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## The resistivity of liquid rare earths

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**Résumé.** — La résistivité de plusieurs terres rares liquides a été calculée par l'approximation des matrices  $t$  des ions individuels. La correspondance entre la théorie et l'expérience est satisfaisante. Nous démontrons que l'interaction entre les électrons et les spins ioniques ne joue qu'un rôle négligeable.

**Abstract.** — The resistivities of various liquid rare earths were calculated in a single-site  $t$ -matrix approximation. Good agreement with experiment is achieved. Spin disorder scattering is shown to be unimportant in the liquid state.

The experimental resistivity data of liquid rare earths (RE) shows the following behavior [1, 2] :

The resistivity  $\rho$  increases across the series of the trivalent RE's. The temperature coefficient (TC) changes from slightly positive for La to slightly negative for Lu. The divalent Eu and Yb behave exceptionally : Eu has the highest and Yb the lowest  $\rho$ -value of all liquid RE's. They both have negative TC's.

We have calculated  $\rho$  for La, Eu, Gd, Yb and Lu in a single-site scattering approximation. The interaction between a conduction electron and the ions contains a potential and an exchange contribution :

$$H = \sum_n [V_{MT}(r - R_n) + J(r - R_n) s \cdot S_n]. \quad (1)$$

Here  $s$  is the electron spin and  $S_n$  the 4f-spin of an ion at position  $R_n$ . The muffin-tin potentials  $V_{MT}$  were constructed in the usual way [3]. The s-f-exchange function  $J$  was taken from Freeman's work for crystalline Gd [4].

We first sketch our calculations for a system without s-f-exchange. The single site expression for  $\rho$  is

$$\rho = \frac{3 \pi \Omega_0}{4 \hbar e^2 v_F^2 k_F^4} \int_0^{2k_F} dq q^3 S(q) |t(q)|^2 \quad (2)$$

$\Omega_0$ ,  $k_F$  and  $v_F$  being atomic volume, Fermi wave vector and velocity, respectively. The static structure factor  $S(q)$  is taken from experiment [5] and the  $t$ -matrix is determined by the phase shifts  $\delta_l$  of  $V_{MT}$ . Typically  $\delta_0$  and  $\delta_1$  are negative,  $\delta_2$  shows resonance-like behavior and  $\delta_3$  is very small. In the same approximation the integrated density of states (DS) is given by the free electron part  $N_0$  plus a single-site correction :

$$N(E) = N_0(E) + \frac{2}{\pi} \sum_l (2l + 1) [\delta_l(E) - \delta_l(0)]. \quad (3)$$

$E_F$  is determined by requiring  $N(E_F)$  to be equal to the valence.

For Eu and Yb we obtained the Fermi wave vector according to

$$k_F^2 = 2 m E_F. \quad (4)$$

This is the only choice consistent with the free electron (FE) boundary conditions used to evaluate  $\delta_c$  [6]. It corresponds to using a FE conduction band with  $E(k) = k^2/2 m$ . The relation

$$k_F^3 = 3 \pi^2 n_c \Omega_0 \quad (5)$$

yields an effective number  $n_c$  of conduction electrons per ion. The difference in  $\rho$  between Eu and Yb can be traced back to differences in the atomic potentials. Using  $S(q)$  for two different temperatures, as measured by Waseda *et al.* [5], we calculated  $d\rho/dT$  and indeed found negative TC's in good agreement with experiment.

For La, Gd and Lu the choice (4) for  $k_F$  would yield too high values for  $n_c$  and  $\rho$ . This is due to the fact that the bottom energy  $E_B$  of the conduction band lies higher than the muffin-tin zero in these substances, as band structure calculations for the crystals show. Therefore we use the partial s-p-DS

$$N_{sp}(E) \equiv N_0(E) + \frac{2}{\pi} \sum_{l=0}^1 (2l + 1) [\delta_l(E) - \delta_l(0)] \quad (6)$$

to determine  $n_c$  according to  $n_c = N_{sp}(E_F)$ . Eq. (5) then yields  $k_F$ , and  $E_B$  is obtained from

$$E_B = E_F - k_F^2/2 m. \quad (7)$$

This value of  $k_F$  is, however, inconsistent with the free electron boundary conditions [6]. Thus we constructed *renormalized* muffin-tin potentials  $V_{MT}$  the zero of which now lies at  $E = E_B$ . The phase shifts of  $V_{MT}$  were then used to calculate  $\rho$ .

