Photoemission study of $CoSe_2$

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Introduction

Exchange-enhanced Pauli paramagnet $CoSe_2$ with pyrite-type structure, is an end-point material of $Co(S_xSe_{1-x})_2$ system (x=0). CoS_2 (x=1) is a ferromagnetic metal with the Curie temperature T_C of 124 K. T_C rapidly decreases by a substitution of Se for S and the system becomes paramagnetic by 12 % substitution. In this study, we have invesigated the valence-band electronic structure of $CoSe_2$ by the Co 3p-3d resonant photoemission spectroscopy.

Experimental

The Co 3p-3d resonant photoemission experiments for $CoSe_2$ were carried out on the beamline BL-3B. The photoemission spectra were measured with DCMA at room temperature. The total energy resolution of the photoemission spectra was ~0.3 eV. Samples used in the present experiments were polycrystalline $CoSe_2$. The appropriate amount of Co and Se elements was kept at 900 ˚C for 3 weeks. The clean surfaces of the samples were obtained by scraping with a diamond file under ultra-high vacuum and the photoemission spectra were in situ measured.

Results

Figure 1 shows a series of valence-band photoemission spectra of $CoSe_2$ measured at hν=30~67 eV including the Co 3p-3d excitation region. The photoemission spectrum at hν=30 eV exhibits a main peak at 1.0 eV with a shoulder on the lower binding energy side and two broad structures around 3 and 6.5 eV. With increasing hν from 30 to 50 eV, a feature of the photoemission spectra drastically changes. The main peak at 1.0 eV is remarkably enhanced, while two broad structures are considerably suppressed. From the energy-dependent photo-ionization cross sections, the main peak at 1.0 eV with the shoulder is mainly due to the Co 3d states, and two broad structures around 3 and 6.5 eV are mainly attributed to the Se 4p bands. Above hν=50 eV, the feature of the photoemission spectra is almost unchanged. Broad structures in the spectra at hν=60 and 67 eV denoted by vertical arrows are attributed to the emission of the Co MVV Auger electrons. Resonance enhancement of the spectra was not observed in the Co 3p-3d excitation region so much.

Figure 2 shows theoretical Co partial DOS (Co-pDOS) of $CoSe_2$ (solid line) [1] together with the photoemission spectrum measured at hν=50 eV. The convoluted curve is also shown by a dashed line. On the basis of the band-structure calculation, the main peak and shoulder in the experimental spectrum are assigned to be the fully occupied t_{2g} and partially filled e_g bands, respectively. Although the basic feature of the spectrum is in qualitative agreement with the convoluted curve with respect to two structures near the Fermi level and 1.0 eV, the energy position of the t_{2g} bands of the theoretical Co-pDOS is markedly higher than that obtained from the experimental result. The disagreement of the energy position of the t_{2g} bands between the experimental and theoretical Co pDOS's suggests that the electron correlation is important for $CoSe_2$.

References

[1] H. Yamada et al., J. Mag. Mag. Mat. **177-181**, 607 (1998).

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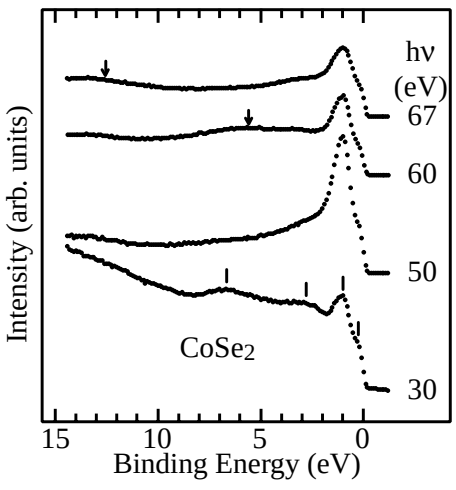

Fig.1. Photoemission spectra of $CoSe_2$.

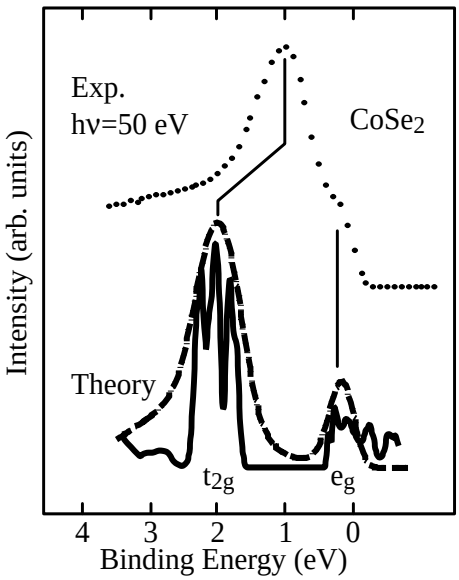

Fig.2. Comparison between experiment and theory.