Proc. of the 9th Rare Earth Research Conf., Vol. I (1971)

DAVI-HL 71-1136

STUDIES IN LANTHANIDE OXIDE FLUORIDES

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KEYNOTE ADRESS

EFFECTS OF PRESSURE ON THE ELECTRONIC STRUCTURE OF THE SAMARIUM MONOCHALCOGENIDES*

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ABSTRACT

A program for the calculation of the electronic band structures of the rare-earth monopnictides and monochalcogenides is discussed and reviewed. Explicit calculational results are then presented for SmS and SmTe, both for their normal lattice parameters and for reduced lattice parameters corresponding to experimentally obtainable pressures. These calculations strongly indicate that the mechanism for the recently observed pressure-induced semiconductor-to-metal transition in SmS is 4f electron delocalization, but the mechanism for a like transition in SmTe is a simple band-gap closing with pressure.

I. INTRODUCTION AND GENERAL DISCUSSION

The samarium solid-state compounds SmS, SmSe, and SmTe are of interest not only because of their own unique and specific physical properties, but also due to their belonging to a large general class of solid-state compounds. This class is the NaCl-structured monopnictides (N, P, As, Sb, Bi) and monochalcogenides (S, Se, Te) of the rare-earth elements, and contains an exceedingly rich diversity of solid-state properties as one moves his consideration from compound to compound within the class. Generally speaking, all members of the class are refractory; e.g., PrS melts at about 2500°K. At the same time, the class contains individual members representing just about every range of electrical conductivity, from good metals to wide-gap semiconductors. Metallic examples are HoP and DyP,[1] but HoN and DyN are semiconductors with band gaps of about 1 eV.[2] Diverse magnetic properties also exist as one moves through the class of compounds. TmN does not order magnetically, while GdN is a ferromagnet; but GdP is an antiferromagnet, while other compounds like HoP are ferrimagnetic.[3]

Of course, the similarities and differences in the physical properties of this class of rare-earth compounds are directly relatable to the electronic structures of the individual compounds; i.e., they are related to the actual details of the compounds' electronic band structures. However, such actual correlations between properties and band structures have been lacking, mainly because few realistic band structure calculations have been reported for the compounds in this class, a notable exception to this statement being

*Research sponsored by the U. S. Atomic Energy Commission under contract with Union Carbide Corporation.