

Infrared Study of the Valence Transition Compound YbInCu₄ using Cleaved Surfaces

The physical properties of intermetallic compounds containing rare earth elements, most typically Ce or Yb, are often strongly influenced by the electrons in the $4f$ orbital of the rare earth elements. At high temperatures of the order of room temperature, the f electrons are basically localized at the rare earth atom, since the wave function of the $4f$ orbital is strongly confined in the inner portion of the atom. However, at low temperatures of the order of ~ 10 K or lower, the f electrons may become itinerant (delocalized) through hybridization with the conduction electrons. The resulting hybridization state generally has a much larger effective mass m^* than the rest electron mass due to a strong Coulomb interaction acting on the f electrons. For many such “heavy fermion” compounds, the crossover from the localized to the itinerant characteristics of f electrons occurs gradually and continuously as the temperature is lowered. YbInCu₄, however, shows a first order phase transition at $T_v \sim 42$ K, where a sudden change in the Yb valence is observed from ~ 3 above T_v to ~ 2.9 below T_v . Many physical properties such as the lattice constant, electrical resistivity and magnetic susceptibility also show sudden changes at T_v . YbInCu₄ has attracted a great deal of attention for showing such a first-order transition between localized and itinerant regimes, since most other heavy fermion compounds show only a gradual crossover as mentioned above.

We carried out an infrared (IR) reflectivity study of YbInCu₄ to probe the changes in the microscopic electronic structure associated with this transition [1]. Hancock *et al.* [2] previously reported a detailed IR reflectivity study on YbInCu₄ using mechanically polished samples. They clearly observed large spectral changes between the reflectivity spectra [$R(\omega)$] below and above T_v . Below T_v , the optical conductivity obtained from $R(\omega)$ showed a pronounced mid-infrared peak, which was attributed to optical excitation within the hybridization state of the f electrons [2]. However, the data showed a gradual evolution of the optical spectra with temperature, in contrast to the result expected for a first-order phase transition. There have also been interesting photoemission results [3] reported on YbInCu₄, which showed that the electronic structures and the valence in this compound are extremely sensitive to surface conditions. Motivated by these developments, we used *cleaved* samples to measure $R(\omega)$ of YbInCu₄. Since YbInCu₄ does not yield a large flat surface by cleaving, we needed to measure the $R(\omega)$ on small

specular surfaces on cleaved (fractured) pieces of YbInCu₄. The typical dimensions of the specular surfaces were 0.1–0.5 mm. We carried out the measurement at the IR beamline BL43IR. Owing to the high brilliance of the IR synchrotron radiation from SPring-8 and using an IR microscope available at BL43IR, a spot size of ~ 15 μm was obtained at the sample position. This allowed us to measure the $R(\omega)$ of the cleaved surfaces very easily.

Figure 1 shows the measured $R(\omega)$ spectra of both cleaved and polished surfaces of YbInCu₄ single crystals taken from the same batch. The $R(\omega)$ spectra and their temperature evolutions are qualitatively similar for both cases. However, the cleaved sample data show larger spectral changes between below and above 50 K. In addition, the magnitude of $R(\omega)$ is much lower for the cleaved sample than for the polished one. Figure 2 shows the detailed evolution of $R(\omega)$, integrated over 0.2–0.5 eV, as a function of temperature. For the polished sample, a gradual temperature change is seen, in agreement with a

