Insulator-metal phase transition coupled with structural deformation in electron-doped VO_2 thin films

D. Okuyama[1], K. Shibuya[1], Y. Kitagawa[2], R. Kumai[3], T. Suzuki[1], Y. Yamasaki[3], H. Nakao[3], Y. Murakami[3], M. Kawasaki[1,2], Y. Taguchi[1], T. Arima[4] and Y. Tokura[1,2]

[1]Cross-Correlated Materials Research Group (CMRG), and Correlated Electron Research Group (CERG), RIKEN-ASI, Wako 351-0198, Japan

[2]Department of Applied Physics, University of Tokyo, Tokyo 113-8656, Japan

[3]Condensed Matter Research Center and Photon Factory, Institute of Materials Structure Science, KEK, Tsukuba 305-0801, Japan

[4]Department of Advanced Materials Science, University of Tokyo, Kashiwa 277-8561, Japan

VO_2 has been attracting much interest as a typical material showing an insulator-metal transition above room temperature (∼340 K). In the insulator-metal transition, concomitant structural phase transition from tetragonal (rutile) to monoclinic (with alternate V-dimer) takes place with the emergence of (0 1/2 1/2) superlattice and (0 k l): k+l=*odd* forbidden reflections. A recent work on W-doped VO_2 thin films fabricated on TiO_2(001) substrate shows that the insulator phase (Insulator1) is suppressed as the electron doping proceeds [1]. In the W concentration (x) of 0.07≤ x ≤0.10 ($V_{1-x}W_xO_2$), metallic state was observed for the whole temperature range below room temperature. Furthermore, 0.10≤ x, another insulator phase (Insulator2) appears at low temperatures. For clarifying the driving mechanism of these Insulator1-Metal-Insulator2 transitions with electron doping, we performed synchrotron x-ray diffraction experiments at BL3A, PF.

Upon entering into the Insulator1 phase, we observed structural transition from tetragonal (rutile) to monoclinic with alternate V-dimer shown in Fig. 1, which is the same as the monoclinic structure of the bulk VO_2. In the metallic sample with x=0.08, no phase transition takes place. Associated with the transition to Insulator2, we observed an expansion of c-lattice constant analogous to that observed in Insulator1. However, (0 1/2 1/2) reflection was not observed, while the extinction rule for (0 0 odd) is broken. These structural data indicate that the crystal symmetry is not tetragonal but lower symmetry without alternate dimer of V ions. Furthermore, we found persistent x-ray induced structure and insulator-metal phase transition at several low-temperature points both in Insulator1 and Insulator2 phases as marked with cross symbols in the figure.

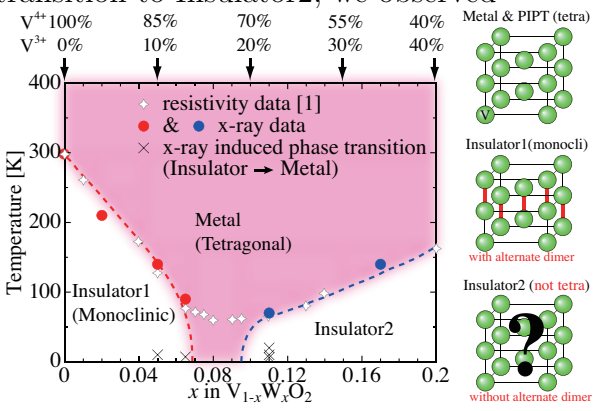

Figure 1: Phase diagram and corresponding crystal structure on W-doped VO_2 thin films.

[1] K. Shibuya, M. Kawasaki, and Y. Tokura, Appl. Phys. Lett. **96**, 022102 (2010).

[2] K. Shibuya, D. Okuyama, R. Kumai, Y. Yamasaki, H. Nakao, Y. Murakami, Y. Taguchi, T. Arima, M. Kawasaki, and Y. Tokura, Phys. Rev. B **84**, 165108 (2011).