**Crystal Structure of Uranium Monosilicide: A High Temperature Time-of-Flight Neutron Diffraction Study**

Tashiema L. Ulrich[1], Sven C. Vogel[1], Joshua T. White[1], Elizabeth S. Sooby[2]

[1]*Materials Science and Technology Division, MST-8, Los Alamos National Laboratory, P.O. Box 1663, Los Alamos, NM 87544 USA, tlwilson@lanl.gov*

[2]*Department of Physics and Astronomy, University of Texas at San Antonio, One UTSA Circle, San Antonio, TX 78249 USA*

**Abstract:**

The crystal structure of the uranium monosilicide (a = 10.622(1) Å, c = 24.389(7) Å, space group *I4/mmm*) has been determined from room temperature to 1100 °C using high temperature time-of-flight neutron diffraction on the High Pressure Preferred Orientation (HIPPO) diffractometer at Los Alamos Neutron Science Center (LANSCE). It was found to contain 6 U atoms occupying the 4e, 8f, 8j, 16n and 16m Wyckoff sites and 8 Si atoms occupying the 2a, 4c, 4e, 8h, 16n and 16m Wyckoff sites. The Si atoms on the 2a and 4e sites have partial occupancy of 0.7 and 0.4, respectively, giving a stoichiometry of $U_{68}Si_{67}$ ($USi_{0.99}$). The average linear coefficient of thermal expansion as well as the atomic displacement parameters have also been determined for this compound.