Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Synthesis of Hf_8O_7, a new binary hafnium oxide, at high pressures and high temperatures[1] BJORN WINKLER, LKHAMSUREN BAYARJARGAL, WOLFGANG MORGENROTH, NADINE SCHRODT, Frankfurt University, VICTOR MILMAN, BioVia, CHRISTOPHER STANEK, BLAS UBERUAGA, 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_8O_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_6O, 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 α-Hf transforms to β-Hf around 2160(150) K and 18.2 GPa and β-Hf remains stable up to at least 2800 K at this pressure.

[1]Funding was provided by DFG projects Wi1232 and Ra2585, BMBF projects 05KS7RF1, 05K10RFA, and 05K13RF1, Los Alamos National Laboratory

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Date submitted: 11 Nov 2016 Electronic form version 1.4