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Photoemission Spectroscopy on Single Crystal Uranium (001) C.P. OPEIL, R.K. SCHULZE, R.C. ALBERS, B. MIHAILA, K.B. BLAGOEV, M.E. MANLEY, J.C. LASHLEY, J.L. SMITH, (Los Alamos National Laboratory), P.B. LITTLEWOOD, (Cavendish Laboratory, University of Cambridge) — We have conducted XPS and UPS measurements ($173 \le T \le 873$ K) on high quality single-crystal U(001) and compared them with WIEN2K code electronic band structure calculations. We report significant correspondence between theory and experiment for binding energy (BE) < 4 eV and report anomalous splitting of the $6p_{1/2}$, $6p_{3/2}$ bands at BE = 13-30 eV. Spectrometer resolution allows observation of a shift in spectral weight in the U6d-U5f electrons upon comparison of He I (21.21 eV) and He II (40.80 eV) spectra at T = 173 K. ARPES experiments confirm that our electron structure result is a representative bulk effect. LEED patterns indicate a well-ordered orthorhombic crystallographic surface structure. Additionally, our experiments show a temperature correlation between the U work function and the brittle to ductile transition at ~ 450 K. Recent resistivity and specific-heat data will be discussed.

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