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To cite this version:
F. Marabelli, P. Wachter, E. Walker. ELECTRONIC STRUCTURE OF CeCu6 AND LaCu6. Journal de Physique Colloques, 1988, 49 (C8), pp.C8-771-C8-772. 10.1051/jphyscol:19888348. <jpa-00228528>

HAL Id: jpa-00228528
https://hal.archives-ouvertes.fr/jpa-00228528
Submitted on 1 Jan 1988
ELECTRONIC STRUCTURE OF CeCu₆ AND LaCu₆

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Abstract. — We present the first optical reflectivity measurements on the a – c plane of a single crystal of the heavy fermion CeCu₆ and on a polycrystalline sample of LaCu₆. The measurements have been made between 12 eV and 1 meV at temperatures between 5 K and 300 K. Whereas the spectrum of LaCu₆ does not change at low temperature, a strong difference is revealed in CeCu₆ due to the interaction with the f states. In particular a new structure appears at very low energies which we ascribe to f-f transitions across a gap, however, the Fermi level lies in a narrow f-like band of high density of states.

Amongst the heavy fermion compounds CeCu₆ is a very interesting material presenting an enormous γ value of the specific heat [1, 2] and having no magnetic order down to very low temperatures [3, 4]. Unfortunately its complicate crystal structure with a large anisotropy prevented band calculation up to now. The problems arise from the difficulty to consider on the one hand the interactions between the electrons in the correct form, on the other hand the coherence effects due to the lattice periodicity of the interaction [5]. Therefore, it is important to perform experiments which give information about the ground state properties of these materials. Far infrared spectroscopy supplies a great help to clarify the electronic structure by measuring with high resolution and at very low energies and low temperature the intensity and the energy distribution of the elementary excitations of the system and in this way yields information on the ground state, complementary to the one obtained by specific heat or by some other kind of spectroscopy, e.g. point contact spectroscopy [6]. As far as we know, we present the first optical reflectivity measurements on a single crystal of CeCu₆. In order to have a reference in the analysis of our data we measured also the reflectivity of a polycrystalline sample of LaCu₆ at room as well as at low temperature.

The reflectivity shown in figure 1 has been measured in the range of energy from 1 meV and 12 eV by using four spectrometers. The different runs of measurements link very well between them having large superpositions and the differences being always less than 1 %. To prevent oxidation of the surface both samples have always been kept in vacuum or in helium atmosphere and the surface has always been freshly polished before the measurements. In the far infrared we used a Fourier spectrometer equipped with a liquid helium cooled germanium bolometer. The crystal and the reference gold mirror were mounted in a cryostat with helium exchange gas which permitted a temperature variation between 5 and 300 K. The measurements are reproducible to within 1 %.

In order to obtain the optical conductivity we performed a Kramers-Kronig transformation of the reflectivity. At room temperature and for energies lower than 1 meV the reflectivity has been extrapolated down to zero energy by using the Hagens Rubens relation and the measured dc-conductivity. At low temperature the extrapolation of the reflectivity of CeCu₆ is more difficult. In any case the shape of the optical conductivity in the meV range is not drastically changed by the extrapolation and the structure at 5 meV is practically unaffected. We chose the extrapolation in such a way as to have the reflectivity values consistent with the statical conductivity and the Kramers-Kronig relation.

The spectra of both materials present the same features at high energies: we ascribe the two transitions at 2.8 and 5 eV (insert of Fig. 2) to excitations of the 3d electrons of copper since they are found also in pure copper and they are confirmed by XPS measurements on CeCu₆ [7].

If we look at the spectra of LaCu₆ in figure 2 we observe two structures, respectively, at 50 meV and at 90 meV. Also CeCu₆ exhibits structures at these ener-
gies. In the lack of band calculations and of measurements of the phonon dispersion it is difficult to assign these structures to electronic transitions, but, considering the strength of the transitions we ascribe the peak at 90 meV to electronic transitions between the conduction band and the d states of La or Ce and the one at 50 meV to a phonon excitation. The spectrum of CeCu$_6$ shows also a third structure which is well visible at low temperature. By subtracting the spectra of CeCu$_6$ and LaCu$_6$ at low temperature we calculated the energy of this transition to be 0.27 eV and the oscillator strength to be about 0.6. This new excitation must be related to the f-electron of the Cerium ion and probably corresponds to an f-d transition (because of the strong oscillator strength) or to the well known spin-orbit splitting of Ce.

The features of the LaCu$_6$ spectra at low frequencies are determined by the free carrier contribution. The only change at low temperature concerns the energy at which the conductivity sharply rises to the static value. This is consistent with a lowering of the scattering rate, in agreement with the resistivity measurements [8]. CeCu$_6$ at room temperature shows the same features, but one observes important deviations from the values of LaCu$_6$ indicating a strong interaction with the f-level of cerium. This interaction is responsible for the drastic changes in the conductivity spectrum of CeCu$_6$ at low temperature. Below 20 K an enhanced peak appears at about 5 meV and a deep minimum in the optical conductivity at about 1 meV indicates the formation of a gap above $E_F$ and of a narrow quasiparticle band at the Fermi level. The unscreened plasma frequency of the carriers in this band calculated by our data results in about 150 meV and if we analyse this value together with the enhanced value of the specific heat according to the formulae $\omega_p^2 \propto k_F^3/m^*$ and $\gamma \propto k_F m^*$ we obtain 1.2 quasiparticles per cerium in the band, with an effective mass of 700 electronic masses.

The oscillator strength of the excitation at 5 meV is 0.023, a rather low value indicating transitions between strongly hybridized f-states which have a certain d-admixture.

In conclusion our study of the optical properties of CeCu$_6$ and LaCu$_6$ gives evidence of the role of the f-states of cerium in determining the electronic structure of the material.

The most important result is the indication that the f-states hybridize with the conduction band and form very narrow bands of quasiparticles in the vicinity of the Fermi level, in agreement with d.H.-v.A. measurements [9]. There are at least two bands separated by a gap of about 5 meV and optical transitions are observed between the partially filled and the empty one. This is also consistent with the observed Schottky anomaly [1] in the specific heat.

A value for the unscreened plasma frequency of the carriers in these bands has been obtained of 150 meV. The number of carriers is about 1.2 quasiparticles per formula unit.

f-d or spin-orbit splitting transitions are observed at 270 meV, whereas the phonon excitation and other transitions at 90 meV and at higher energy do not seem to be affected by the f electrons.