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Electronic Structure of Antiferromagnet CeCoSi Revealed by VUV-ARPES

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Strongly correlated electron systems have been known to show various emergent physical properties, as have been studied over recent decades. In such systems, a duality of "localization" and "itinerancy" of constituent electrons is the key to understand them; well localized *f*-electrons get to be itinerant when hybridized with conduction electrons (*cf*-hybridization). Magnetic or electronic ordered states develop when *cf*-hybridization is weak, while heavy-fermion emerges from strong *cf*-hybridization, namely in itinerant *f*-electron systems. The transition point from an ordered state to a heavy-fermion system defined in parametric space at zero temperature is called the quantum critical point (QCP). QCP has attracted a lot of theoretical and experimental attention for a few decades because some exotic phenomena, such as non-Fermi liquid, superconductivity, and Kondo destruction, have been reported in the vicinity of it [1].

Ternary cerium intermetallic compound, CeCoSi, has a tetragonal crystal structure (P4/nmm No. 129) (see Fig.1(a)). Antiferromagnetic (AFM) and antiferroquadrupole (AFQ) ordered phases were reported to take place at 9.4 K and 12 K at ambient pressure respectively, though the determination of the precise phase diagram has been controversial yet. The AFM transition temperature does not change against applied pressure very much, while that of the AFQ phase is stabilized up to 40 K at 1.6 GPa and vanishes around 2.4 GPa, implying the existence of QCP in the relevant pressure range [2, 3]. The different behaviors in AFM and AFQ phase indicate the existence of distinct mechanisms with different *cf*-hybridization strength because the large sensitivity to the applied pressure is often seen in rare-earth intermetallic compounds near the QCP [4, 5]. To reveal the mechanism of the AFQ phase, the information of the momentum-dependent *cf*-hybridization is important. Motivated by this, we have performed an angle-resolved photoemission spectroscopy (ARPES) of CeCoSi and its reference material, LaCoSi to elucidate the effect of *cf*-hybridization on the Fermi surfaces or band structures at HiSOR BL-9A.

The ARPES images of CeCoSi along the $\bar{\Gamma}-\bar{X}$ and $\bar{\Gamma}-\bar{M}$ lines (see Fig.1 (b)) measured using *s*-polarized light with its photon energy (*hv*) of 16eV are shown in Figs. 1(c) and 1(e), respectively. The results for LaCoSi are also depicted in Figs. 1(d) and 1(f) for comparison. We find a pair of bands crossing the Fermi level (E_F) as denoted with β along the $\bar{\Gamma}-\bar{X}$ and β' along the $\bar{\Gamma}-\bar{M}$ line for both CeCoSi and LaCoSi. It is recognized that the dispersion is quite anisotropic, where band β' is less steep (heavier) with an estimated effective mass of 13 m_e as compared with β (5.7 m_e). We have to note here that these bands are quite sensitive to light polarization. They actually disappear when excited with the *p*-polarized light, suggesting Co $3d_{x^2-y^2}$ orbital character. The band structures of LaCoSi and CeCoSi show a good agreement; the band structure of CeCoSi is well-reproduced by shifting the E_F about -0.1 eV, which suggests that the contribution of *f*-electrons to the Fermi surfaces are negligible, or the *f*-electrons in CeCoSi are well localized at ambient pressure.

Figures 2(a) and 2(b) show the magnified picture of the β band near E_F for CeCoSi and LaCoSi, respectively. The "kink" like structure is observed only for CeCoSi and its second derivative image visualizes a flat band and a gap in the β band. The flat band is not seen in LaCoSi and therefore can be ascribed to Ce *4f* band. Since the gap opens at the crossing point of the flat band, it is thought that this gap is caused by *cf*-hybridization. Moreover, the flat band causing the *cf*-hybridization lies at about 11 meV below E_F which is identical with the size of the *f*-level crystal electric field (CEF) splitting caused through excitation as determined by the inelastic neutron scattering [6]. Therefore, it is thought that the *cf*-hybridization takes place between the Co $3d_{x^2-y^2}$ and the excited CEF level. Since AFQ moment becomes active only in the inter-orbital space made between the ground state and excited state, we believe that this hybridization is the key to understand the mechanism of the pressure-induced AFQ phase.

