Soft x-ray angle-resolved photoemission study of $CeRu_2X_2$ (X = Si, Ge)

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CeT_2X_2 (T = Ni, Cu, Ru; X = Si, Ge) with a $ThCr_2Si_2$ crystal structure shows a variety of interesting phenomena such as anisotropic superconductivity, heavy fermion bahabior, and magnetic ordering. Among them, $CeRu_2Si_2$ and $CeRu_2Ge_2$ are known as a heavy fermion system with the Kondo temperature (T_K) of ~20 K, and a ferromagnet with the Curie temperature of ~8 K. A hybridization strength between the localized Ce 4f state and the itinerant valence-band states, which reflects T_K, is expected to be weaker for $CeRu_2Ge_2$ than for $CeRu_2Si_2$. Actually, we have so far revealed that T_Ks are estimated as ~20 and < 1 K for $CeRu_2Si_2$ and $CeRu_2Ge_2$ from the bulk-sensitive angle-integrated Ce 3d-4f resonance photoemission [1]. In order to further clarify the valence-band electronic structures, Fermi surfaces, and the *c-f* hybridization effect to them in detail, we have performed the soft x-ray angle-resolved photoemission (ARPES) study of $CeRu_2Si_2$ and $CeRu_2Ge_2$.

The photoemission measurements were performed at BL25SU. The excitation photon energy (hv) was 700-890 eV. The overall energy resolution was set to 100-300 meV. The base pressure was about 4 x 10^{-8} Pa. In order to obtain clean (001) surfaces, the single crystalline samples were cleaved *in situ* at the measuring temperature of 20 K.

Figure 1 shows the hv dependence of the second derivative of the ARPES spectra for $CeRu_2Ge_2$ measured at the polar angle θ of ~1° with the energy and angular resolution of 300 meV and ±0.25°, respectively. It is recognized that several peaks disperse in an energy region from the Fermi level (E_F) to -6 eV with half-period of ~70 eV. This value is consistent with an expected period of the dispersion along the (001) direction derived from the lattice constants [2] and the formula $k_z = (E_K\cos^2\theta + V_0)^{0.5}$, where k_z, E_K and V_0 stand for the momentum along the surface normal within the crystal, the photoelectron kinetic energy, and inner potential, respectively. Therefore, our result demonstrates that k_z is well resolved as a function of hv even at kinetic energies of 700-900 eV and a "three-dimensional" Fermi surface mapping is feasible by the soft x-ray ARPES. On the other hand, we have found that the ARPES spectrum at Γ(000) can be obtained at hv~755 eV, which is deviated from the expected hv from the above formula. This is caused by a momentum transfer effect from the incident photon to the photoelectron.

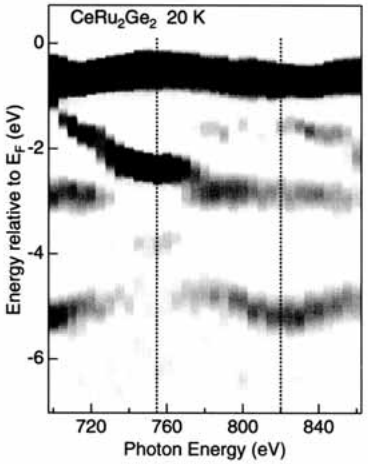

Fig. 1 hv dependence of the second derivative of the ARPES spectra at the polar angle of ~1° for $CeRu_2Ge_2$, where hv is set from 700 to 860 eV, reflecting the band dispersions along the (δ,δ,0)-(δ,δ,π) direction (δ~0.16π).

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Bulk Sensitive Photoemission Studies of Two Quasi-1d Metallic Oxides

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Angle-resolved photoemission spectroscopy (ARPES) measurements have been performed along the chain direction of quasi-one-dimensional (quasi-1d) $LiMo_6O_{17}$ and β'-$Cu_{0.66}V_2O_5$. The measurements were made on cleaved surfaces of single-crystalline samples under the base pressure of 2 x 10^{-10} Torr, using the angular mode of a SCIENTA-200 analyzer.

Damage was induced by the photons for both samples, much more severely than in our measurements previously made with low photon energies. For the case of β'-$Cu_{0.66}V_2O_5$, it was practically impossible to obtain any meaningful data, because the lineshapes of the spectra changed within 1 hour, which is not sufficient to obtain any high resolution ARPES data.

The rate of the damage was slower for $LiMo_6O_{17}$ (~ 4 hours), which enabled us to obtain ARPES spectra at 500eV by changing the position of the sample to a non-damaged position after initial measurements were done. The lineshapes of the 500eV ARPES spectra are the same as those of low photon energy spectra, which solidifies our interpretation that the bulk shows Luttinger liquid features.

The damage that occurred with the proposed samples provided an opportunity to measure two other important and interesting samples: $BaVS_3$ and LiV_2O_4.

$BaVS_3$ is a quasi-1d conductor that seems to undergo a smooth metal-insulator transition at 70K. However, the one-dimensionality is marginal in the metallic phase in that the conductivity along the chain direction is only 4 times larger than along the interchain direction. The resistivity is almost temperature independent in the metallic phase with a weak minimum at ~130K. We have measured angle-integrated PES using the transmission mode of the analyzer at the temperatures below and above the transition temperature. Our data contradict band calculations in which a band crossing the Fermi energy (E_F) provides a sharp density of states at E_F. No distinct Fermi edge was observed in the metallic phase spectra, even with the high photon energy where the surface sensitivity of the spectra is minimized. Rather, from 20K to 150K, an E_F gap of ~ 70meV is steadily filled by spectral weight transfer over a range 0.5eV below E_F, as occurs in the Mott insulator phase of V_2O_3.

We also have obtained preliminary PES spectra of LiV_2O_4, the only known *d*-electron heavy-fermion system. The measurements were done on the cleaved surface of a single crystalline sample of LiV_2O_4, and showed a much different lineshape compared to the previously reported PES spectra made with low photon energy on a polycrystalline samples. Thus there is now strong motivation to make a detailed PES, ARPES and XAS study using various photon energies and varying temperatures.