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Valence-band Electronic Structure of FeSi studied by high-resolution Angle-Resolved Photoelectron Spectroscopy (ARPES)

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Among transition metal mono-silicides: MSi (M=Cr, Mn, Fe, Co, Ni), FeSi has been intensively studied as one of the possible candidates for the d-electron Kondo insulators. While FeSi has an insulating ground state, electric conductivity shows a semiconductor to insulator crossover at 300K. Another interesting feature is the temperature dependence of its magnetic susceptibility, which rises nearly exponentially up to 500K making a broad maximum followed by a Curie-Weiss law at even high temperatures. To explain these unusual electric and magnetic properties, many theoretical models have been discussed so far. They are for example, thermally excited spin-fluctuation theory, phenomenological models assuming two narrow *d* bands in the vicinity of the band gap. Such a model density of states is quite similar to those for Kondo insulator description, and due to this similarity, it was often claimed that FeSi is the first Kondo insulator containing no *f*-electrons.

A number of valence band photoemission spectroscopy studies have been performed to elucidate the electronic structures near the Fermi level (E_F) [2]. In spite of careful measurement with sufficiently high-energy resolution smaller than the expected semiconductor band gap, results are not conclusive about the existence of the band gap [3]. Recently, Klein *et al*. made an effort to cleave a single crystal at (001) plane and observed ARPES spectra [4]. Though the sample surface consists of several faces, they observed that the spectral features are almost consistent with calculated band structure along the ΓXMΓ plane in the Brillouin zone showing a sharp peak feature at 300meV below E_F. In the following, we present the valence band structures of FeSi(001) single crystal surface observed by ARPES and discuss on the electronic structures of this material.

Experiments were carried out at CASSIOPEE beamline of SOLEIL. The ARPES apparatus consists of a sample preparation chamber equipped with an Auger electron spectrometer (AES) and a low energy electron diffraction (LEED) apparatus and an analysis chamber with a hemispherical electron energy analyzer (SCIENTA R4000). Clean FeSi(001) single crystal surface was obtained by the procedure described elsewhere [5].

Figure 1 sows the valence band structure of FeSi(001) single crystal surface observed along the Γ-X direction in the Brillouin zone, where the Fe 3*d* originated valence band shows a very small energy dispersion. The results are basically consistent with the calculated valence band structure with an energy gap very close to the E_F. The obtained band dispersion well reproduces the theoretical calculation, except the reduction of the bandwidth of about 30% due to the renormalization effect.

This work resolves the controversial evidences, which have been provided for the arguments of the Kondo-like interaction in this material.

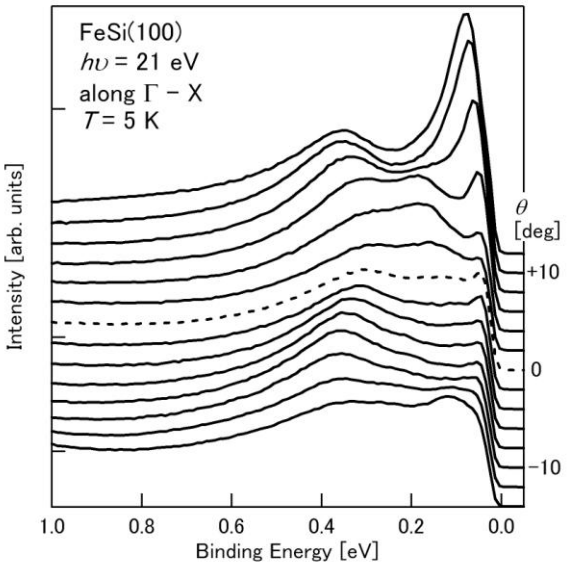

Fig. 1. ARPES spectra of FeSi(100).

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