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An Experimental Approach to a Simplified Band Structure of the Rare Earth Metals*

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ABSTRACT

From specific heat data it was concluded that the normal trivalent rare earth metals have a density of states at the Fermi surface of 1.5 to 2.5 states/eV/atom. Interpretation of the Hall coefficient data on the basis of a two band model suggests that the number of holes in the 6s band varies from 0.001 to 0.040. For those rare earths which have negative Hall coefficients the density of states is found to be directly proportional to the number of holes in the 6s band. The band structures of these metals is thought to consist of a nearly filled 6s band which overlaps a 5d band containing slightly more than one electron. The 4f electrons are thought to occupy discrete energy levels or very narrow one-electron bands. From these analyses Hall coefficients were predicted for terbium, holmium and scandium from the known electronic specific heat constants.

The band structures of cerium, europium and ytterbium are different from the normal rare earth metals. γ-Ce has band structure nearly like those of the normal metals, except that the one-electron 4f band lies just below the Fermi level (0.076 eV below). This low lying band explains several unusual properties of γ-Ce. α-Ce has three overlapping bands, the 6s, 5d and the narrow one-electron 4f band. The 6s band contains about two electrons, the 5d about 1 2/3 electrons and the 4f about 1/3 electron. This model accounts for the unusually high electronic specific heat constant. Europium

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and ytterbium appear to have a 6s band (containing about 1. 5 electrons) which overlaps the 5d band (containing about 0. 5 electron). A virtual 4f bound state model which had been proposed for cerium and ytterbium does not appear to be applicable to γ-Ce and ytterbium, but may be valid for α-Ce.

1. INTRODUCTION

A number of the physical properties from which we can obtain both direct and indirect information concerning the band structures of metals, have been measured for most of the rare earth metals. It was thought that it would be desirable to review and examine these data and try to tie them together. For this purpose the very low and room temperature heat capacities, Hall coefficients, magnetic susceptibilities, spectral data and electrical resistivities of these metals and some of their alloys were examined.

2. MAGNETIC MEASUREMENTS

The magnetic susceptibility measurements of the rare earth metals indicate directly the number of 4f electrons a particular element may have. By subtracting the number of 4f electrons from the number of electrons outside of the xenon rare gas core, one arrives at the number of electrons available for bonding, i. e. the number of valence electrons. Examination of the magnetic susceptibility data of the rare earth metals, as summarized by Arajs and Colvin [1] and Gschneidner [2], shows that all of the rare earth metals are trivalent, except for europium and ytterbium (which are divalent), and possibly cerium and samarium. A critical analysis of the magnetic behavior and other properties (metallic radii, diffuse neutron scattering values and Hall coefficients) of the cerium allotropes by Gschneidner and Smoluchowski [3] led them to conclude that the valence for both the normal face-centered cubic cerium (γ) and hexa-