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Pressure-Induced Antifluorite-to-Anticotunnite Phase Transition in Lithium Oxide AMY LAZICKI, University of California at Davis, Lawrence Livermore National Laboratory, CHOONG-SHIK YOO, Lawrence Livermore National Laboratory, WILLIAM EVANS, Lawrence Livermore National Laboratory, WARREN PICKETT, University of California, Davis, RICHARD SCALETTAR, University of California, Davis — Using synchrotron angle-dispersive x-ray diffraction (ADXD) and Raman spectroscopy on samples of Li_2O pressurized in a diamond anvil cell, we observed a reversible phase change from the cubic antifluorite (α, Fm3m) to orthorhombic anticotunnite (β, Pnma) phase at 50($\pm$5) GPa at ambient temperature. This transition is accompanied by a moderate volume collapse of 5.4 ($\pm$0.8)% and large hysteresis upon pressure reversal (P_{down} at $\sim$25 GPa). Contrary to a recent study, our data suggest that the high-pressure β-phase (B_o = 188 $\pm$12 GPa) is substantially stiffer than the low-pressure α-phase (B_o = 90$\pm$1 GPa). A relatively strong and pressure-dependent preferred orientation in β-Li_2O, resulting in changes diffraction intensities, is observed. The present result is in accordance with the systematic behavior of antifluorite-to-anticotunnite phase transitions occurring in the alkali-metal sulfides. This work has been supported by LLNL, University of California, under the auspices of the U.S. DOE under Contract No. W-7405- ENG-48 and by the Stockpile Stewardship Academic Alliances Program under grant DOE DE-FG03-03NA00071, and by the NSF(ITR 031339) at UCD.

Amy Lazicki
University of California at Davis, Lawrence Livermore National Laboratory

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