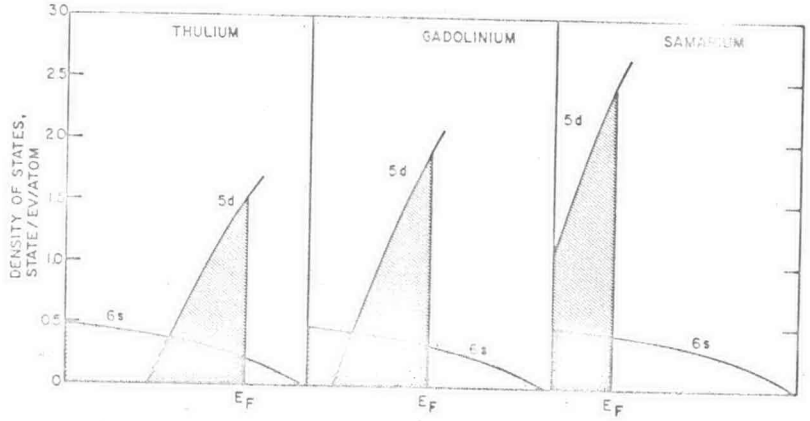

Fig. 5. The simplified band structures of three of the rare earth metals which have negative Hall coefficients.

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.

6. 1 α- and β- LANTHANUM.

Lanthanum at room temperature generally consists of a mixture of two allotropes, face-centered cubic (β-La) and hexagonal (α-La), unless special precautions are taken to obtain one or the other allotrope. The α-β transformation occurs on heating at about 580°K (310°C) and on cooling at about 490°K (220°C). The transformation on cooling $\beta \rightarrow \alpha$ is sluggish and very seldom goes to completion. All of the experimental data, which were analyzed to determine the band structure of lanthanum, are from samples which contain both phases. Thus it is impossible to know the correct value of the density of states of either α or β-La. It is, however, possible to determine the density of states of α-La relative to β-La. This is outlined below.

Suhl and Matthias [30] have given a relationship between the density of states and the superconducting transition temperature, T_s, for a superconductor (*e.g.* lanthanum) containing some paramagnetic impurity atoms (*e.g.* gadolinium). Rewriting their Eqn. (29) as:

$$\frac{dT_s}{dc} = -\frac{\pi^2}{7} J^2 S(S+1) \frac{N(E)}{k} \qquad (13)$$

where c is the concentration of the paramagnetic impurity in a/o, J the exchange energy of the spin coupling between a paramagnetic ion and a conduction electron, S the spin of the paramagnetic ion and k the Boltzmann constant. Since J is quite difficult to evaluate, only an order of magnitude value can be obtained for N(E). But for lanthanum the value of dT_s/dc is known for gadolinium impurities in both α and β-La. If we make the reasonable assumption that J is identical for these two cases, then we see that the term $(\pi^2/7k)J^2 S(S+1)$ is a constant, and that

$$\frac{N(E)_\alpha}{N(E)_\beta} = \left(\frac{dT_s}{dc}\right)_\alpha \Big/ \left(\frac{dT_s}{dc}\right) \qquad (14)$$