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Transport and optical properties of CeTe₂

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Abstract

The electrical resistivity, magnetic susceptibility, specific heat and reflectivity of single crystal CeTe₂ were measured. A weak anisotropy appears in these measurements. Its carrier concentration is extremely low and the valence of Ce is evaluated as trivalence. Its resistivity is abnormal, which seems to be due to the p–f mixing or/and dense Kondo effects. Owing to these effects its magnetic structure phase is complex such as Ce-monopnictides.

Polytellurides strongly differ from Se-rich selenides and S-rich sulfides. The RX₂ (R is rare earth; X is O, S, Se and Te) composition is usually attributed to these compounds. In many cases, however, nonstoichiometries occur from either a deficiency or an excess of X. Therefore, little study on the stoichiometry of RX₂ has been carried out up to now. To investigate the intrinsic physical property of RX₂, we have grown single crystal CeTe₂ among RX₂ by using mineralization in an evacuated and sealed tungsten crucible at 1500°C. CeTe₂ has the tetragonal structure, of the Fe₂As type, with lattice parameters $a = 4.653$ and $c = 9.305$ Å. From Wang et al. the interatomic distances in NdTe₂ are [1]: Te(a)–Te(a) 3.187 Å; Te(a)–Te(b) 4.036 Å; Te(b)–Te(b) 4.009 Å; Te–Nd 3.26 to 3.38 Å. These Te atoms are at very short distances from one another and form very compact layers of Te, in which they are directly bonded by covalency. In contrast, the Te(b) are at large distances from the other Te atoms and not bonded together; they are only bonded to the five R atoms.

Fig. 1 shows the temperature dependence of inverse magnetic susceptibilities ($1/\chi$) with $H\parallel c$ -plane and $H\perp c$ -plane. In the lower temperature region, since $1/\chi$ has a weak broad peak, crystalline field interaction seems to be small. Both are in higher temperature region almost linear with temperature, which suggests that there is no crystalline field effect. Its slope indicates that the Ce-ion has a trivalence. The paramagnetic Curie temperature (Θ_p) is evaluated to be about 0 K for $H\perp c$ -plane but about -50 K for $H\parallel c$ -plane, which seems to be due to the antiferromagnetic exchange interaction. χ below 4 K has an infinite value for $H\perp c$ -plane but becomes saturated for

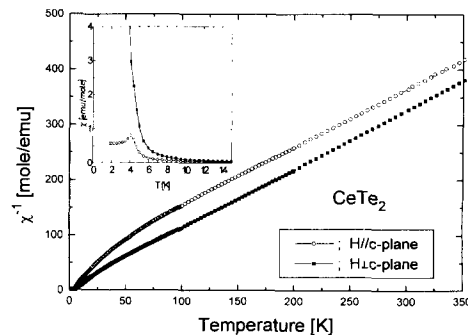


Fig. 1. Temperature dependence of inverse magnetic susceptibilities ($1/\chi$) with $H\parallel c$ -plane and $H\perp c$ -plane for CeTe₂.

$H\parallel c$ -plane. These results suggest that the magnetic moment perpendicular to the c -axis is reduced by an antiferromagnetic exchange interaction such as Kondo interaction.

Fig. 2 shows the temperature dependence of electrical resistivity (ρ) with $I\parallel c$ -plane and $I\perp c$ -plane. Since resis-

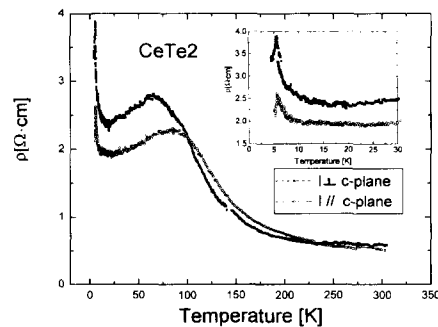


Fig. 2. Temperature dependence of electrical resistivity (ρ) with $I\parallel c$ -plane and $I\perp c$ -plane for CeTe₂.

