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Bulk-sensitive photoemission study of $A\mathrm{Cu_3Ru_4O_{12}}$ (A=Ca, Na, and La) with heavy-fermion behavior

Takaaki Sudayama,[1] Yuki Wakisaka,[1] Kou Takubo,[1] Takashi Mizokawa,[1,2] Wataru Kobayashi,[3] Ichiro Terasaki,[3]
Soutarou Tanaka,[4] Yoshiteru Maeno,[4] Masashi Arita,[2] Hirofumi Namatame,[2] and Masaki Taniguchi[2,5]
[1]*Department of Physics & Department of Complexity Science and Engineering, University of Tokyo, Kashiwa, Chiba 277-8561, Japan*
[2]*Hiroshima Synchrotron Radiation Center, Hiroshima University, Higashihiroshima, Hiroshima 739-0046, Japan*
[3]*Department of Applied Physics, Waseda University, Tokyo 169-8555, Japan*
[4]*Department of Physics, Graduate School of Science, Kyoto University, Kyoto 606-8502, Japan*
[5]*Graduate School of Science, Hiroshima University, Higashihiroshima, Hiroshima 739-8526, Japan*
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We have studied the *d*-electron heavy-fermion states in $A\mathrm{Cu_3Ru_4O_{12}}$ (A=Ca, Na, and La) using x-ray photoemission spectroscopy and high-resolution photoemission spectroscopy at bulk-sensitive photon energy (7 eV). The bulk-sensitive photoemission measurements for A=Ca, Na, and La show that a resonancelike structure within a pseudogap commonly evolves in the low-temperature range where the Kadowaki-Woods relation holds. The origin of the resonancelike peak and the heavy-fermion behavior is basically attributed to the hybridization between the Cu 3*d* and Ru 4*d* orbitals. The *A*-site substitution controls the filling of the Cu 3*d* and Ru 4*d* hybridized bands. Interestingly, while the resonancelike peak position roughly follows the rigid-band shift for A=Na and La, the resonancelike peak deviating from the rigid-band behavior is located just at the Fermi level as expected in a Kondo system. The difference in the resonancelike peak near the Fermi level is correlated with that in the Cu 2*p* core-level spectra.

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I. INTRODUCTION

Perovskite-type transition-metal oxides and their relatives show remarkably rich electric and magnetic properties.[1] In particular, *A*-site ordered perovskite $AA'_3B_4\mathrm{O}_{12}$ has transition-metal ions at A' and B sites and the $B\mathrm{O}_6$ octahedra are tilted to produce a pseudosquare planar coordination for the A' site. The novel *A*-site ordered perovskite compounds have attracted a great deal of attention both in experimental and theoretical studies due to its interesting and unexpected properties. Among them, $\mathrm{CaCu_3Mn_4O_{12}}$ shows over a wide range of temperatures very large magnetoresistance at low magnetic fields.[2] $\mathrm{CaCu_3Ti_4O_{12}}$ has been reported as having the largest dielectric constant ever measured over a wide range of temperatures.[3–5]

Recently, Kobayashi *et al.* and Ramirez *et al.* found that $\mathrm{CaCu_3Ti_{4-x}Ru_xO_{12}}$ shows an insulator-to-metal transition around $x\sim 3$ and that the end member $\mathrm{CaCu_3Ru_4O_{12}}$ exhibits a *d*-electron heavy-fermion behavior with electronic specific-heat coefficient γ of 28 mJ/(Cu mol K^2).[6,7] While Ramirez *et al.* attributed the insulator-to-metal transition to the valence change from Cu^{2+} to Cu^{+}, Kobayashi *et al.* concluded that the Cu valence stays at +2 across the insulator-to-metal transition. In addition, the magnetic susceptibility of $\mathrm{CaCu_3Ru_4O_{12}}$ has a broad peak at $\sim$200 K and its resistivity is dominated by the T^2 term below 25 K satisfying the Kadowaki-Woods relation. These measurements imply that the heavy-fermion behavior comes from the Kondo mechanism just as that in the *f*-electron heavy-fermion systems.[6] It has been suggested that the hybridization between the itinerant electrons originating from the Ru 4*d* orbitals and the localized Cu^{2+} electrons with $S=1/2$ spins contributes to the Kondo behavior. In addition, the previous x-ray photoemission spectroscopy (XPS) result[8] also indicates that the mechanism of mass enhancement of $\mathrm{CaCu_3Ru_4O_{12}}$ is different from that of other *d*-electron heavy-fermion systems such as $\mathrm{LiV_2O_4}$, in which only V 3*d* electrons have important roles.[9,10] Very recently, Tanaka *et al.* reported that $\mathrm{NaCu_3Ru_4O_{12}}$ and $\mathrm{LaCu_3Ru_4O_{12}}$ also show *d*-electron heavy-fermion behavior with γ of 25 and 45 mJ/(Cu mol K^2). $A\mathrm{Cu_3Ru_4O_{12}}$ (A=Na, Ca, and La) show the Kadowaki-Woods relation and the Wilson ratio similar to those of *f*-electron heavy-fermion systems, indicating that the correlation effects in the itinerant Ru 4*d* bands are important for the *d*-electron heavy-fermion state in $A\mathrm{Cu_3Ru_4O_{12}}$.[11]

