Structures and Stability of U-Bearing Phases for Nuclear Energy Applications

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Uranium (U) compounds are important materials for nuclear energy applications. They serve as reactor fuels in a nuclear power plant and as host phases for disposal of high-level waste and spent nuclear fuel in a geological repository. Since the associated radiation and decay heat may alter the properties of these phases, it is essential to study their structures and stability at relevant conditions. In this study, we employed synchrotron X-ray diffraction, absorption spectroscopy and neutron scattering to characterize both the crystal and local structures of several U-bearing compounds, and used high-temperature oxide-melt drop-solution calorimetry to measure their thermodynamic stability. The determined phase stability can be related to the corresponding structural characteristics, deriving structure-stability relations that have implications to the behavior of these phases in the environments encountered in nuclear energy applications.