8.2 YTTERBIUM.

The electronic specific heat constant and Hall coefficient for ytterbium suggest the band structure shown in Fig. 8a, where the density of states at the Fermi level is 0.78 states/eV/atom and the 5d band has 0.56 electrons (and conversely the 6s band has 0.56 holes).

Bridgman [45], Stager and Drickamer [46], Hall and Merrill [47] and Souers and Jura [48] have found that as pressure is applied ytterbium slowly changes from a good conductor to a poor conductor to a semiconductor, and finally at 39 kb it abruptly changes back to a good conductor. The proposed band structures for these behaviors is shown in Figs. 8a through 8d. The band structure of face-centered cubic ytterbium at atmospheric pressure is shown in Fig. 8a. As pressure is applied the bands shift with respect to each other as is shown in Fig. 8b. Then as more pressure is applied the bands continue to shift and finally a gap is formed between the completely filled 6s and the empty 5d band (Fig. 8c), giving rise to the semiconducting properties of ytterbium. The energy gap, as measured on impure (as semiconductors are concerned) ytterbium by Souers and Jura [48], is about 0.85 eV. As the pressure is increased to 39 kb, the resistance suddenly decreases by a factor 10 to 13 and ytterbium is now a better conductor than it was at atmospheric pressure. Hall's and Merrill's data [47] show that face-centered cubic ytterbium transforms to body-centered cubic ytterbium at this pressure, with about a change in the metallic radius from 1.81 to 1.74A. McWhan and Jayaraman [49] have shown that this change in the metallic radii is almost entirely accounted for by the change in coordination (the discrepancy of 0.01A can easily be accounted for by experimental error). On the basis of this evidence we suggest that the band structure of body-centered cubic ytterbium at pressures greater than 39 kb is similar to that shown in Fig. 8d. Hall coefficients and possibly magnetic susceptibility measurements of high pressures would be extremely useful in confirming this model.

Rocher [29] suggested that the 39 kb transformation* in ytterbium was due to the transition of about one half of a 4f electron per atom to the valence band. He was able to correlate the data, which were available at that time, in terms of a virtual 4f bound state model with a partially occupied one electron 4f level. More recent X-ray studies of Hall and Merrill [47] and the subsequent interpretation of their atomic size data by McWhan and Jayaraman [49] have shown that ytterbium undergoes a crystal structure change, but no valence change at 39 kb. Because of this it would appear that the virtual 4f bound state model is not applicable to ytterbium at high pressures.

9. CONCLUSION

The above band models proposed for the rare earth metals are greatly simplified and it is amazing that the high temperature specific heat and Hall coefficient data give such consistent results. The biggest disappointment is that very low temperature specific heat data, except for the non-magnetic metals, do not seem to yield any reliable data concerning the band structures of these metals.

Before very high purity rare earth metals (99.99+a/o pure with respect to all impurities) become available to make direct Fermi surface measurements, there are a number of careful experiments that can be performed on these metals, which should give us some reliable data on their band structure. Low temperature elastic constant measurements on single crystals would yield an independent method for determining the Debye temperature and thus the lattice contribution to the specific heat. Specific heat measurements at very

* Rocher used 65 kb for this transition in his paper. This larger value is taken from Bridgman [45], which was the only value available to Rocher at that time. Bridgman's transition pressure is high because (1) his ytterbium was probably not as pure as that available to later investigators [46, 47, and 48], and (2) his pressure scale was too high compared to the presently acceptable pressure scale.