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Band gap closure in yttrium hydride under high pressure AKIHIKO MACHIDA, AYAKO OHMURA, TETSU WATANUKI, KATSUTOSHI AOKI, Synchrotron Radiation Research Center, JAERI, Japan, SATOSHI NAKANO, KENICHI TAKEMURA, Advanced Materials Laboratory, NIMS, Japan
— Trivalent rare-earth metals demonstrate spectacular change in electronic properties by hydrogenation. With increase in hydrogen concentration beyond $x \sim 2.7$, yttrium hydride, YH_x, shows metal-insulator phase transition with structural change from the fcc to hcp of yttrium metal lattice. Band gap opening due to orbital hybridization between $1s$ (H) and $4d$ (Y) has theoretically been proposed for the metal-insulator transition. Theoretical studies have also predicted that the volume reduction by applying hydrostatic pressure would lead to metallization in association with band gap closure. We have investigated structural properties of yttrium hydrides by means of x-ray diffraction and infrared absorption beyond a predicted metallization pressure of $\sim$ 18 GPa. Hydride specimen was prepared by hydrogenation reaction of yttrium powder or foil with liquid hydrogen in a diamond anvil cell at room temperature. With increase in pressure beyond $\sim$ 10 GPa, the hcp lattice of YH_3 transforms gradually to a fcc structure. Infrared spectra show peak position change in the hydrogen vibrational region of 450-1500 cm^{-1} above $\sim$ 11 GPa, corresponding to the x-ray diffraction results. The H-Y bonding state and expected metallization are discussed on the basis of the high pressure experimental results obtained x-ray diffraction and infrared absorption.

Akihiko Machida
Synchrotron Radiation Research Center
Japan Atomic Energy Research Institute

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