

samarium, thulium and lutetium (Fig. 2). For ytterbium the Hall coefficient indicates 0.56 holes in the 6s band and this number of electrons in the 5d band, assuming the ratio of the mobilities to be 0.1.

The relationship between the Hall coefficient (or more precisely the atomic Hall coefficient per unit volume, NeR_H) and the number of holes in the 6s (5s for yttrium) band for a mobility ratio of 0.1 is shown in Fig. 3 for those rare earth metals which have negative Hall coefficients. This behavior is not at all unreasonable, in view of the positions of the almost straight lines shown in the bottom of Fig. 2. That is, the larger (more negative) the Hall coefficient the smaller the number of positive carriers (holes) in the 6s (or 5s) band.

6. BAND* STRUCTURE OF THE NORMAL TRIVALENT RARE EARTH METALS

From the above data it should be possible to construct a simple band structure for the rare earth metals. The Hall coefficient data suggest that the 6s band has approximately 0.01 hole, and the electronic specific heat constant data suggest a density of states of about 2.0 states/eV/atom at the Fermi surface. A closer examination of these data (Fig. 4) show that the density of states increases as the number of holes in the 6s band (and as the number of electrons in the 5d band) increase. This is what one might expect, but the agreement shown in Fig. 4 is much better than one could possibly hope for, considering the assumptions made in determining the density of states values especially for magnetic rare earth metals and in applying Sondheimer two band model to obtain the number of holes in the s band. It is also interesting to note that there is no regular or systematic variation of the density of states or the number of holes in the s band for these metals, as is observed for most of the physical

* When we talk about a particular type band, such as the 6s, we really mean a band which has s-like character.

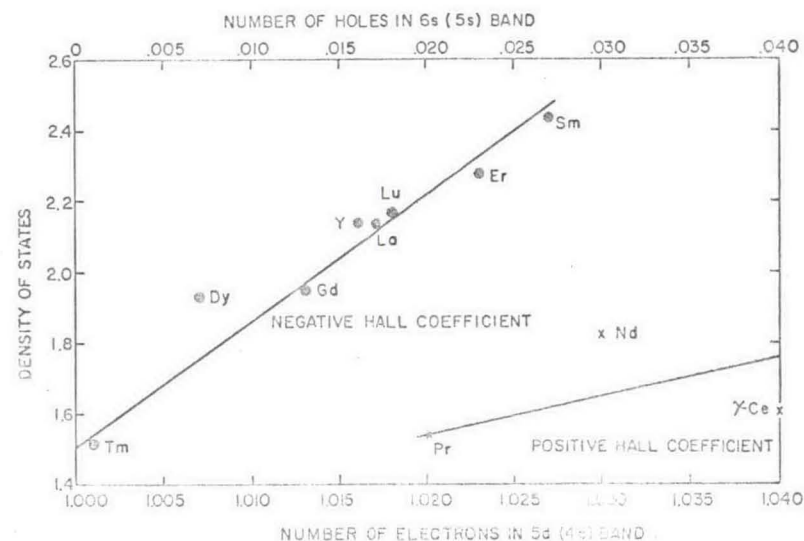


Fig. 4. The density of states at the Fermi level vs the number of holes in the s band (number of electrons in the d band).

properties of these metals. Nor does there seem to be any dependence on the spin, or the projection of the spin on the lowest J state, or the orbital angular quantum number, or the total angular quantum number.

From the data shown in Fig. 4, the band structures of three representative rare earth metals, which have negative Hall coefficients, are shown in Fig. 5. Thulium, which has the lowest density of states, has the smallest number of holes in the 6s band, and samarium, which has the largest density of states, has the largest number of holes in this band. The other metals, which have density of states values which are intermediate between these two extremes, have band structures represented more or less by gadolinium. It is noted that, if the band structures shown in Fig. 5 are correct, then