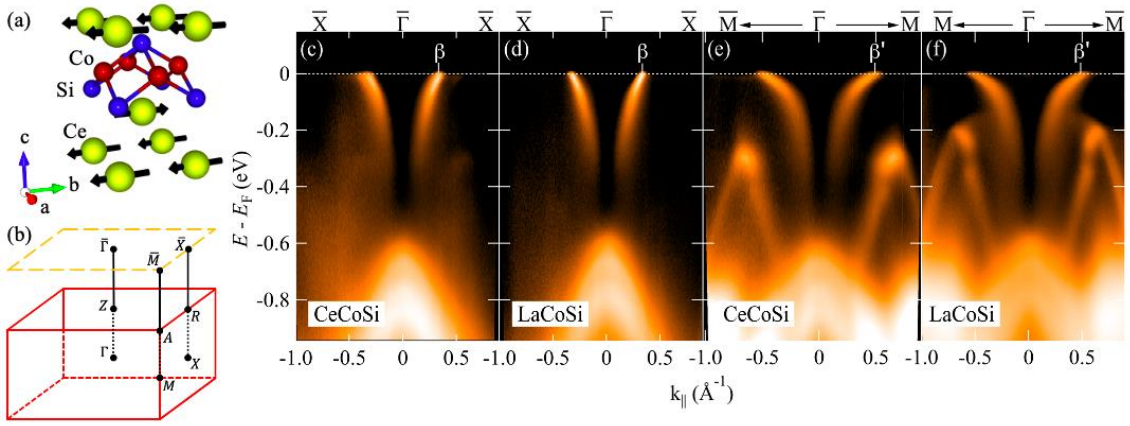

FIGURE 1. (a) Crystal structure of CeCoSi. Black arrows show magnetic moments in the AFM phase. **(b)** Bulk and surface Brillouin zones of *R*CoSi (*R* = La, Ce). **(c)-(f)** ARPES spectra of CeCoSi and LaCoSi along $\bar{\Gamma} - \bar{X}$ and $\bar{\Gamma} - \bar{M}$ lines.

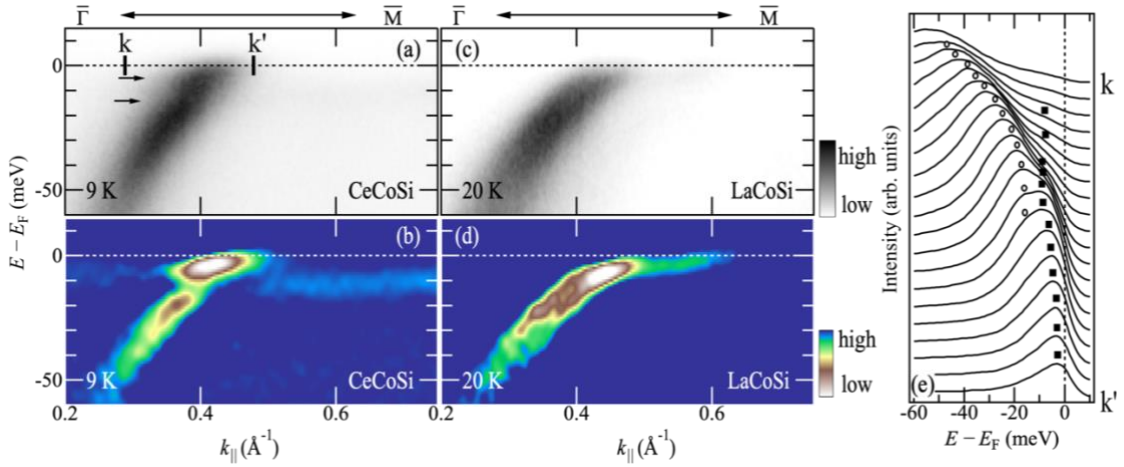

FIGURE 2. (a), (c) Band structures of the β band of CeCoSi and LaCoSi along $\bar{\Gamma} - \bar{M}$ line near E_F. Two black arrows in (a) show characteristic energies of "kink" like structure. **(b), (d)** Second derivative spectra of panels (a) and (c). **(e)** Energy distribution curves in the region between cut k and k' shown in panel (a). Open circles and black squares show peak structures derived from the β band and the flat band, respectively.

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