

Hydrogen Ordering of Layered Perovskite Oxyhydrides $\text{Sr}_2\text{VO}_{4-x}\text{H}_x$

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The Sr_2VO_4 is a representative layered K_2NiF_4 -type perovskite oxide composed of two-dimensional networks of corner-shared VO_6 octahedra [1]. The types of structures are well-known to exhibit various intriguing physical phenomena such as high- T_c superconductor $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$. The Sr_2VO_4 is a Mott insulator with a d^1 electronic configuration and indicates an antiferromagnetic ordered state with an orbital ordering transition around 97 K [2]. Recently, the hydrogen anion doped samples, $\text{Sr}_2\text{VO}_{4-x}\text{H}_x$ ($0.0 \leq x \leq 1.01$), were synthesized by the advanced high-hydrogen pressure method with controlling of the hydrogen/oxygen amounts [3]. The bipolar element hydrogen enables to change the valence states from -1 to $+1$. Moreover, the spatial spread of the H $1s$ -orbital is sensitive to the chemical environment. These unique characters are expected to provide new phenomena for mediating electronic and magnetic interactions.

Synchrotron powder X-ray diffraction measurements were performed for $\text{Sr}_2\text{VO}_{4-x}\text{H}_x$ using the curved imaging plate diffractometer (BL-8A) at KEK-PF. The X-ray powder-diffraction structural analysis with RIETAN-FP program [4] using high-resolution synchrotron radiation source provides the oxygen content with doping the hydrogen.

Figure 1 shows the crystal structures of $\text{Sr}_2\text{VO}_{4-x}\text{H}_x$ with various hydrogen contents. On refining the crystal structure, we checked the occupation of oxygen in the O1 and O2 sites, resulting in what we found the oxygen defect on the O1 site. Because the amount of hydrogen was obtained by integrating the thermal desorption spectrum, from the amount of oxygen vacancies on the structural refinement we can estimate the amount of hydrogen in the sample. The findings of the oxygen defect on O1 site is not the emergence of the defect but the site-selective doping of the hydrogen atom on the O1 site [3]. Moreover, the decrease of the bond length of V-O1/H1 was observed with increasing the hydrogen content.

Over the $x_{\text{nom}} = 1.0$, the tetragonal-orthorhombic transition was observed in the structural refinement by the neutron and X-ray diffraction measurements [3]. This is an interesting experimental finding of a new polymorph in the layered perovskite, which is originated by the doping and the ordering effect of the implanted hydride in

crystal. Taking account of the V-O-V magnetic interactions, the $\text{Sr}_2\text{VO}_{4-x}\text{H}_x$ is regarded as the two (one)-dimensional d^1 (d^2) magnet in $x=0$ (1.0).

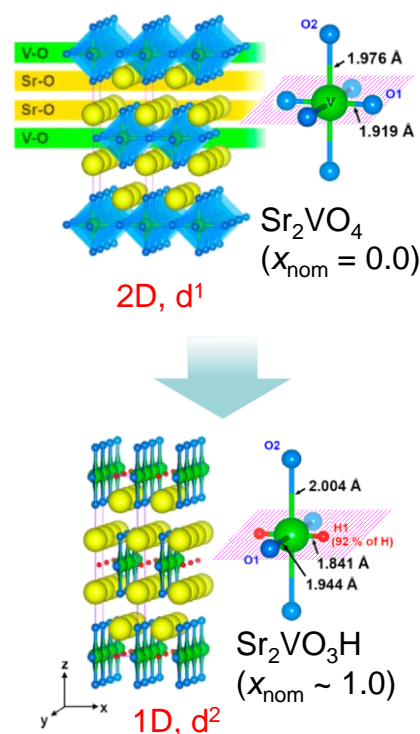


Fig.1 Crystal structures of $\text{Sr}_2\text{VO}_{4-x}\text{H}_x$ for $x = 0.0$ and 1.0 . They are regarded as the two-dimensional d^1 magnet and the one-dimensional d^2 magnet for $x = 0.0$ and 1.0 , respectively.

References

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