Observation of metal-insulator transition in VO_2 by soft and hard x-ray photoelectron spectroscpy

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VO_2 is a 3d transition-metal oxide which undergoes the metal-insulator transition (MIT) at about 340K.The crystal structure changes from the monoclinic structure in the low temperature insulating phase to the rutile tetragonal structure in the high temperature metallic phase. It has been long debated whether these structural changes are due to electron-lattice interaction (resulting in a Peierls insulator) or electron-electron interaction (resulting in a Mott-Hubbard insulator). We have already performed the soft x-ray photoelectron spectroscopy (SX-PES) on VO_2 single crystals at BL25SU of SPring-8. Surface contributions are noticeable in the SX-PES spectra, although spectral changes were observed across MIT. To elucidate the bulk electronic structures of VO_2, We have performed the hard x-ray photoelectron spectroscopy (HAX-PES) on VO_2 single crystals at BL19LXU of SPring-8. For the spectra near the Fermi energy, a quasiparticle peak is observed in good agreement with the results of a cluster extension of dynamical mean-field theory (C-DMFT). [1] The HAX-PES results are consistent with the results of C-DMFT calculations. One can conclude that the insulating phase in VO_2 is a Peierls insulator affected by strong Coulomb interactions.

[1] S. Biermann et al. Phys. Rev. Lett. **94,** 026404 (2005).