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In situ diffraction studies of $\mathbf{H}_x\mathbf{VO}_2$ and $\mathbf{D}_x\mathbf{VO}_2$[1] D. NATELSON, Rice University, Department of Physics and Astronomy, 6100 Main St., Houston, TX 77005, N. TUMANOV, V. BAN, Y. FILINCHUK, IMCN, Universite Catholique de Louvain, Louvain-La-Neuve, Belgium, H. JI, Rice University, Department of Physics and Astronomy, 6100 Main St., Houston, TX 77005, J. WEI, Tulane University, Department of Physics, New Orleans, LA 70118, M.W. SWIFT, University of California at Santa Barbara, Department of Physics, Santa Barbara, CA 93106, A.H. NEVIDOMSKYY, Rice University, Department of Physics and Astronomy, 6100 Main St., Houston, TX 77005 — Vanadium dioxide exhibits a first-order phase transition at around 338 K between a high temperature, tetragonal, metallic state (T) and a low temperature, monoclinic, insulating state (M1), driven by electron-electron and electron-lattice interactions. Intercalation of VO2 with atomic hydrogen has been demonstrated, with evidence that this doping suppresses the transition. However, the effects of intercalated H on the crystal structure of the resulting hydride had not been examined in detail. Here we report synchrotron and neutron diffraction studies of this material system, mapping out the structural phase diagram as a function of temperature and hydrogen content. In addition to the original T and M1 phases, we find two orthorhombic phases, O1 and O2, which are stabilized at higher hydrogen content. We present density functional calculations that confirm the metallicity of these states. The intercalation of hydrogen above a critical fraction suppresses the metal-insulator transition entirely.

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