Optical study on electronic structure of the locally non-centrosymmetric CeRh$_2$As$_2$

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The electronic structures of the heavy-fermion superconductor CeRh$_2$As$_2$ with the local inversion symmetry breaking and the reference material LaRh$_2$As$_2$ have been investigated by using experimental optical conductivity ($\sigma_1(\omega)$) spectra and first-principal DFT calculations. In the low-temperature $\sigma_1(\omega)$ spectra of CeRh$_2$As$_2$, a 4f–conduction electron hybridization and heavy quasiparticles are clearly indicated by a mid-infrared peak and a narrow Drude peak. In LaRh$_2$As$_2$, these features are absent in the $\sigma_1(\omega)$ spectrum, however, it can nicely be reproduced by DFT calculations. For both compounds, the combination between a local inversion symmetry breaking and a large spin-orbit (SO) interaction plays an important role for the electronic structure, however, the SO splitting bands could not be resolved in the $\sigma_1(\omega)$ spectra due to the small SO splitting size.

I. INTRODUCTION

Materials with non-centrosymmetric crystal structure and crystal surfaces with inversion symmetry breaking have recently attracted attention for novel physical properties combined with spin-orbit interaction (SOI) [1]. By using the SOI and the electric field gradient generated by the spatial symmetry breaking, a spin-polarized current originating from spin-polarized bands is generated and is regarded to be useful for spintronics applications. A breaking of local inversion symmetry also generates a toroidal current owing to the Dzyaloshinsky-Moriya interaction [2] and a Cooper pair with a helical spin structure, which produces a superconducting state with a high critical field [3]. Actually, an extremely spin structure, which produces a superconducting state generated by the spatial symmetry breaking, a spin-polarized band splitting such as the Rashba effect [18, 19], which can be directly observed by an angle-resolved photoelectron spectroscopy (ARPES) [20] and (magneto-optical) infrared spectroscopies [21, 22]. ARPES studies on non-centrosymmetric heavy fermions such as CeIrSi$_3$ [23] and UIr [24], have been reported theoretically [10, 16] and experimentally [17]. However, the electronic structure of the material, which is the most basic information for the discussion of the physical properties, has not been investigated experimentally so far, although the electronic structure using DFT calculations has been reported [13, 14].

A locally non-centrosymmetric crystal structure can produce a local electric field to the electron orbitals. With a large SOI, the local electric field induces the band splitting such as the Rashba effect [18, 19], which can be directly observed by an angle-resolved photoelectron spectroscopy (ARPES) [20] and (magneto-optical) infrared spectroscopies [21, 22]. ARPES studies on non-centrosymmetric heavy fermions have been performed on CeIrSi$_3$ [23] and UIr [24]. However, so far, no studies of optical conductivity were reported for this type of materials.

FIG. 1. Crystal structure of $R$Rh$_2$As$_2$ ($R = Ce, La$) with the space group of P4/mmm depicted by using VESTA [5]. Rh 1 and Rh 2 are located at different sites and therefore have different effects on the electronic structure (see Figs. 3 and 6).
FIG. 2. Temperature-dependent reflectivity ($R(\omega)$) spectra of the as-grown (001) surfaces of CeRh$_2$As$_2$ and LaRh$_2$As$_2$ in the photon energy $\hbar\omega$ range of 0.01–1.2 eV. Fine structures of CeRh$_2$As$_2$ at the photon energies $\hbar\omega$ of about 15, 23, and 32 meV originate from TO phonons (not discussed here). (Inset) Wide-energy-range $R(\omega)$ spectra of CeRh$_2$As$_2$ and LaRh$_2$As$_2$ in the $\hbar\omega$ range of 0.1–30 eV at 300 K. Both spectra are almost identical suggesting the similar electronic structure at room temperature.

