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**Phase relations and hardness trends of ZrO<sub>2</sub> and HfO<sub>2</sub> at high pressure** YAHYA AL-KHATATBEH, New Mexico State University, KANANI LEE, Yale University, BORIS KIEFER, New Mexico State University — We use high-resolution synchrotron x-ray powder diffraction and Density-Functional Theory to investigate the phase stability, equations of state (EOS), and mechanical hardness of ZrO<sub>2</sub> and HfO<sub>2</sub>. For the equilibrium phase of ZrO<sub>2</sub> at ambient conditions (MI), we provide a new experimental 2<sup>nd</sup>-order Birch-Murnaghan EOS that is comparable to results obtained from Brillouin measurements, but significantly different from previous high-pressure experiments: ambient-pressure bulk modulus  $K_0$  of 210 ( $\pm 28$ ) GPa. For the high-pressure OI-ZrO<sub>2</sub> phase, we find that  $K_0 = 290$  ( $\pm 11$ ) GPa which is 19-32% higher than previously determined. The cotunnite OII phase is observed to be the most stable phase up to at least 54 and 100 GPa at room temperature after laser heating to  $\sim 1800$  ( $\pm 200$ ) K for ZrO<sub>2</sub> and HfO<sub>2</sub>, respectively. The OI  $\rightarrow$  OII phase transition in both ZrO<sub>2</sub> and HfO<sub>2</sub> yields a volume collapse of  $\sim 10\%$ . Using scaling relations we obtain the hardness of OII-ZrO<sub>2</sub> of  $\sim 10$  GPa. As Hf and Zr have similar ionic radii, neither phase is likely to qualify as superhard.

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