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tivity in measured temperature is very large and at 300 K is 300 times larger than that of Yb_4As_3 [2], which indicates that carrier concentration is $\sim 10^{17}$ per mole, the temperature dependence of ρ shows abnormal metallic behavior. This is different from the behavior of LaTe_2 , which is reported to be a p-type semiconductor by Ramsey et al. [3]. This situation is similar to Ce-monopnictides, especially CeP and CeN [4]. Note that in Ce-monopnictides this situation is well explained as a p–f mixing effect by Takahashi et al [4]. Both have a sharp peak due to the ferromagnetic transition at 5.6 K and a broad one, at a temperature of 90 K for $I\parallel c$ -plane and 65 K for $I\perp c$ -plane. Above this temperature, similar to Yb_4As_3 [3], the resistivity decreases with increasing temperature, which seems to be due to the carrier decrease as well as Kondo scattering. Below the temperature the resistivity decreases with temperature. It is thought that the decrease is due to carrier increase owing to nonlinear p–f mixing because of the short distance between Ce-ions and Te-ions, which is similar to the behavior in CeSb [4] or/and coherent Kondo behavior.

The measured specific heat (C) versus temperature and the entropy calculated from the specific heat are shown in Fig. 3. A sharp peak with a shoulder appears at 4.35 K (T_c), which is due to a ferromagnetic transition from the magnetic susceptibility and another one at 2.3 K. The origin of this peak and the shoulder is not clear but they seem to be due to the p–f mixing or/and dense Kondo effects. The entropy at T_c has $R\ln 2$, which indicates that the ground state of Ce^{3+} is a doublet. Since the crystalline field splitting is expected to be small, we cannot decide whether the doublet is normal or not.

Fig. 4 shows the photon energy dependence of the measured reflectivity (R) and the imaginary part (ϵ_2) of the calculated dielectric constant with $E\parallel c$ -plane and $E\perp c$ -plane at 300 K. In reflectivities we cannot find plasma reflection due to carriers down to 0.5 eV. This indicates that the number of carriers is simply estimated to be far smaller than 0.05 per mole, compared with LaSb [5]. For an analysis of the origin of the peaks, we evaluated the effective number of electrons (N_{eff}) accompanied in each

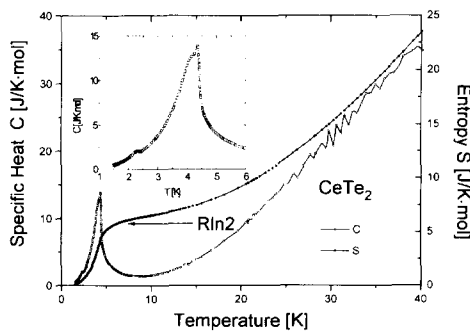


Fig. 3. Temperature dependence of the measured specific heat (C) and the entropy calculated from the specific heat for CeTe_2 .

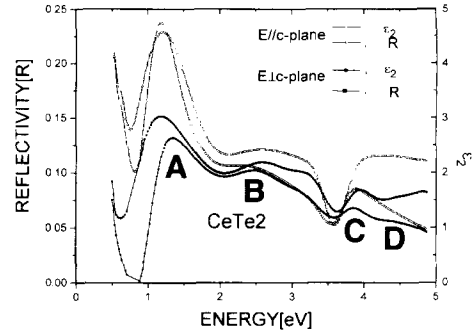


Fig. 4. Photon energy dependence of measured reflectivity (R) and imaginary part (ϵ_2) of calculated dielectric constant with $E\parallel c$ -plane and $E\perp c$ -plane at 300 K for CeTe_2 .

transition (peak in ϵ_2). Peak A seems to be due to the transition from the valence p-band near the Fermi energy (E_F) to the $5d_{12g}$ -band near E_F inferred from the N_{eff} -value and the energy position of the peak corresponding to the transition in LaSb [5]. Since peak B is relatively wide (half width of about 2eV) it seems to be mainly due to the d–f transition, in which the d-character is occupied through p–d mixing and the unoccupied 4f-state is expected to have many energy levels spreading over a couple of eV through f–d mixing. The origin of peak C is presumed to be 4f–5d transition because the peak is sharp. In the energy region above peak D the main p–d transition seems to occur, because N_{eff} increases fast. Since the origins, however, are still not clear now, more experiments and band calculations are needed.

From the above, we think that CeTe_2 , although it has an extremely low carrier concentration, is a Kondo system with magnetic ordering. Thus, we can conclude that original free carriers are not important to the formation of the Kondo state. The best simple explanation for us is that f-electrons change character from the atomic localized state by mixing to a more extended state to cover the original free carriers to make a singlet ground state. More theoretical and experimental research is necessary to solve this new problem.

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