We investigated the fundamental electronic structure of the locally non-centrosymmetric heavy-fermion material CeRh$_2$As$_2$ by measuring the optical conductivity ($\sigma(\omega)$) spectra and comparing them with first-principal DFT calculations. As a reference material without 4$f$ electrons, we also investigated LaRh$_2$As$_2$ in order to discuss the electronic structure without the effect of the hybridization between conduction and 4$f$ electrons ($c$–$f$ hybridization). Firstly, the obtained $\sigma(\omega)$ spectrum of LaRh$_2$As$_2$ is compared with the DFT calculations for the fundamental electronic structure without 4$f$ electrons. Next, the $\sigma(\omega)$ spectrum of CeRh$_2$As$_2$ is compared with the corresponding calculation results. Finally, the temperature-dependent $\sigma(\omega)$ spectra of CeRh$_2$As$_2$ is compared with other heavy fermion materials to discuss the evolution of the $c$–$f$ hybridization.

II. EXPERIMENT AND CALCULATION METHODS

Single-crystalline CeRh$_2$As$_2$ and LaRh$_2$As$_2$ samples were synthesized by the Bi-flux method [4]. The optical reflectivity $R(\omega)$ measurements have been performed using the as-grown (001) plane. Near-normal-incident $R(\omega)$ spectra were acquired in a wide photon-energy range of 8 meV–30 eV to ensure accurate Kramers-Kronig analysis (KKA) [26]. Infrared (IR) and terahertz (THz) measurements at the photon energy $\hbar\omega$ regions of 8 meV–1.5 eV have been performed using conventional near-normal reflectivity measurement setups to obtain absolute $R(\omega)$ at an accuracy of ±0.3 % with a feedback positioning system in the temperature range of 10–300 K [27]. To obtain the absolute $R(\omega)$ values, the in-situ gold evaporation method was adopted. Obtained $R(\omega)$ spectra of CeRh$_2$As$_2$ and LaRh$_2$As$_2$ are shown in Fig. 2. In the photon energy range of 1.5–30 eV, the $R(\omega)$ spectrum was measured only at 300 K by using the synchrotron radiation setup at the beamline 3B of UVSOR-III Synchrotron [28], and connected to the spectra for $\hbar\omega \leq 1.5$ eV for KKA. In order to obtain $\sigma(\omega)$ via KKA of $R(\omega)$, the spectra were extrapolated below 8 meV with a Hagen-Rubens function [$R(\omega) = 1 - \{2\omega/(\pi\sigma_{DC})\}^{1/2}$] due to the metallic $R(\omega)$ spectra, and above 30 eV with a free-electron approximation $R(\omega) \propto \omega^{-4}$ [29]. Here, the values of the direct current conductivity ($\sigma_{DC}$) were adopted from the experimental values [4]. The extrapolations were confirmed not to severely affect to the $\sigma(\omega)$ spectra at around 100 meV, which are the main part in this paper.

First-principal DFT calculations have been performed by using the WIEN2k code including SOI [30] to explain the experimentally obtained $\sigma(\omega)$ spectra. Lattice parameters obtained from room-temperature x-ray diffraction measurements shown in Table I were adopted to the calculations. The obtained band structure of CeRh$_2$As$_2$ was consistent with the recent report [13, 15]. $\sigma(\omega)$ spectra of the interband transitions have also been calculated by using the WIEN2k code. For the discussion of LaRh$_2$As$_2$, we also performed DFT calculations on the basis of a hypothetical ThCr$_2$Si$_2$-type crystal structure, assuming the same lattice constants as for the original CaBe$_2$Ge$_2$-type structure.