In this work, we report on results of XPS and high-resolution photoemission spectroscopy with bulk-sensitive photon energy (7 eV) of $A\mathrm{Cu_3Ru_4O_{12}}$ (A=Ca, Na, and La) with the heavy-fermion behavior and discuss the variation of electronic structure by the *A*-site substitution as well as possible mechanism of the mass enhancement.

II. EXPERIMENTS

The polycrystalline samples of $\mathrm{CaCu_3Ru_4O_{12}}$, $\mathrm{NaCu_3Ru_4O_{12}}$, and $\mathrm{LaCu_3Ru_4O_{12}}$ were prepared by a solid-state reaction as described in the literatures.[6,11] The polycrystalline samples were fractured *in situ* to obtain clean surfaces for photoemission measurements. XPS measurements were carried out at room temperature using JPS9200 spectrometer (JEOL, Japan). Monochromatic Al $K\alpha$(1486.6 eV) was used as the x-ray source. The pass energy of the electron analyzer was set to 10 eV. The total-energy resolution including the x-ray source and the electron analyzer was about 0.6 eV. The binding energy was calibrated using the Fermi edge and the Au 4*f* core level of the gold reference sample. The base pressure of the chamber was 1×10^{-7} Pa. High-resolution photoemission measurements were carried out at beamline 9A, Hiroshima Synchrotron Radiation Center (HiSOR) using high-resolution hemispherical electron-energy analyzer R4000 (Gammadata-Scienta, Sweden). The total-energy resolution including both the electron-energy analyzer and the monochromator was set to 4 meV at $h\nu=7$ eV. The binding energy was calibrated using the Fermi edge of the gold reference sample. The base pressure of the chamber was 1×10^{-8} Pa.

III. RESULTS AND DISCUSSION

A. XPS results

Figure 1(a) shows XPS result at 300 K for the valence-band spectra of $NaCu_3Ru_4O_{12}$ and $LaCu_3Ru_4O_{12}$ with that of $CaCu_3Ru_4O_{12}$. The peak at ~0.5 eV, the broad structure at ~6 eV, and the peak at ~2.5 eV are derived from the Ru $4dt_{2g}$ band (hybridized with the O 2*p* states), the O 2*p* band (hybridized with the Ru 4*d* states), and the Cu 3*d* states, respectively.[8] The gross features of $NaCu_3Ru_4O_{12}$ and $LaCu_3Ru_4O_{12}$ are similar to those of $CaCu_3Ru_4O_{12}$. The effect of carrier doping by the replacement of *A*-site Ca^{2+} by $Na^+(La^{3+})$ does not appear prominently in the overall valence-band structure.

