P10

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ARPES study of the mechanically polished FeSi [001] surface

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FeSi is a nonmagnetic semiconductor at low temperatures. With increasing temperature, the magnetic susceptibility rises and the temperature dependence of the electric resistivity shows a crossover from the semiconducting state to the metallic state at ~300 K [1,2]. Thus, FeSi can be viewed as the Kondo insulator [3]. In order to investigate the electronic structure and electron-electron correlation effect in FeSi, the angle reserved photoemission spectroscopy (ARPES) measurements on FeSi [001] surface were carried out at HiSOR BL-1.

FeSi clean surface was successfully by mechanical polishing in air, and Ar ion sputter and annealing in the UHV chamber. After that procedure, the clear 1x1 LEED images were seen for the [001] surfaces (Fig.1).

Figure 2 shows the valence band dispersion along k_z (perpendicular to the sample surface), obtained by normal emission ARPES spectra from hv = 25 to 135 eV at 25 K. Assuming that the inner potential V_0 is 17 eV, the observed band structure are in agreement with the result of the GGA calculation along Γ -X line of the BZ (dashed curves). According to the result, it is found that one can examine the electronic band structure around Γ -X and X-M in the 4th bulk BZ with hv = 51 and 72 eV. respectively. We carried out the ARPES measurement with hv = 72 eV as shown in the Fig. 3. There are two dispersion bands between E_F and -1 eV, which approximately correspond to the calculated band structures along X-M (dashed curves). However, the observed dispersion bandwidths are narrower than the calculated ones. In particular, the observed bandwidth near E_F is approximately 0.6 times narrower than the calculated bandwidth. A similar bandwidth narrowing is found in the band structure along Γ -X (Fig. 2). We suppose that the bandwidth shrinking is derived from the strong electron-electron interaction.

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- [2] M. B. Hunt et al., Phys Rev. B 50,14933 (1994).
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Fig.1 LEED image of FeSi [001] for E = 100 eV.



Fig.2 Plot of the normal emission ARPES intensity of FeSi [001] along k_z . Dashed curves represent the calculated band structures along ΓX .



Fig.3 Plot of the ARPES intensity with hv = 72 eV. Dashed curves represent the calculated band structures along XM.