Our results are listed in table I. The agreement with experiment is quite satisfactory. It is interesting to note that  $n_c$  increases systematically from La to Lu. This fact, which is the very reason for the increase of  $\rho$ , is consistent with band structure calculations by Duthie and Pettifor [7] yielding the same trend for the number of electrons in s-like Bloch states. Our  $n_c$ -values also explain the  $T$ -dependence of  $\rho$ : Lu has a slightly negative TC since  $2k_F$  is almost equal to  $k_p$ , the first peak in  $S(q)$  [8]. Moreover it accounts for the negative TC for alloys like LaSn, CeIn, GdSn etc. [2].

Table I. — Resistivities of various liquid rare earths.

Element	$n_c$	$\rho_{\text{calc}}$ ( $\mu \Omega \text{ cm}$ )	$\rho_{\text{exp}}$ ( $\mu \Omega \text{ cm}$ )
—	—	—	—
Eu	1.93	221	244
Yb	1.83	135	108
La	0.92	133	135
Gd	1.14	209	195
Lu	1.42	239	224

A striking feature of the liquid RE's is the absence of a maximum in  $\rho$  for Gd, suggesting that spin disorder scattering is unimportant. Indeed, our  $\rho_{\text{calc}}$  show the same degree of agreement with experiment for all elements, although s-f-exchange was omitted. Including it, the single-site scattering problem can be solved in a representation in which  $J = S + s$  is diagonal [9]. One obtains two scattering amplitudes,  $t^{(+)}$  and  $t^{(-)}$ , for  $J = S \pm 1/2$ . Assuming complete disorder in the ionic spins yields :

$$\rho = \frac{3 \pi \Omega_0}{4 \hbar e^2 v_F^2 k_F^4} \int_0^{2k_F} dq q^3 \times [S(q) R_1(q) + R_2(q) - R_1(q)], \quad (8)$$

where

$$R_1 = |((S + 1) t^{(+)} + S t^{(-)}) / (2S + 1)|^2$$

$$R_2 = ((S + 1) |t^{(+)}|^2 + S |t^{(-)}|^2) / (2S + 1). \quad (9)$$

In Born approximation (8) can be split into

$$\rho = \rho_{\text{pot}} + \rho_{\text{mag}}.$$

Kasuya [10] found  $\rho_{\text{mag}} \approx 60 \mu \Omega \text{ cm}$  for solid Gd.

We calculated the influence of spin-disorder scattering through s-f-exchange for liquid Gd in various approximations :

(i) In Born approximation  $\rho_{\text{mag}}$  is about  $3 \mu \Omega \text{ cm}$ . The large difference between this and Kasuya's value is due to  $v_F$ : Kasuya averaged  $v_F$  over the Fermi surface of crystalline Gd, whereas our  $v_F$ , the FE-value for about 1.1 electrons per ion is several times larger than Kasuya's average.

(ii) We included some (ferromagnetic) short range correlations between adjacent ionic spins. This even reduces  $\rho_{\text{mag}}$ .

(iii) The full calculation of  $\rho$  according to (8) yields  $\rho = 221 \mu \Omega \text{ cm}$  for the same potential used in table I for potential scattering alone. Thus s-f-exchange enhances  $\rho$  by about  $12 \mu \Omega \text{ cm}$  in the single-site approach.

Concluding, we find that our calculations indeed show a relatively weak influence of spin-disorder scattering on  $\rho$  for liquid RE's. The intriguing aspect, however, is that experimental data point to a continuous decrease of  $\rho_{\text{mag}}$  with increasing temperature, even in the solid [1]. More details of our calculations will be presented elsewhere.

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