The Ru 3*d* core-level XPS results of $NaCu_3Ru_4O_{12}$ and $LaCu_3Ru_4O_{12}$ are shown in Fig. 1(b) together with that of $CaCu_3Ru_4O_{12}$. The sharp well-screened peak around 280.9 eV is accompanied by the broad poorly screened feature[12] around 282.3 eV as observed in various Ru oxides.[8,13,14] The sharp well-screened peak is shifted to the lower binding-energy side in going from $NaCu_3Ru_4O_{12}$ to $LaCu_3Ru_4O_{12}$. The Ru 3*d* core-level binding-energy shift can be caused by chemical-potential shift due to the carrier doping and by change in the chemical shift due to the Ru valence change. The La substitution for Na can introduce electrons in the Ru 4*d* band and the chemical potential can be shifted to the higher binding-energy side. However, the direction of the expected binding-energy shift due to the chemical-potential shift is opposite to the experimental result. In addition, since the density of states at the Fermi level (E_F) is extremely high in the present system, the chemical-potential shift should be negligibly small if it exists. Assuming that the formal Cu valence is +2, the La substitution for Na may decrease the formal Ru valence from +4.25 to +3.75. The decrease of the formal Ru valence can shift the Ru 3*d* peak to the lower binding-energy side, consistent with the experimental result.

Figure 1(c) shows the Cu 2*p* core-level XPS spectra of $NaCu_3Ru_4O_{12}$ and $LaCu_3Ru_4O_{12}$ with that of $CaCu_3Ru_4O_{12}$. In addition to the charge-transfer satellite (labeled as A, dominated by the d^9 configuration in the final states), the main peak has two components that can be assigned as the poorly screened structure (B, $d^{10}\underline{L}$, $\underline{L}$ represents an O 2*p* hole) and the well-screened structure (C, d^{10}).[15] The line shape of the charge-transfer satellite indicates that the Cu valence is basically close to +2. When the Cu valence is close to +2, the Cu 3*d xy* orbital, that is the highest energy level among the Cu 3*d* orbitals, is close to half filling and, consequently, close to the orbital-selective Mott transition for the Cu 3*d xy* band. Structure C of $CaCu_3Ru_4O_{12}$ is substantially enhanced compared to those of $NaCu_3Ru_4O_{12}$ and $LaCu_3Ru_4O_{12}$. This indicates that, even at 300 K, more Cu 3*d* electrons are involved in the density of states around E_F in the Ca system than in Na and La systems. Therefore, in

