## The Influence of Structural Disorder and Phonon on Metal-To-Insulator Transition of VO<sub>2</sub>

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**Abstract :** We used temperature-dependent X-Ray absorption fine structure (XAFS) measurements to examine the local structural properties around vanadium atoms at the V K edge from VO<sub>2</sub> films. A direct comparison of simultaneously-measured resistance and XAFS from the VO<sub>2</sub> films showed that the thermally-driven structural phase transition (SPT) occurred prior to the metal-insulator transition (MIT) during heating, whereas these changed simultaneously during cooling. XAFS revealed a significant increase in the Debye-Waller factors of the V-O and V-V pairs in the {111} direction of the R-phase VO<sub>2</sub> due to the phonons of the V-V arrays along the direction in a metallic phase. A substantial amount of structural disorder existing on the V-V pairs along the c-axis in both M<sub>1</sub> and R phases indicates the structural instability of V-V arrays in the axis. The anomalous structural disorder observed on all atomic sites at the SPT prevents the migration of the V 3d<sup>1</sup> electrons, resulting in a Mott insulator in the M<sub>2</sub>-phase VO<sub>2</sub>. The anomalous structural disorder, particularly, at vanadium sites, effectively affects the migration of metallic electrons, resulting in the Mott insulating properties in M<sub>2</sub> phase and a non-congruence of the SPT, MIT, and local density of state. The thermally-induced phonons in the {111} direction assist the delocalization of the V 3d<sup>1</sup> electrons in the R phase VO<sub>2</sub> and the electrons likely migrate via the V-V array in the {111} direction as well as the V-V dimerization along the c-axis. This study clarifies that the tetragonal symmetry is essentially important for the metallic phase in VO<sub>2</sub>. **Keywords :** metal-insulator transition, XAFS, VO<sub>2</sub>, structural-phase transition

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