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Phase transformations in transition metal oxides for electronic device applications

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Transition metal oxides (TMO) are currently used in a variety of electronic devices and have been considered for a number of emergent technologies. The unfilled d-shells of transition metals are responsible for many unusual properties of these oxides and in particular, a multitude of phase transitions that range from structural to electronic. The recently developed ability to grow layers of TMOs with the atomic precision by means of physical vapor deposition has led to discovery of many fascinating phenomena that cannot be easily realized in bulk materials and to integration of these oxides on semiconductors. In this talk I will review briefly the ferroic ordering and metal-to-insulator transition in TMOs focusing primarily on the Peierls transition in NbO_2. I will discuss the basic properties of NbO_2 and our efforts in growing single crystal NbO_2 on several oxide substrates. For practical applications relying on the metal-to-insulator transition, the band gap and phase purity of the material are of key importance. I will discuss our present understanding of the electronic structure of the low-temperature insulating phase of NbO_2, which is based on photoemission spectroscopy, spectroscopic ellipsometry and density functional theory [1-3]. I will also explain how to distinguish under-oxidized and over-oxidized phases using a combination of first principles modeling with the core-level and valence band spectroscopy [4].

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