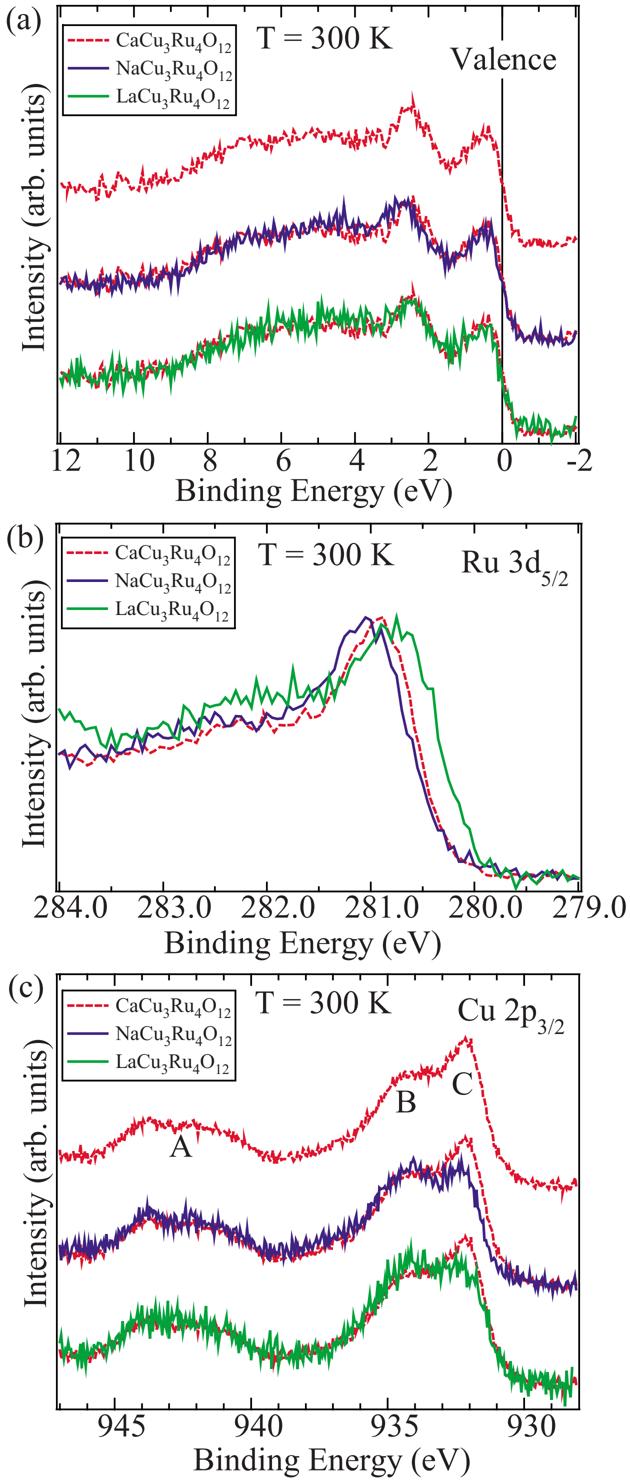

FIG. 1. (Color online) (a) Valence-band XPS spectra of $NaCu_3Ru_4O_{12}$, $LaCu_3Ru_4O_{12}$, and $CaCu_3Ru_4O_{12}$ taken at 300 K. (b) Ru 3*d* photoemission spectra of $NaCu_3Ru_4O_{12}$, $LaCu_3Ru_4O_{12}$, and $CaCu_3Ru_4O_{12}$ taken at 300 K. (c) Cu 2*p* photoemission spectra of $NaCu_3Ru_4O_{12}$, $LaCu_3Ru_4O_{12}$, and $CaCu_3Ru_4O_{12}$ taken at 300 K.

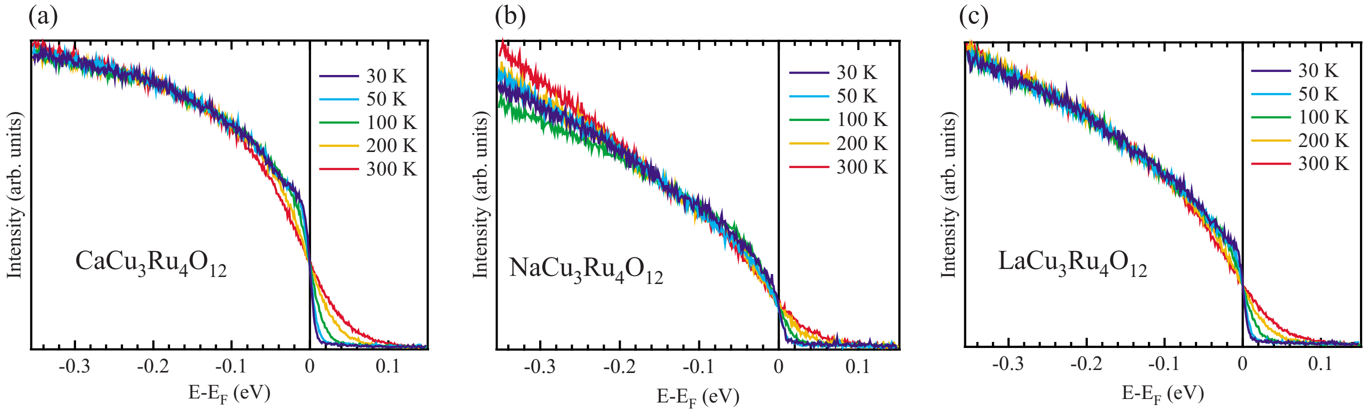

FIG. 2. (Color online) Temperature dependence of the angle-integrated photoemission spectra near the Fermi level for (a) $CaCu_3Ru_4O_{12}$, (b) $NaCu_3Ru_4O_{12}$, and (c) $LaCu_3Ru_4O_{12}$.

$CaCu_3Ru_4O_{12}$, the Cu 3*d* *xy* orbital is close to half filling and the Cu 3*d* electrons are delocalized just like the 4*f* or 5*f* electrons in the ground states of the *f*-electron heavy-fermion systems. In this picture, the closeness to the orbital-selective Mott transition and the resulting Kondo-like effect is more important in the Ca system than in the Na and La systems and the Cu 3*d* contribution around E_F can be larger than the prediction of the band-structure calculation[16] in the Ca system. Here, it should be noted that the enhancement of Cu 3*d* contribution in the Ca system does not mean the enhancement of heavy-fermion mass in the Ca system. A kind of hybridization gap may open in one of the Ru 4*d* bands due to the Kondo-like effect and the heavy-fermion mass could be reduced.

