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Properties of MBE-grown NbO₂ thin films ALEX DEMKOV, ANDY O'HARA, AGHAM POSADAS, University of Texas at Austin — Niobium dioxide or NbO₂ a sister compound of the more celebrated VO₂, belongs to the class of transition metal oxides that undergo a temperature-driven metal-to-insulator transition. Using density functional theory, we explore the electronic properties of both the high-temperature metallic rutile and the low-temperature insulating distorted rutile phases. We investigate the nature of the transition and predict a large carrier concentration change even at the high transition temperature of 1080 K. We also grew thin NbO₂ films on LSAT(111) single crystal substrates using molecular beam epitaxy. The films show very good crystallinity with a single out-of-plane orientation by x-ray diffraction, and exhibit a smooth surface with the presence of three epitaxial domains as observed by reflection high energy electron diffraction. The NbO₂ stoichiometry is confirmed by x-ray photoemission measurements of the Nb 3d core level as well as the valence band.

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