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High Pressure Crystalline Structure and Resistance of Vanadium Dioxide to 13.5 GPa[1] NATHANIEL BRADY, University of Alabama at Birmingham, KANNATASSEN APPAVOO, Vanderbilt University, JEFFERY MONTGOMERY, YOGESH VOHRA, University of Alabama at Birmingham, RICHARD HAGLUND, Vanderbilt University, DAVID HILTON, University of Alabama at Birmingham — We have investigated the insulator-to-metal transition in thin film vanadium dioxide as a function of pressure at ambient temperature using a designer diamond anvil cell (DAC). Four-point probe resistance measurements show a monotonic decrease over the entire pressure range studied with no significant discontinuity. High-pressure X-ray diffraction measurements observe an M_1 ($P2_1/c$) phase at 0 GPa, an M_2 (C2/m) phase from 0.8 GPa to 1.1 GPa, and a reentrant M_1 phase from 1.1 GPa to 13.5 GPa. Crystal refinement above 1.1 GPa shows a monotonically decreasing a, b and c lattice constants and a minimum in the monoclinic angle, β, near 8.5±0.5 GPa. The atomic positions show that the first V-V nearest neighbor distance (d) decreases over the entire pressure range, the second nearest neighbor distance (s) increases until 5 GPa after which it is constant with $s \approx f \approx 3.2$ Å. The next most closely spaced V-V distance (f), which corresponds to V atoms in different unit cells, is approximately constant across the entire pressure range measured.

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