In comparison, the Cu 3*d* electrons are less active around E_F in the Na and La systems although their Cu 3*d* orbitals hybridize with the Ru 4*d* and O 2*p* orbitals to some extent by considering the calculated band structure of $CaCu_3Ru_4O_{12}$.[16] For $NaCu_3Ru_4O_{12}$, one can speculate that holes doped by the substitution of Na for Ca are trapped in the Cu site and form Zhang-Rice singlets ($d^9\underline{L}$). In such a case, the weakening of the half fillingness would suppress the Kondo-like effect. Consequently, the Cu 3*d* contribution around E_F would be reduced in going from the Ca system to the Na system. As for $LaCu_3Ru_4O_{12}$, it is also possible that the Cu sites grab oxygen holes from the Ru sites to form Zhang-Rice singlets and that the Kondo channel is suppressed. The increase of the Ru 3*d* screening from the Na system to the La system can be understood by considering the calculated density of states that has a peak above E_F.[16] In $LaCu_3Ru_4O_{12}$, electrons doped by the substitution of La for Na (or Ca) fill the states just below the peak and E_F is located near the peak.[11] In the following discussion, let us denote the peak in the density of states as van Hove singularity (vHs).

B. Near-E_F bulk-sensitive photoemission results

Figure 2 shows the temperature dependence of bulk-sensitive photoemission spectra for $ACu_3Ru_4O_{12}$ (A=Ca, Na, and La) taken at $h\nu$=7 eV. The spectra are normalized to the integrated intensities from −0.2 to −0.1 eV. In the Na system, the temperature dependence of the spectral weight between −0.3 and −0.2 eV is attributed to a change in the background signal due to secondary electrons, which is derived from some instabilities of surface regions or grain boundaries in polycrystalline samples. The background signal increases with increasing temperature suggesting that the surface quality is degraded with increasing temperature. However, the bulk-sensitive photoemission spectra near E_F are reasonably thought to represent the bulk electronic states below the surface regions or the grain boundaries. This assumption is supported by the high-temperature data in Fig. 3 as discussed in the next paragraph.

Since the transport data of $ACu_3Ru_4O_{12}$ show typical Fermi-liquid behavior, the photoemission spectra can be divided by the Fermi-Dirac distribution function to extract the temperature dependence of density of states. In the present analysis, we first fitted the photoemission spectra of the gold reference sample to model functions with Fermi-Dirac distribution function at respective temperatures. We then divided the photoemission spectra of $ACu_3Ru_4O_{12}$ by the model functions[17] to obtain the density of states as plotted in Fig. 3. Here, the data up to $3k_BT$ above E_F are plotted where sufficiently large signal-to-noise ratio is available. At high temperatures (200 and 300 K), the density of states near E_F is just flat for A=Ca, Na, and La. The flat density of states is obtained for A=Na in which surface degradation at high temperatures is concerned. This observation supports the assumption that the bulk-sensitive photoemission spectra near E_F represent the bulk electronic states below the surface regions or the grain boundaries even for A=Na.

In the data set taken at 50 K shown in Fig. 3(d), the resonancelike peak of $CaCu_3Ru_4O_{12}$ is just located at E_F while that of $NaCu_3Ru_4O_{12}$ is located at ~8 meV above E_F. As for $LaCu_3Ru_4O_{12}$, the resonancelike peak is likely to be located at ~3 meV above E_F although the poor signal-to-noise ratio prevents the precise evaluation of the peak position.

