

## Observation of Erbium Deuteride formation via in-situ D<sub>2</sub> loading

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### Abstract

Acuity of neutron scattering to the deuterium isotope enables structure analysis of hydride materials with sensitivity to site occupancy. We have made use of this sensitivity to monitor the deuterium loading of Er metal at various temperatures and D<sub>2</sub> pressures with simultaneous collection of neutron diffraction patterns. Our setup employed a fused-silica reaction vessel equipped with vacuum and D<sub>2</sub> gas-handling. The reaction vessel was heated in-situ using a vanadium heating element. Samples of Er powder were heated in vacuum to temperatures ranging from 250 to 450°C and D<sub>2</sub> loading was performed at pressures ranging from 0.01 Torr up to 500 Torr. We report initial results for D<sub>2</sub> loading experiments which document the formation of ErD<sub>2</sub> (fluorite) in-situ at 450°C and 10 Torr. In addition, we will present evidence for deuterium octahedral site occupancy via D<sub>2</sub> overpressures and the subsequent removal of octahedral deuterium via vacuum, with the entire sequence of overloading and pumping performed at temperature (450°C). We quantify lattice parameters, site occupancies, and isotropic atomic displacement parameters and discuss them with respect to the stability of the deuterated materials. We will also present evidence of in-situ formation of the hexagonal ErD<sub>3</sub> phase in the 250°C temperature range with various D<sub>2</sub> pressures.

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