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Transport properties and crystal field energy in CeTe

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Résumé. — Nous avons mesuré la résistivité électrique de CeTe en fonction de la température, audessus de 4,2 K. Les résultats sont analysés à l'aide d'un modèle prenant en compte la diffusion inélastique des porteurs libres par les ions cérium. Un bon accord entre la théorie et l'expérience est obtenu. La valeur déduite $\Delta \simeq 26$ K est d'un ordre de grandeur plus faible que celle prédite par la théorie des charges ponctuelles ce que nous avons attribué à l'existence d'une forte hybridation f-d.

Abstract. — We report resistivity measurements of CeTe as a function of temperature above 4.2 K. The results are analysed in the framework of a model taking into account the inelastic scattering of the free carriers which can exchange the energy Δ with the Ce scattering centre. A very good agreement between theory and experiment is obtained. The deduced value $\Delta \simeq 26$ K is one order of magnitude smaller than predicted by the point charge model, which we attribute to the existence of a strong d-f hybridization.

1. Introduction.

CeTe crystallizes in the NaCl structure ($a \simeq 6.361$ Å). This compound is a type II antiferromagnet below the Néel temperature $T_N = 2$ K [1, 2]. Due to the cubic symmetry, the ${}^2F_{5/2}$ ground state of the free Ce³⁺ ion is split in a Γ_7 doublet and a Γ_8 quartet separated by an energy $\Delta = E(\Gamma_8) - E(\Gamma_7)$ [3]. Birgeneau *et al.* [4] showed that, among the rare earth monochalcogenides and pnictides, the cerium compounds are quite unique, because the crystal field energy is much smaller than the value predicted by the point charge model ($\simeq 240$ K). It is then of particular interest to get accurate determination of Δ in CeTe.

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Recently, we reported on a model to calculate the electrical properties of Ce compounds [5]. This model takes into account both the elastic and the inelastic scattering of the free carriers. The inelastic process arises from the exchange of the energy Δ between the free carrier and the Ce scattering centre during the collision and is then very sensitive on Δ . This model was used to determine the value of Δ in CeSb [5] and CeSb_{1-x}Te_x for x < 0.05 [6].

In this paper, we report thermal variations of the resistivity of CeTe in the paramagnetic configuration. The agreement between the theory of [5] and experiments is very good. The deduced value of the crystal field energy is then compared with previous data and discussed.

2. Experiments.

The crystal growth and electrical measurement techniques were described elsewhere [2, 5]. The sample used for the experiments was single phased. Plasma emission and microprobe analysis revealed that it was stoichiometric (Ce/Te $\simeq 1 \pm 0.02$). The thermal variations of the resistivity $\rho(T)$, between 4.2 K and 50 K is shown in figure 1. In the whole temperature range investigated, the resistivity increases with temperature from 315 $\mu\Omega$ cm at 5 K to 450 $\mu\Omega$ cm at 40 K. In the range 40 K < T < 300 K, ρ increases linearly with temperature. In particular, we did not observe any Kondo effect. The resistivities, we have found for CeTe, are thus significantly larger than those observed in CeS [7], but have the same order of magnitude as in CeAs [8, 9]. This is a surprising result, because based on a simple consideration of valence one would predict the cerium monochalcogenides to be more conducting than the monopnictides.

An inflexion point of the curve $\rho(T)$ is observed at $T_{\rm M} = 8$ K, which corresponds to the maximum of $\frac{\partial \rho}{\partial T}(T)$ reported in figure 2.

3. Discussion.

The resistivity ρ can be decomposed into three independent parts

$$\rho = \rho_{\rm m} + \rho_{\rm ph} + \rho_{\rm r} \tag{1}$$

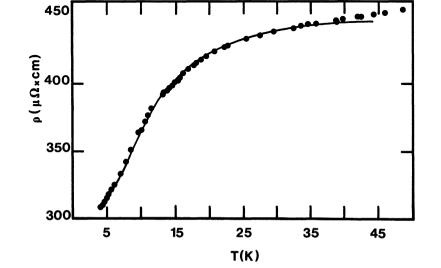


Fig. 1. — Thermal variation of the electrical resistivity of CeTe between 4.2 K and 50 K. The full curve is theoretical. Dots are experimental data.

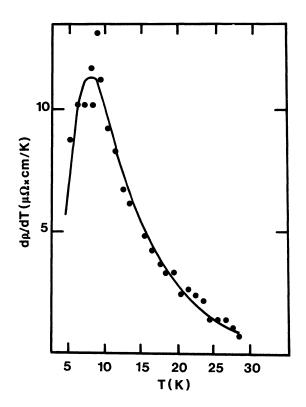


Fig. 2. — Thermal variation of the first derivative of the resistivity with respect to temperature. The full curve is theoretical. Dots are experimental data.

