American Mineralogist, Volume 93, pages 1090–1098, 2008

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

STEEVE GRÉAUX,[1,*] LAURENT GAUTRON,[1,†] DENIS ANDRAULT,[2,3] NATHALIE BOLFAN-CASANOVA,[3] NICOLAS GUIGNOT,[4,‡] AND JULIEN HAINES[5]

[1]Laboratoire des Géomatériaux et Géologie de l'Ingénieur, Université Paris-Est Marne la Vallée, France
[2]Institut de Minéralogie et de Physique des Milieux Condensés, Paris, France
[3]Laboratoire Magmas et Volcans, Université Blaise Pascal, Clermont-Ferrand, France
[4]European Synchrotron Radiation Facility, Grenoble, France
[5]Institut Charles Gerhardt Montpellier, Université de Montpellier, Montpellier, France

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