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B K emission spectra for MgB_2 and $Mg_{0.8}Al_{0.2}B_2$

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Introduction

Recently, MgB_2 was shown to be a superconductor with Tc=39 K by Nagamatsu *et al* [1] . Since the discovery, the nature of the superconductivity in MgB_2 has been studied. The results suggest strongly that MgB_2 is a conventional BCS-type phonon-mediated superconductor. Within the related materials, Al-doped MgB_2 was one of the objects whose superconductivity was earlier estimated by theoretical and experimental aspects [2] . To confirm these results, soft-X-ray emission (SXE) spectroscopy is a useful method. Since the SXE spectrum reflects the partial density of states (PDOS) of the valence band, B K emission for MgB_2 shows the PDOS of the B 2p band. B 2p is a dominant component at the Fermi level, which is closely related with the Tc of superconductors. Thus B K emission spectra of MgB_2 and Al-doped MgB_2 ($Mg_{0.8}Al_{0.2}B_2$) provide much information of the superconductivity in MgB_2.

Experiments

The samples were sintered polycrystals of MgB_2 and $Mg_{0.8}Al_{0.2}B_2$. Phase purity and the Tc of the samples were estimated before the SXE measurements. X-ray diffraction patterns showed that all the samples were of a hexagonal phase with the lattice constants a=0.3086 nm and c=0.3524 nm for MgB_2 and slightly larger for $Mg_{0.8}Al_{0.2}B_2$. The temperature-dependent magnetization measurements showed that the Tc of the samples were 39 K for MgB_2 (x=0) and 29 K for $Mg_{0.8}Al_{0.2}B_2$, respectively. SXE experiment was performed at BL-16B. The FWHM of the incident SR soft X-ray at 191.1 eV was 0.5 eV, and of the spectrometer we used was 0.8 eV. Samples were filed in the preparation chamber before the measurements to remove surface contaminations.

Results and discussion

Figure 1 shows the B K emission spectra measured for MgB_2 and $Mg_{0.8}Al_{0.2}B_2$. The spectrum for MgB_2 (solid circles) has a main peak around 183 eV and Rayleigh scattering peak around 191eV. The spectral shape almost resembles the PDOS obtained by the band calculation of MgB_2. Compared with this spectrum, that for $Mg_{0.8}Al_{0.2}B_2$ (open circles) shifts about 0.3 eV towards the lower energy side.

The reason of the peak shift is explained as follows; B 2p band, which is shown by the B K emission spectrum, can separate into σ and π bands. The σ band is pulled up by ionized Mg, which results in a hole-doping into the σ band. The peak of the B K emission spectrum of MgB_2 is contributed from the σ band around the M and L point in Brilluan zone, positioned about 2 eV below the Fermi level. The B-B in-plainer bonding is shortened by Al doping. It causes the σ bonding to be tight, and results in lowering of the σ band. This effect may cause the shift of the spectra qualitatively.

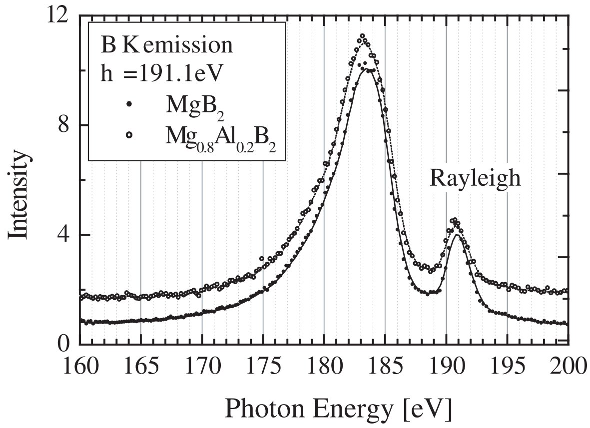

Figure 1: B K SXE spectra for MgB_2 and $Mg_{0.8}Al_{0.2}B_2$. The peak at about 191 eV in each spectrum is due to the elastic scattering of the incident soft X-rays.

References

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