World Academy of Science, Engineering and Technology
International Journal of Industrial and Systems Engineering
Vol:11, No:11, 2017

The Influence of Structural Disorder and Phonon on Metal-To-Insulator Transition of VO_2

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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_2 films. A direct comparison of simultaneously-measured resistance and XAFS from the VO_2 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_2 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_1 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 $3d^1$ electrons, resulting in a Mott insulator in the M_2-phase VO_2. The anomalous structural disorder, particularly, at vanadium sites, effectively affects the migration of metallic electrons, resulting in the Mott insulating properties in M_2 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 $3d^1$ electrons in the R phase VO_2 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_2.

Keywords : metal-insulator transition, XAFS, VO_2, structural-phase transition
Conference Title : ICISET 2017 : International Conference on Innovative Science, Engineering and Technology
Conference Location : Cape Town, South Africa
Conference Dates : November 02-03, 2017