Electronic structure of SmN, DyN, and GdN

B. RUCK, S. GRANVILLE, A.R.H. PRESTON, D.H. HOUSDEN, H.J. TRODAHL, MacDiarmid Institute for Advanced Materials and Nanotechnology, Victoria University of Wellington, Wellington, New Zealand, A. BITTAR, Industrial Research Limited, Lower Hutt, New Zealand, J.E. DOWNES, Department of Physics, Macquarie University, NSW, Australia, K.E. SMITH, Department of Physics, Boston University, Boston, MA, P. LARSON, W.R.L. LAMBRECHT, Department of Physics, Case Western Reserve University, Cleveland, OH — The rare-earth nitrides lie on the boundary between metals and insulators, and as such present an exciting challenge to both experiment and theory. Incorporating the localized and correlated 4f electrons into band structure calculations is difficult, while the propensity of the rare-earth nitrides to oxidize in atmosphere impedes experimental studies. Here we present nitrogen K-edge x-ray absorption and emission measurements from SmN and DyN films grown in-situ at the synchrotron beamline, supported by resistivity and magnetization results. The x-ray data show a clear gap between the occupied and unoccupied states, implying that the materials are semiconducting. The density of states are in excellent agreement with band structure calculations performed in the LSDA+U scheme, as long as a rigid 1 eV upward shift is applied to the conduction band.