

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

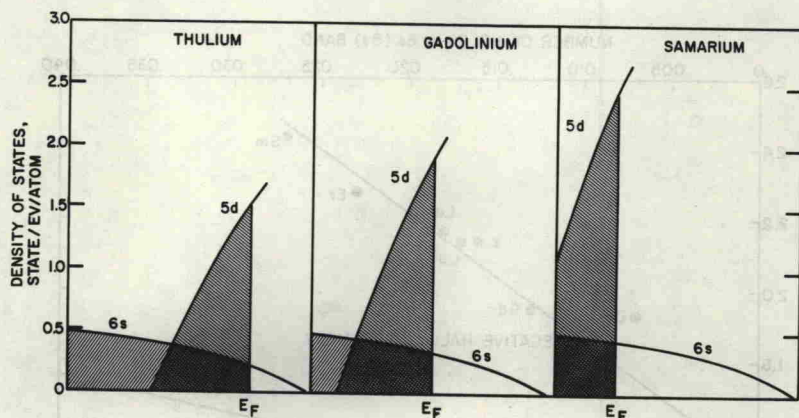


Fig. 5. The simplified band structures of three of the rare earth metals which have negative Hall coefficients.

the relative positions of the 6s and 5d bands with respect to each other must shift from one element to another. Furthermore, it is concluded that there is no broad 4f band which overlaps the 6s and 5d bands; most likely, the 4f electrons occupy discrete levels, or very narrow one electron bands as proposed by Mott. [28]

For the rare earth metals, which have positive Hall coefficients, the density of states are significantly smaller for a corresponding number of holes in the 6s band (Fig. 4). Thus one would expect the band structures of praseodymium and neodymium to be slightly different from those shown in Fig. 5, but the general conclusions mentioned above for the metals which have negative Hall coefficients are expected to apply to praseodymium and neodymium. Discussion of the band structure of γ -Ce is deferred to section 7.1.

The band structures proposed here for the rare earth metals are in general agreement with the conclusions arrived at by Rocher [29] in his analysis of the electronic and magnetic properties of these metals, except for the metals cerium and ytterbium, which will be discussed later.