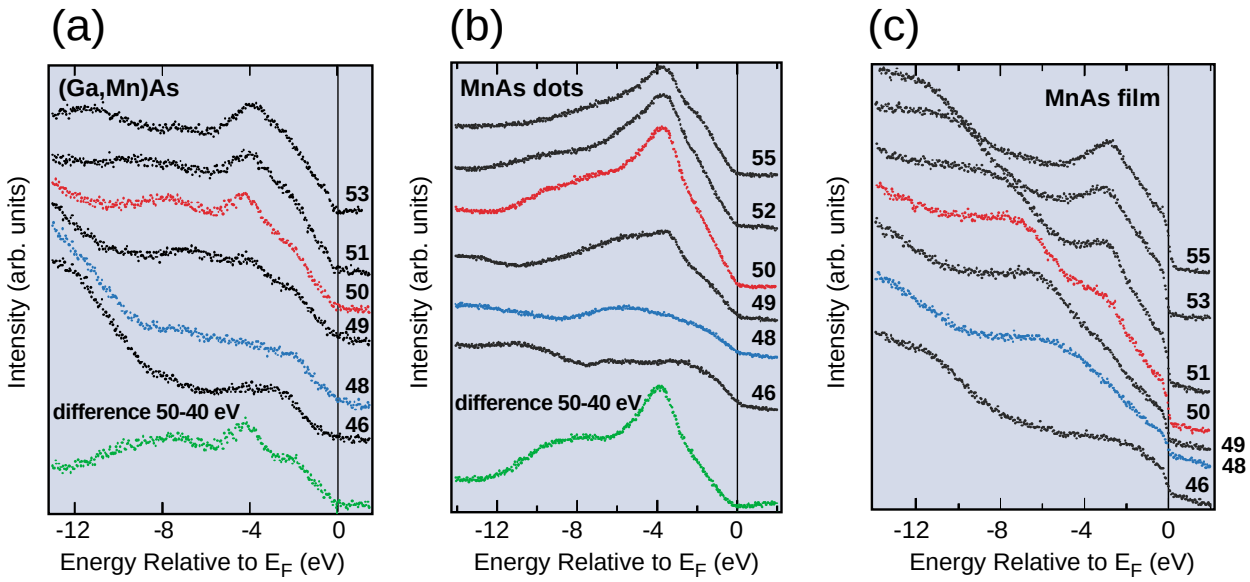

Figure 4
In situ photoemission spectra of (Ga,Mn)As, zinc-blende MnAs dots, and NiAs-type MnAs film.