

Structural characterization of natural UO_2 at pressures up to 82 GPa and temperatures up to 2200 K

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ABSTRACT

Uranium is one of the main heat sources in the Earth, as about 25% of the total heat is produced by the radioactive decay of U. The location of U in the deep mantle is then essential for a better understanding of the geodynamics and thermal behavior of the Earth. For the first time, the crystal structure of natural simple dioxide UO_2 uraninite has been studied by X-ray diffraction with synchrotron radiation (ESRF, Grenoble, France), in situ in a laser-heated diamond-anvil cell at pressures and temperatures relevant to the deep Earth's mantle. Fluorite-type UO_2 displays a new sequence of phase transitions at high P and T , with a cubic modified fluorite $Pa\bar{3}$ observed at 18 GPa, and an orthorhombic $Pbca$ structure from 33 GPa up to 82 GPa. Using a second-order Birch-Murnaghan equation of state, we calculated room-pressure bulk modulus $K_0 = 166(7)$ GPa with pressure derivative $K'_0 = 4.0$ for the $Pa\bar{3}$ structure, and $K_0 = 225(8)$ GPa with $K'_0 = 4$ for the $Pbca$ structure. The expected $Pnma$ cotunnite structure was not observed but is not excluded at pressures higher than 82 GPa. Since UO_2 displays a $Pbca$ structure stable up to 82 GPa and presents a density much higher than the average density of the surrounding mantle, UO_2 could be a host of U in the deep lower mantle.

Keywords: Heat sources, uranium oxide, X-ray diffraction, crystal structure, deep mantle