

where the subscripts  $\alpha$  and  $\beta$  designate  $\alpha$ -La and  $\beta$ -La respectively. The value of  $(dT/dc)_\alpha$  is  $-4.5^\circ\text{K}$  per 1 a/o [31] and  $(dT_s/dc)_\beta$  is  $-5.1^\circ\text{K}$  per 1 a/o [16]. Substituting these values into Eqn. (14) we find  $N(E)_\beta = 1.13N(E)_\alpha$ , or in other words the density of states of  $\beta$ -La (face-centered cubic) is 13 per cent larger than that of  $\alpha$ -La (hexagonal).

## 6.2 PREDICTION OF HALL COEFFICIENTS.

The Hall coefficients of terbium, holmium and scandium have not been measured, however, it is possible to estimate these values from their measured electronic specific heat constants,  $\gamma$ . If the density of states,  $N(E)$ , is calculated from  $\gamma$  by using Eqn. (3), we can determine the number of holes in the s band from Fig. 4, which in turn can be used to find  $N_eR_H$  from Fig. 3. Once  $N_eR_H$  is known it is a simple matter of calculating the Hall coefficient,  $R_H$ . The predicted values of the Hall coefficients (in units of volt-cm/amp-Oe) are:

Tb	$-0.11 \times 10^{-12}$
Ho	$-1.5 \times 10^{-12}$
Sc	$-0.32 \times 10^{-12}$

It is interesting to note that as the final pages of this paper were being written an abstract [32] of a Russian publication on some transport and magnetic properties of scandium became available. This abstract [32] noted that scandium has a Hall coefficient of  $-0.30 \times 10^{-12}$ , which is in very good agreement with the predicted value.

In a similar manner the Hall coefficient of  $\beta$ -La with respect to that of  $\alpha$ -La can be estimated from the result shown earlier that  $N(E)_\beta = 1.13 N(E)_\alpha$ . It is found that  $(R_H)_\beta \approx 0.4 (R_H)_\alpha$ , and since a sample containing a mixture of both  $\alpha$  and  $\beta$ -La phases had a  $R_H$  value of  $-0.8 \times 10^{-12}$ , it is obvious that the Hall coefficient of  $\beta$ -La will be less negative than that of  $\alpha$ -La.

## 7. BAND STRUCTURE OF CERIUM

Cerium metal has four allotropic modifications, two are face-centered cubic, one body-centered cubic and one hexagonal. The normal room temperature face-centered cubic form,  $\gamma$ -Ce, and the hexagonal form,  $\beta$ -Ce, have been suggested to have a valence of 3.05 [3] and presumably the high temperature body-centered cubic  $\delta$ -Ce has also a similar valence. At low temperatures ( $\sim 120^\circ\text{K}$  and 1 atm) or at high pressure ( $\sim 7.5$  kb and  $298^\circ\text{K}$ )  $\gamma$ -Ce form transforms to the second face-centered cubic modification,  $\alpha$ -Ce, with a large contraction in volume (17 to 12 per cent depending on pressure and temperature). This large volume change has been suggested by many to be due to the transfer of the 4f electron in cerium to the 5d band (see ref. 3 for a complete review of the pertinent literature). Gschneidner and Smoluchowski [3] have concluded from their examination of the physical properties of cerium and cerium-rich alloys that the valence of  $\alpha$ -Ce is 3.67 at 1 atm and  $116^\circ\text{K}$ . Also in support of this valence for  $\alpha$ -Ce are the calculations of Waber *et al.* [33]. If these values are correct or nearly so, we may ask ourselves what is the band picture for  $\alpha$ - and  $\gamma$ -Ce?

### 7.1 $\gamma$ -CERIUM.

In order to explain the valence of 3.06 for  $\gamma$ -Ce one might suggest that there is a 4f one electron band which overlaps the 6s and 5d bands near the Fermi energy, such that about 0.06 of a hole exists in the 4f band and that the magnitude of the density of states is still governed by the 5d level. The order of magnitude of most of the observed physical properties of the cerium does not rule out this model. It is difficult to determine the sign and order of magnitude of the Hall coefficient on the basis of three overlapping bands since no mathematical solution has been proposed for this model. Infrared studies of  $\gamma$ -Ce at  $298^\circ\text{K}$  by Wilkins, *et al.* [34] revealed a large absorption at 15.5 microns, which they have not explained, and a number of minor peaks at shorter wave