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XPS characterization scheme for phase-pure epitaxial NbO_2 TOBIAS HADAMEK, AGHAM POSADAS, ALEX DEMKOV, University of Texas at Austin — NbO_2 shows a semiconductor-to-metal transition with an associated structural transition of Peierls type. NbO_2 and Nb_2O_5 or mixtures thereof have also shown electrically induced insulator-to-metal transitions. To shed light on the nature of the electrically induced insulator-to-metal transition it is important to grow high phase purity NbO_2 and Nb_2O_5 and compare electrical measurements with mixed niobium oxides and with different electrode materials. Processing NbO_2 and avoiding surface oxidation requires ultra-high vacuum (UHV) conditions. Niobium oxide thin films where grown in UHV by molecular beam epitaxy on 111-oriented STO substrates and analyzed by X-ray photoelectron spectroscopy (XPS). It was shown that the NbO_2 3d core level spectrum exhibits an asymmetric spin-orbit peak pair with more spectral weight on the high binding energy side. Based on the shape of the Nb 3d core levels, peak positions relative to the oxygen O 1s peak, and the valence band shape and height ratio of the niobium $4d_{xy}$ split-off band to the oxygen 2p band, an identification scheme for NbO_2 by XPS was devised. Complementary the NbO_2 phase was confirmed by reflection high-energy electron and x-ray diffraction analysis.

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