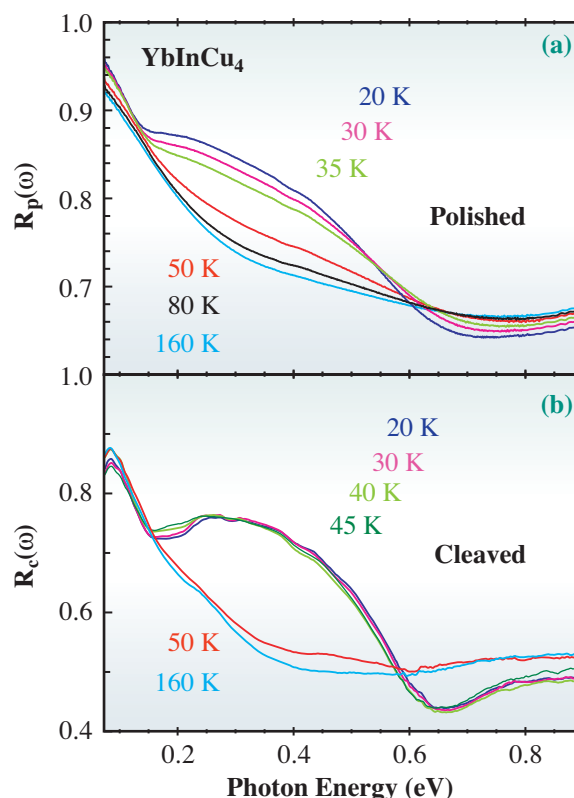


Fig. 1. Temperature dependence of reflectivity spectra $R(\omega)$ for (a) polished and (b) cleaved YbInCu₄.

previous report [2]. However, the cleaved sample data undergoes a sudden change at ~ 45 K, during which the change in $R(\omega)$ occurs within a temperature range of about 2 K. In addition, a hysteresis of about 1 K was observed between the cooling and warming data (not shown here). These results for the cleaved surfaces are consistent with the sudden changes observed for other physical properties at T_v . They also demonstrate that the microscopic electronic

structure indeed undergoes a first-order transition in this compound. The gradual temperature evolution observed for the polished sample is probably due to the compositional and/or site disorder, since it was previously reported that the transition temperature in this compound is very sensitive to even a small deviation from the ideal 114 composition, and to a site disorder between the In and Yb sites.

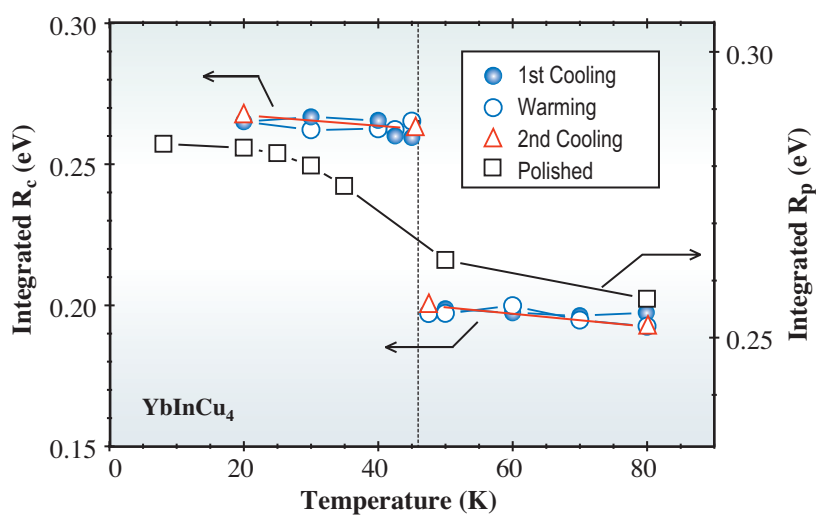


Fig. 2. Detailed temperature dependences of the reflectivity for cleaved and polished samples. The polished sample shows a much more gradual evolution with changing temperature than the cleaved sample.

Hidekazu Okamura

Graduate School of Science and Technology,
Kobe University

E-mail: okamura@kobe-u.ac.jp

References

- [1] H. Okamura, T. Watanabe, M. Matsunami, N. Tsujii, T. Ebihara, H. Sugawara, H. Sato, Y. Onuki, Y. Isikawa, T. Takabatake, T. Nanba: *J. Phys. Soc. Jpn.* **76** (2007) 023703.
- [2] J.N. Hancock *et al.*: *Phys. Rev. Lett.* **92** (2004) 186405; *Phys. Rev. Lett.* **92** (2004) 186405.
- [3] H. Sato *et al.*: *Phys. Rev. Lett.* **93** (2004) 246404.