In the low-temperature range below 100 K, the density of states of $ACu_3Ru_4O_{12}$ (A=Ca, Na, and La) has a resonancelike peak near E_F within a pseudogap of ~50 meV. Interestingly, the formation of the resonancelike peak is very similar to that observed in another *d*-electron heavy-fermion system LiV_2O_4.[18] In LiV_2O_4, a resonancelike peak located

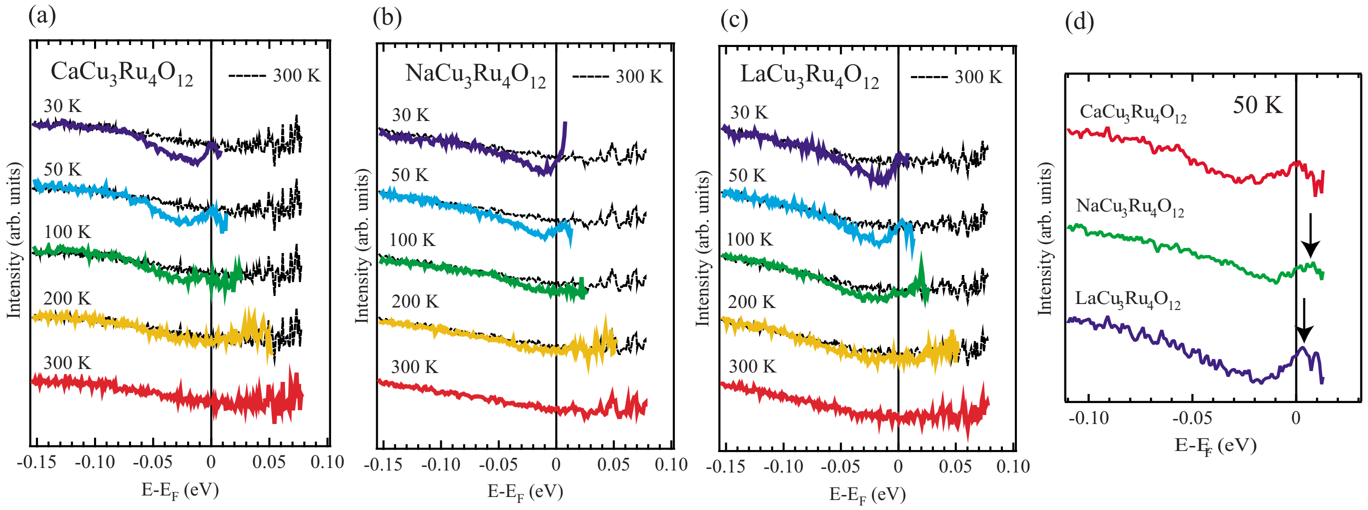

FIG. 3. (Color online) Temperature dependence of the photoemission spectra near the Fermi level divided by fitting functions of gold spectra for (a) $CaCu_3Ru_4O_{12}$, (b) $NaCu_3Ru_4O_{12}$, and (c) $LaCu_3Ru_4O_{12}$. The spectra taken at 300 K are shown by the black dashed curves and are compared to the spectra taken at 30, 50, 100, and 200 K. (d) Photoemission spectra at 50 K of $CaCu_3Ru_4O_{12}$, $NaCu_3Ru_4O_{12}$, and $LaCu_3Ru_4O_{12}$. The peak positions are indicated by the arrows for the Na and La systems.

above E_F gradually disappears with increasing temperature. It is expected that the resonancelike peak with peculiar temperature dependence is deeply related to the heavy-fermion behaviors in the transition-metal oxides. In the next section, let us discuss the origin of the resonancelike peak based on the Kondo picture and the band picture.

C. Possible origins of the heavy-fermion state

In $CaCu_3Ru_4O_{12}$, the evolution of the resonancelike peak at E_F below 100 K [see Fig. 3(a)] is exactly expected in a Kondo system with Kondo temperature of ~100 K. The Cu valence is close to +2 in $CaCu_3Ru_4O_{12}$ and, therefore, the Cu 3*d* *xy* band is almost half filled. In such case, the Cu 3*d* *xy* electrons can be localized due to the orbital-selective Mott transition. Then the localized Cu 3*d* *xy* electrons can hybridize with the Ru 4*d* band to form the heavy-fermion state just at E_F with the approximate electron-hole symmetry. On the other hand, in $NaCu_3Ru_4O_{12}$, the resonancelike peak above E_F is not consistent with the Kondo picture. The difference in the resonancelike peaks between the Na system and the Ca system is consistent with the differences in the magnetic susceptibility and in the Cu 2*p* core-level spectra.