III. RESULTS AND DISCUSSION

The measured $R(\omega)$ spectra of CeRh$_2$As$_2$ and LaRh$_2$As$_2$, shown in Fig. 2 at various temperatures, were used for KKA in order to obtain their $\sigma(\omega)$ spectra as shown in Fig. 3. At 300 K, $\sigma(\omega)$ of both materials monotonically increase with decreasing $\hbar\omega$ suggesting a typical metallic character. The spectrum of CeRh$_2$As$_2$ at 300 K is very similar to that of LaRh$_2$As$_2$, as demonstrated by almost identical $R(\omega)$ spectra in the inset of Fig. 2. This suggests fully localized Ce 4$f$ states at 300 K. With decreasing temperature, the spectra strongly change and new features emerge: A double-peak structure (“mid-IR peak”) appears at 0.12 and 0.4 eV in CeRh$_2$As$_2$, whereas in LaRh$_2$As$_2$, a weak single peak becomes visible at 0.45 eV. The mid-IR peak is usually observed in many Ce compounds and suggests the emergence of the $c$–$f$ hybridization [31]. The peak appearing in LaRh$_2$As$_2$ does not obviously originate from the $c$–$f$ hybridization, but can be explained by the electronic structure of LaRh$_2$As$_2$. 


TABLE I. Lattice parameters of CeRh$_2$As$_2$ and LaRh$_2$As$_2$ used for the DFT calculations. The parameters were obtained by x-ray diffraction methods.

| Sample | CeRh$_2$As$_2$ | LaRh$_2$As$_2$ |
|--------|----------------|----------------|
| Crystal structure | CaBe$_2$Ge$_2$-type | $P_2_1/mnm$ (No. 129) |
| Lattice constant |  |
| a (Å), b (Å), c (Å) | 4.283(1), 4.283(1), 9.865(2) | 4.3137(2), 4.3137(2), 9.8803(4) |
| Position | X | Y | Z | X | Y | Z |
| Ce, La | 0.25 | 0.25 | 0.254686(3) | 0.25 | 0.25 | 0.2543(2) |
| Rh 1 | 0.75 | 0.25 | 0 |
| Rh 2 | 0.25 | 0.25 | 0.617418(4) | 0.25 | 0.25 | 0.6159(2) |
| As 1 | 0.75 | 0.25 | 0.5 |
| As 2 | 0.25 | 0.25 | 0.864075(7) | 0.25 | 0.25 | 0.871(9) |

**FIG. 3.** Temperature-dependent optical conductivity ($\sigma_1(\omega)$) spectra of CeRh$_2$As$_2$ and LaRh$_2$As$_2$.

**A. Electronic structure of LaRh$_2$As$_2$**

Figure 4 shows the band calculation results of LaRh$_2$As$_2$ near the Fermi energy ($E_F$) with and without SOI. The main effect of including the SOI appears as a spin-orbit (SO) splitting near $E_F$ along the $M-X$ and $A-R$ lines (see the red encircled regions in Fig. 4). The bands mainly originate from the 4$d$ states of Rh 1 as shown in the partial density of states depicted in Fig. 4. The SO splitting is much smaller than that of LaPt$_3$Si [32] and BiTeI [22]. The different SO splitting size probably originate from the different orbital moments (4$d$ for Rh, 5$d$ for Pt, and 6$p$ for Bi), locally/globally non-centrosymmetric crystal structure, and/or the different dimensionality, three-dimensional LaRh$_2$As$_2$ and LaPt$_3$Si, and two-dimensional BiTeBr.

Figure 5 shows the experimental $\sigma_1(\omega)$ spectrum of LaRh$_2$As$_2$ at $T = 10$ K together with spectra obtained from the DFT calculation results (Fig. 4) either with SOI (red solid line) or without SOI (blue solid line). The free charge carrier response (Drude peak, grey solid line) evaluated from $\sigma_{DC}$ of LaRh$_2$As$_2$ is also shown. The experimental $\sigma_1(\omega)$ spectrum (denoted by “Experiment” in Fig. 5) is much larger than the expected Drude curve suggesting the existence of other components due to interband transitions overlapping on the Drude curve. These interband transitions are indicated by the thick solid line (denoted by “Experiment - Drude” in Fig. 5), which was derived by subtraction of the Drude curve from the $\sigma_1(\omega)$ spectrum. The interband transition spectrum has a broad peak at around $\sim 0.1$ eV and a sharp peak at $\sim 0.5$ eV.

