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New routes to nitrogen-rich transition metal nitrides: Synthesis of novel polymorphs of Hf_3N_4 ASHKAN SALAMAT, Harvard University, A.L. HECTOR, B.M. GRAY, Southampton University, S.A.J. KIMBER, European Synchrotron Radiation Facility, P. BOUVIER, CNRS, P.F. MCMILLAN, University College London — One of the most obvious features of transition metal nitride chemistry is that the maximum formal oxidation state of the metal is rarely as high as in the corresponding oxides or fluorides. Much of the interest in the high oxidation phases stems from the desire to identify the next generation of photocatalytic materials with tuneable bandgaps. Experiments in the laser heated diamond anvil cell (LHDAC) between the direct reaction of metals and nitrogen have previously produced a number of important new main group nitride phases. This technique has also demonstrated its potential for formation of new nitrogen-rich transition metal nitride phases. Alternative methods with the development of "soft" routes to new phases with high nitrogen content also offer the possibility of obtaining metastable phases through topotactic conversions. Using LHDAC *in situ* with synchrotron angle dispersive diffraction techniques we have crystallised at high pressures and temperatures two novel polymorphs of Hf_3N_4. Starting with an amide-derived nanocrystalline Hf_3N_4 sample we have identified a novel tetragonal ($I4/m$) polymorph at 15 GPa and 1500K and a second high pressure orthorhombic (*Pnma)* polymorph at 30 GPa and 2000 K. This study demonstrates that the combination of precursor-based synthesis and high-pressure crystallization could be very productive in synthesis of such nitrogen-rich phases.

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