 $\rho_{\rm m}$ is the magnetic contribution to the resistivity associated with the diffusion of the free carriers by thermal spin fluctuations of Ce ions. $\rho_{\rm m}$ has been calculated elsewhere [5]. Above the Néel temperature $T_{\rm N}$, ρ has the following value :

$$\rho = \rho_0 \frac{5}{3} \frac{A}{Z} \left\{ 1 - \frac{8[e^{-\delta/3} + e^{2\delta/3}] \log \left| \frac{1+c}{1-c} \right|}{Ac[\cosh(\delta) - 1]} \right\}^{-1}$$

$$c = \left\{ 1 + \frac{21Z}{2A[\cosh(\delta) - 1]} \right\}^{1/2}; \quad \delta = \frac{A}{k_{\rm B}T}$$

$$A = 13 e^{-\delta/3} + \frac{5}{2} e^{2\delta/3}$$

$$Z = 4 e^{-\delta/3} + 2 e^{2\delta/3}$$
(2)

The scaling parameter ρ_0 gives the strength of the exchange coupling between the spin of the free carrier and that of the Ce ions. $k_{\rm B}$ is the Boltzmann constant. The term $\rho_{\rm ph}$ is associated with the diffusion of the free carriers by the phonons. This term has been studied with some details in [6], and is responsible for a linear increase of ρ at high temperature. In the temperature range investigated in the present paper, however, this term is negligible ($T \leq 30$ K):

$$\rho_{\rm ph} \sim 0. \tag{3}$$

The last term, in (1), is the residual resistivity. In the previous studies of CeSb [5], ρ_r was determined experimentally from the resistivity data at temperature $T \ll T_N$ where $\rho_m \simeq 0$. For CeTe, however, T_N is much smaller ($T_N = 2$ K instead of 16 K in CeSb) and such low temperature ($T \ll T_N$) could not be reached with our experimental set. Consequently, we could not determine experimentally the value of the residual resistivity ρ_r which then appears as an additional unknown parameter. To get rid of this parameter, we can take advantage of the fact that it does not depend on $\frac{\partial \rho}{\partial t}$

temperature and study the temperature derivative $\frac{\partial \rho}{\partial T}$ rather than the resistivity itself. From (3), we find :

$$\frac{\partial \rho}{\partial T} \simeq \frac{\partial \rho_{\rm m}}{\partial T} \tag{4}$$

which, according to (2), is only a function of ρ_0 , Δ and T. $\frac{\partial \rho}{\partial T}$ goes through a maximum at a temperature T_M defined by

$$\frac{\partial^2 \rho_{\rm m}}{\partial T} = 0. \tag{5}$$

Since ρ_0 is only a scaling factor, (5) is an implicit equation giving T_M as a function of Δ . Moreover, (2) only depends on the ratio $\Delta/k_B T$ and not on Δ and T separately so that the solution of (5) takes the form $\Delta/k_B T_M = \alpha$, where α is a constant. We have calculated α numerically. The result reads :

$$k_{\rm B} T_{\rm M} \simeq 0.312 \,\varDelta \,. \tag{6}$$

Since $\frac{\partial \rho_m}{\partial T}$ variations are similar to those of the specific heat [5], (6) is expected to relate the energy

 Δ to the temperature $T_{\rm M}$ of specific heat. Such a peak was observed by Hulliger *et al.* [8] who found experimentally $k_{\rm B} T_{\rm M} \simeq 0.377 \Delta$, very close to our result. This corroborates the validity of our model to calculate $\rho_{\rm m}$ (Eq. (2)). From equation (6) and the experimental value $T_{\rm M} \simeq 8$ K, we find $\Delta \simeq 26$ K, which value is in very good agreement with previous determinations [8]. ρ_0 can then be deduced by fitting the experimental curve $\partial \rho / \partial T$ by the theoretical law deduced from (2) and (4). The result is $\rho_0 = 22 \ \mu\Omega$ cm. The corresponding theoretical curve is reported in figure 2. It is worth noticing that, even if we have, *a priori*, three unknown parameters, namely ρ_0 , ρ_r and Δ , the parameter Δ can be derived independently from (6), which is a significative advantage over the calculation techniques we have previously used [6].

The value of Δ strongly disagrees with the predictions of the point charge model [4]. The same disagreement exists for cerium monopnictides. In particular, Kasuya *et al.* [10] claimed that the crystal field splitting in CeSb is very small due to the strong exchange coupling between the holes in the valence band and the 4f state of the Ce ions. In the case of CeTe, such a model is not relevant, since the hole concentration is negligible in this compound.

We have shown [11], however, that a similar reduction of Δ can be produced by a f-d hybridization associated with a coupling between the 4f states and the conduction electrons. We believe the small value of Δ in CeTe provides evidence of the importance of the d-f interaction in cerium compounds.

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