Both calculated $\sigma_1(\omega)$ spectra with and without SOI are almost identical suggesting a weak effect of the SOI on $\sigma_1(\omega)$. This is consistent with the small SOI intensity of LaRh$_2$As$_2$. The two significant peaks at $\hbar\omega \sim 0.2$ eV and $0.45$ eV can be attributed to the experimentally observed peaks at $\sim 0.1$ eV and $\sim 0.5$ eV. They both originate from the bands near the $\Gamma - M$ and $Z - A$ lines in the Brillouin zone (see Fig. 4). The background intensity of the calculated spectra is consistent with that of the experimental spectrum. Therefore, the experimental $\sigma_1(\omega)$ spectrum can be explained well by the DFT calculations.

In order to investigate the effect of the crystal structure, Fig. 5 also shows a $\sigma_1(\omega)$ spectrum calculated by using the centrosymmetric ThCr$_2$Si$_2$-type crystal structure ($I4/mmm$) while keeping the lattice parameters as in the CaBe$_2$Ge$_2$-type structure. The large peak at $\sim 0.5$ eV does not appear and the background spectral intensity is much lower than that of the experimental spectrum. This suggests that both the 0.5 eV peak and the high background intensity are characteristic properties of LaRh$_2$As$_2$ and the locally non-centrosymmetric CaBe$_2$Ge$_2$-type crystal structure.
FIG. 4. Calculated band structure of LaRh$_2$As$_2$ without (left) SOI and with (center) SOI. Spin-orbit split bands are red encircled. Inset depicts symmetry points in the Brillouin zone. (Right) Total density of states and partial density of states of La, Rh 1 and Rh 2 (see Fig. 1) with SOI.

FIG. 5. Optical conductivity ($\sigma_1(\omega)$) spectrum of LaRh$_2$As$_2$ at $T = 10$ K (Experiment, dotted line). Thick line denotes the interband transition part obtained after subtracting the Drude part (grey line) from the $\sigma_1(\omega)$ spectrum. Calculated $\sigma_1(\omega)$ spectra with and without SOI are shown by red and blue lines, respectively. The calculated spectrum of a centrosymmetric ThCr$_2$Si$_2$-type crystal structure (I4/mmm) is also plotted for comparison (dashed green line).

B. Electronic structure of CeRh$_2$As$_2$

Figure 6 shows the calculated band structures of CeRh$_2$As$_2$ with and without SOI. An important effect of the SOI is a splitting of the Ce 4$f$ bands from almost flat bands at $\sim 0.3$ eV into two parts, namely 4$f_{5/2}$ bands at $\sim 0.2$ eV and 4$f_{7/2}$ bands at $\sim 0.5$ eV. The splitting energy is roughly $0.25 - 0.3$ eV, which is a characteristic value for various Ce-based compounds as observed in $\sigma_1(\omega)$ spectra [31, 33] and photoelectron spectra [8, 34].

As in LaRh$_2$As$_2$, the SO split bands appear near $E_F$ along the $M-X$ and $A-R$ lines. The size of SO splitting is larger than that of LaRh$_2$As$_2$. Since the bands originate from the hybridization between the Rh 1 4$d$ and Ce 4$f$ bands (see the partial densities of states of Ce and Rh 1 in the right figure of Fig. 6), the 4$f$ state is considered to be relevant for the SO splitting. Moreover, as flat bands are claimed to be important for the superconductivity [13], the SO splitting may play an important role for the exotic superconductivity in CeRh$_2$As$_2$.

