High pressure behaviour of TbN: an X-ray diffraction and computational study

In the present work, we report an X-ray powder diffraction study of TbN up to an applied hydrostatic pressure of 43 GPa. TbN was found to be stable in the 131 (NaCl structure) within the examined pressure interval, and the zero pressure bulk modulus was determined to be 176(7) GPa. The electronic structure of ferromagnetic TbN has been studied using the linearized augmented plane-wave method. The calculated equilibrium volume and equation of state (EOS) for TbN agree poorly with experiment when the LDA and GGA versions of DFT were used. The agreement between the experimental and theoretical EOS is greatly improved by introducing an orbital dependent U term into the energy-functional. The 4f electrons in TbN-B1 are atomic like and highly correlated, and ferro-magnetic TbN-B1 is found to be a magnetic half-metal. Calculations find the spindown f-electrons in a hypothetical TbN-B2 (CsCl) structure to be itinerant and well described by standard DFT functionals. No pressure-induced phase transitions were found below 250 GPa with the LDA + U and GGA + U methods.