Synthesis of Hf$_8$O$_7$, a new binary hafnium oxide, at high pressures and high temperatures$^1$ BJORN WINKLER, LKHAMSUREN BAYAR-JARGAL, WOLFGANG MORGENROTH, NADINE SCHRODT, Frankfurt University, VICTOR MILMAN, BioVia, CHRISTOPHER STANEK, BLAS UBERA-AGA, Los Alamos National Laboratory — Two binary phases in the system Hf-O have been synthesized at pressures between 12 and 34 GPa and at temperatures up to 3000 K by reacting Hf with HfO$_2$ using a laser-heated diamond anvil cell. In situ X-ray diffraction in conjunction with density functional theory calculations have been employed to characterize a previously unreported tetragonal Hf$_8$O$_7$ phase. This phase has a structure which is based on a fcc Hf packing with oxygen atoms occupying octahedral interstitial positions. Its predicted bulk modulus is 223(1) GPa.

The second phase has a composition close to Hf$_6$O, where oxygen atoms occupy octahedral interstitial sites in a hcp Hf packing. Its experimentally determined bulk modulus is 128(30) GPa. The phase diagram of Hf metal was further constrained at high pressures and temperatures, where we show that $\alpha$-Hf transforms to $\beta$-Hf around 2160(150) K and 18.2 GPa and $\beta$-Hf remains stable up to at least 2800 K at this pressure.

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