Figure 7 shows the experimentally obtained $\sigma_1(\omega)$ spectrum at $T = 10$ K together with the calculated $\sigma_1(\omega)$ spectra with and without SOI. In comparison with the $\sigma_1(\omega)$ spectra of LaRh$_2$As$_2$, the calculated spectra cannot reproduce the experimental spectrum well. The main reason is that the mid-IR peak below $\hbar\omega \sim 0.6$ eV does not appear in the calculation. The experimental mid-IR peak can be attributed to the SO splitting of the Ce 4$f$ states [31], which appears in the unoccupied density of states above $E_F$ as shown in the lower frame of Fig. 7. However, the corresponding mid-IR peak structure does not clearly appear in the $\sigma_1(\omega)$ calculation shown in the upper frame of Fig. 7. The inconsistency suggests that the calculated $c$-$f$ hybridization intensity in the DFT calculations is much smaller than the experimental value because the Kondo interaction between conduction and localized 4$f$ electrons is not included in the calculation.

According to the band calculation in Fig. 6, the signature of the SO splitting along the $\Gamma-M$ line may appear...
at $\hbar \omega \leq 0.1$ eV. In this energy region, there are three phonon peaks at $\hbar \omega = 15.2$, 22.8, and 31.7 meV (see Fig. 2), but no other significant structures except for the Drude peak. Therefore, we conclude that, in the $\sigma_1(\omega)$ spectra, there are no visible signatures for a SO splitting expected in the band structure.

C. $c$-$f$ hybridization of CeRh$_2$As$_2$

The $c$-$f$ hybridization in CeRh$_2$As$_2$ can be characterized by using the temperature dependence of the mid-IR peak. Figure 5 shows the temperature dependencies of the center of gravity $\Delta(\omega) = \langle \omega(T) \rangle - \langle \omega(300 K) \rangle / \langle \omega(300 K) \rangle$, where $\langle \omega(T) \rangle = \int_{\omega_1}^{\omega_2} \omega \sigma_1(\omega)d\omega / \int_{\omega_1}^{\omega_2} \sigma_1(\omega)d\omega$, and the spectral weight transfer $\Delta SW = \int_{\omega_1}^{\omega_2} [\sigma_1(\omega, T) - \sigma_1(\omega, 300 K)]/\sigma_1(\omega, 300 K)d\omega$ of the mid-IR peak of CeRh$_2$As$_2$ relative to those at $T = 300$ K. The integration range was set as $\omega_1 = 0$ eV $\leq \omega \leq \omega_2 = 0.8$ eV, where the spectral change in the lower energy region is almost recovered. In the figure, the evaluated $\Delta(\omega)$ and $\Delta SW$ of two heavy-fermion compounds CeCu$_2$Si$_2$ ($T_K \sim 10$ K) [30] and CeNi$_2$Ge$_2$ ($T_K \sim$ several K) [32] are also plotted for comparison. The temperature dependencies of $\Delta(\omega)$ and $\Delta SW$ correspond to the evolution of the $c$-$f$ hybridization with temperature [31], i.e., an increasing itinerancy corresponds to increasing values of $\Delta(\omega)$ and $\Delta SW$ whereas constant values suggest a localization of the 4f state.

In CeRh$_2$As$_2$, $\langle \omega \rangle$ is constant near 300 K and increases toward low temperatures below $\sim 150$ K, suggesting a rapid development of the $c$-$f$ hybridization below the temperature. This is consistent with the $c$-$f$ hybridization intensity being almost negligible at 300 K, which is demonstrated by almost identical $R(\omega)$ spectra of CeRh$_2$As$_2$ and LaRh$_2$As$_2$ at 300 K (see inset of Fig. 4).

