Electronic structure of $3d^1$ configuration vanadium oxides studied by hard x-ray photoemission spectroscopy

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We investigate the electronic structure of the $3d^1$ configuration vanadium oxides VO_2, $SrVO_3$ and $CaVO_3$ using hard x-ray (7937 eV) photoemission spectroscopy (HX-PES) at undulator beam lne BL29XUL in SPring-8.

VO_2/TiO_2:Nb thin films exhibit a metal-insulator transition (MIT) as a function of temperature at T_{MI} = 295 K. The HX-PES valence band spectra clearly show the opening of a gap at E_F accompanying the MIT. Spectral changes in the V 2*p* and V 1*s* core levels were also observed as a function of temperature. In addition, $3d^1$ configuration metals $SrVO_3$ and $CaVO_3$ are typical materials whose valence band spectra are compared with the dynamical mean-field theory. The *d*-bandwidth can be controlled easily by the V-O-V bond angle, i.e., the *d*-bandwidth *W* of $SrVO_3$ is larger than that of $CaVO_3$. The V 2*p* and 1*s* core level HX-PES of $SrVO_3$ and $CaVO_3$ show clear additional well-screened features. These features originate from bulk screening by coherent band at E_F as observed in other 3*d* transition metal oxides. Comparison between $SrVO_3$ and $CaVO_3$ in HX-PES shows a small increase of the intensity of these well-screened features in $SrVO_3$. The spectra are nicely reproduced by a cluster model calculation, indicating a difference of the parameter V^* for the interaction strength between the central V 3*d* orbitals and the coherent band.