Instead of the Kondo effect, the data of the Na and La systems can be explained by the rigid-band model with the vHs above E_F as recently pointed out by Tanaka *et al.*[11] The resonancelike peak above E_F can be attributed to the vHs and its upward energy shift from the La system to the Na system is derived from the hole doping by Na substitution for La. The ground state predicted by the band-structure calculation is a good starting point to describe the resonancelike peak observed in $ACu_3Ru_4O_{12}$. In the band picture, the vHs state or the heavy-fermion state near E_F exists only in the specific region of the momentum space. This picture is probably applicable to the heavy-fermion behavior and the recent angle-resolved photoemission observation in $(Sr,Ca)_2RuO_4$.[19]

In order to understand the behaviors of $ACu_3Ru_4O_{12}$ (A =Ca, Na, and La) as functions of temperature and doping, one should consider both the vHs and the Kondo-like effect (or the closeness to the orbital-selective Mott transition). As for the doping effect, as basically predicted by the band-structure calculation, the fine structures near E_F (the vHs and the pseudogap) are formed by coherent hybridization between the Cu 3*d* *xy* and Ru 4*d* bands. When the half fillingness of the Cu 3*d* *xy* band is enhanced as in the Ca system, the Kondo-like effect becomes relevant and the deviation from the rigid-band picture becomes apparent.

As for the temperature evolution, when the coherent hybridization between the Cu 3*d* and Ru 4*d* orbitals is lost by thermal fluctuations above 100 K, the vHs and the pseudogap are expected to disappear as observed in the photoemission spectra. Such temperature dependence is similar to that reported in the photoemission studies on LiV_2O_4 (Ref. 18) and $(Sr,Ca)_2RuO_4$.[19] The Kadowaki-Woods relation holds in the low-temperature region where the resonancelike peak is sharp, suggesting that the Kondo-like effect should be considered to explain the temperature evolution in $ACu_3Ru_4O_{12}$ as well as LiV_2O_4 and $(Sr,Ca)_2RuO_4$.

On the theoretical side, the temperature and doping dependence of the single-particle excitation spectra should be reexamined using the Anderson lattice model or the multiband Hubbard model. In the latter model, hybridization between the Cu 3*d* *xy* and Ru 4*d* orbitals should be considered for $ACu_3Ru_4O_{12}$ as in the case of LiV_2O_4.[20] The closeness to the orbital-selective Mott transition of the Cu 3*d* *xy* component would be essential in $ACu_3Ru_4O_{12}$ as emphasized in LiV_2O_4 and $(Sr,Ca)_2RuO_4$.[21,22] In addition, the O 2*p* orbitals would be important in the present system when the Cu 3*d* *xy* band is less than half filling and forms Zhang-Rice singlets with the O 2*p* holes. Therefore, the Kondo and non-Kondo behaviors observed in the present system may lead to recognition as a characteristic phenomenon of a certain class of *d*-electron systems.

IV. CONCLUSION

In summary, we have studied the electronic structure of $A\mathrm{Cu}_3\mathrm{Ru}_4\mathrm{O}_{12}$ (A=Ca, Na, and La) using XPS and high-resolution low-excitation energy photoemission spectroscopy. Cu 2p core-level spectra, which reflect the screening of core-hole charge by the Cu 3d electrons, clarify the difference of the electronic states of $A\mathrm{Cu}_3\mathrm{Ru}_4\mathrm{O}_{12}$ with A=Ca, Na, and La. The Cu 3d xy orbital for A=Ca is closer to half filling than that for A=Na and La and more Cu 3d electrons are involved in the near-E_F states for A=Ca than for A=Na and Ca. The bulk-sensitive photoemission measurements show that the resonancelike structure evolves near E_F in the low-temperature range. The doping dependence of the 3d core-level spectra of these three systems at 300 K, as well as of the photoemission spectra of the Na and La systems near E_F at low temperature, is consistent with the rigid-band picture with the vHs above E_F. However, the deviation from the rigid-band picture is evident in the Ca system and could be related to the Kondo effect or the closeness to the orbital-selective Mott transition. As for the temperature dependence, the resonancelike peak and the pseudogap rapidly disappear above 100 K, indicating that the coherent hybridization between the Cu 3d and Ru 4d electrons is lost at elevated temperatures.

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