The $\Delta SW$ values monotonically increase with decreasing temperature below 300 K. As was shown previously [31], an increase from 300 K to $\sim 100$ K originates from electron-phonon interactions, and the $c$-$f$ hybridization effect appears below the temperature of $\sim 100$ K. In CeRh$_2$As$_2$, the $\Delta SW$ increases at low temperatures, which is consistent with $\Delta(\omega)$. The values of $\Delta(\omega)$ and $\Delta SW$ of CeRh$_2$As$_2$ at the lowest accessible temperature are located in between those of CeCu$_2$Si$_2$ and CeNi$_2$Ge$_2$ suggesting an intermediate $c$-$f$ hybridization intensity $\tilde{V}$, which is included in the Kondo temperature expression

$$T_K \propto \exp[-\tilde{V}^{-2}D_c(E_F)^{-1}],$$

where $D_c(E_F)$ is the density of states of the conduction band at $E_F$ [37]. Hence, compared to CeCu$_2$Si$_2$, the higher $T_K \sim 20-40$ K and smaller $\tilde{V}$ of CeRh$_2$As$_2$ should be related to a larger $D_c(E_F)$. Indeed, such conclusion is consistent with the $\sigma_1(\omega)$ spectral intensity of LaRh$_2$As$_2$ for $\hbar \omega \leq 0.8$ eV, which reflects the density of states near the $E_F$. In this region, $\sigma_1(\omega)$ is enhanced compared to the calculated one using the ThCr$_2$Si$_2$-type structure as shown in Fig. 4 which is also due to a flat Rh 4d band near the $E_F$ as shown in Fig. 4. Therefore, the locally non-centrosymmetric CaBe$_2$Ge$_2$-type crystal structure of CeRh$_2$As$_2$ supports a higher $T_K$ than the ThCr$_2$Si$_2$-type structure of CeCu$_2$Si$_2$. 

FIG. 6. Calculated band structure of CeRh$_2$As$_2$ without (left) SOI and with (center) SOI. Spin-orbit split bands are red encircled. Inset depicts symmetry points in the Brillouin zone. (Right) Total density of states and partial density of states of Ce, Rh 1 and Rh 2 (see Fig. 4 with SOI.)
FIG. 7. Optical conductivity ($\sigma_1(\omega)$) spectrum of CeRh$_2$As$_2$ at 10 K (Experiment, magenta solid line). The Drude curve expected by the experimental electrical resistivity is shown by a gray solid line, and calculated $\sigma_1(\omega)$ spectra with and without SOI are shown by a red marked line and a blue solid line, respectively. The total and partial $f$ density of states above $E_F$ are also plotted in the lower figure for the comparison with the $\sigma_1(\omega)$ spectrum. The $E_F$ of the density of states is set to $\hbar\omega = 0$ eV of $\sigma_1(\omega)$ spectra. The peaks at about 0.2 and 0.5 eV originate from the unoccupied Ce 4$f_{5/2}$ and 4$f_{7/2}$ states.

IV. CONCLUSION

To summarize, optical conductivity $\sigma_1(\omega)$ spectra of a locally non-centrosymmetric heavy fermion superconductor CeRh$_2$As$_2$ and LaRh$_2$As$_2$ as a reference material without 4$f$ electrons were measured and compared with the corresponding DFT calculations. The experimentally obtained $\sigma_1(\omega)$ spectrum of LaRh$_2$As$_2$ can be explained well by the DFT calculations. Besides, the experimental $\sigma_1(\omega)$ spectrum of CeRh$_2$As$_2$ at low temperatures has a stronger $c$-$f$ hybridization intensity than the DFT calculation because the Kondo interaction is effective at low temperatures, which is also seen in the temperature dependence of the $\sigma_1(\omega)$ spectrum. The evidence of the SO splitting due to the locally non-centrosymmetric crystal structure, unfortunately, could not be observed in the $\sigma_1(\omega)$ spectra because of the SO splitting being too small for resolvable spectral features.

FIG. 8. Relative temperature dependence of the change of the center of gravity ($\Delta\langle\omega\rangle$, left axis) and the spectral weight ($\Delta SW$, right axis) of CeRh$_2$As$_2$ and reference materials, CeCu$_2$Si$_2$ and CeNi$_2$Ge$_2$ [31]. These values were normalized to their room-temperature values.

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