（ ※本報告書は英語で記述してください。ただし、産業利用課題として採択されている方は日本語で記述していただいても結構です。）

MLF Experimental Report	提出日 Date of Report 2017, Feb. 24
課題番号 Project No. 2014B0227 実験課題名 Title of experiment Crystal and magnetic structures of the vanadium oxide Sr2VO4 実験責任者名 Name of principal investigator Yoshiaki Kobayashi 所属 Affiliation Nagoya University	装置責任者 Name of responsible person Toru Ishigaki 装置名 Name of Instrument/（BL No.） BL-20 実施日 Date of Experiment 2014, 12, 18 - 2014, 12, 19

試料、実験方法、利用の結果得られた主なデータ、考察、結論等を、記述して下さい。（適宜、図表添付のこと）
Please report your samples, experimental method and results, discussion and conclusions. Please add figures and tables for better explanation.

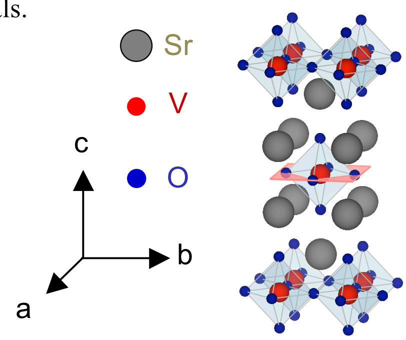
1. 試料 Name of sample(s) and chemical formula, or compositions including physical form.

Sample name: Vanadium oxide with one d-electron in the degenerated orbitals.

Chemical formula: Sr_2VO_4.

Structure: K_2NiF_4 structure (space group I4/mmm) at room temperature.

Sample condition: high purity powder samples prepared in the condition of high temperature and high pressure, and no oxygen deficiency was detected from chemical analysis.



2. 実験方法及び結果（実験がうまくいかなかった場合、その理由を記述してください。）

Experimental method and results. If you failed to conduct experiment as planned, please describe reasons.

We performed elastic neutron scattering measurements to investigate the precise atomic structure in the paramagnetic phase and spin structure in the magnetic ordered phase for the vanadium oxide with one d-electron in the degenerated orbitals, Sr_2VO_4, with no oxygen deficiencies, which has tetragonal structure with space group I4/mmm at room temperature, and temperature reduction brings about tetragonal-to-orthorhombic structural transition at T_{s1}=127 K and the 2nd structural transition from the orthorhombic one to tetragonal structures at T_{s2}=90 K. With further cooling, the Sr_2VO_4 occurs antiferromagnetic transition with Neel temperature (T_N) of 10 K.

The results of our ^{51}V-NMR measurement performed for the Sr_2VO_4 polycrystalline sample provide the potential for existence of the multi vanadium sites or anisotropic magnetic susceptibility. One of purposes of this research is clarify whether or not more than one vanadium sites and planer oxygen sites in the intermediate temperature region between T_{s2} of T_{s1} and in the lower tetragonal phase below T_{s2} from the precise structural analyses.

2. 実験方法及び結果（つづき） Experimental method and results (continued)

And another purpose is to illuminate the spin structure to be until now determined in the antiferromagnetic phase below T_N.

The neutron scattering for the Sr_2VO_4 polycrystalline sample was measured to know its precise oxygen positions. Large ambiguity of the vanadium position would remain if only neutron data were adopted, because vanadium has large absorption coefficient for neutron. To resolve it, we performed the Rietveld analysis of the neutron and x-ray diffraction patterns.

First, we present the results of the crystal structures of Sr_2VO_4. We found that single vanadium site is kept in the wide temperature range through the structural transition temperatures, and that the same structures as ones reported by Yamauchi *et al*. [1] and Zhou *et al*. [2] are realized and no phase with other structures is detected. This fact means that the ^{51}V-NMR spectral features should be interpreted by anisotropic magnetic properties of the one d-electron in the degenerated orbitals due to the effect of the strong spin-orbit coupling.

At this time, we cannot detect the difference of neutron diffraction patterns at 20 K and 4 K, which means that magnetic scattering is quite weak in the antiferromagnetic phase. This is probably attributable to small ordered magnetic moment or short-range correlation length.

At present, it is needed to explain consistently anisotropies of the Knight shift obtained from the ^{51}V-NMR spectra, and the magnetic susceptibility.

Therefore, this neutron diffraction study clarifies that there is only single vanadium site in Sr_2VO_4. We could narrow some ideas to explain the magnetic properties to a scenario.

[1] I. Yamauchi *et al*., Phys. Rev. B 92, 064408 (2015). [2] H. D. Zhou *et al*., Phys. Rev. B **81**, 212401 (2010).