

実験報告書様式(一般利用課題・成果公開利用)

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 MLF Experimental Report	提出日 Date of Report
課題番号 Project No. 2014A0197 実験課題名 Title of experiment Observation of local lattice distortion causing self-doping effect to half metallic ferromagnet CrO ₂ 実験責任者名 Name of principal investigator Katsuaki Kodama 所属 Affiliation Japan Atomic Energy Agency	装置責任者 Name of responsible person Toshiya Otomo 装置名 Name of Instrument/(BL No.) NOVA (BL21) 実施日 Date of Experiment 2014/4/25-27

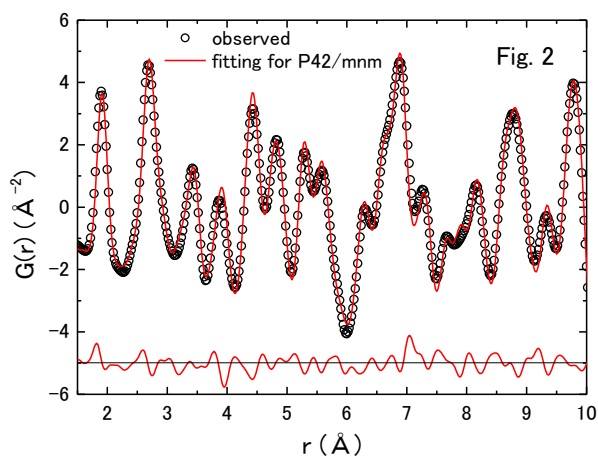
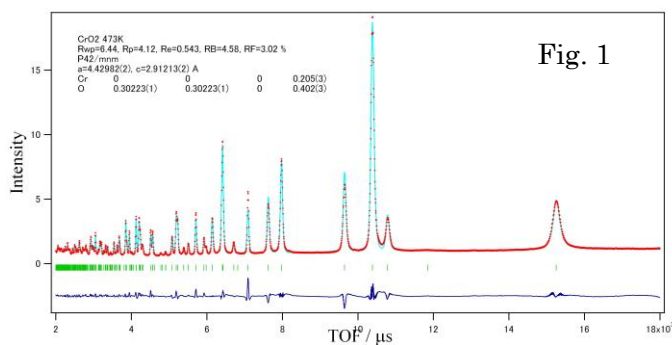
試料、実験方法、利用の結果得られた主なデータ、考察、結論等を、記述して下さい。(適宜、図表添付のこと)
 Please report your samples, experimental method and results, discussion and conclusions. Please add figures and tables for better explanation.

1. 試料 Name of sample(s) and chemical formula, or compositions including physical form.
Powder sample of CrO ₂ (about 1.7g)

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.
<p>The magnetic and transport properties of half metallic ferromagnets CrO₂ have been studied as a candidate of the spintronics materials. However, an origin of the metallic ferromagnetism in CrO₂ remains unsettled. As a mechanism of the metallic ferromagnetism in CrO₂, self-doping effect has been suggested. [1] In the recent NMR measurement, two kinds of Cr sites with different magnetic moments are observed, indicating two kinds of self-doped Cr sites with valences of +4±δ. [2] These results suggest that the self-doped carrier exhibits metallic ferromagnetism through the double exchange type mechanism. Although this scenario can explain metallic ferromagnetism in CrO₂, it is not consistent with the reported crystal structure including only single Cr site.</p> <p>In order to reveal the existence of two kinds of Cr site with different valence due to self-doping effect, we have perform PDF (atomic pair distribution function) analysis on powder neutron diffraction data of CrO₂ obtained by using NOVA. The diffraction data were collected at 50, 370, 410 and 473 K. First, we analyze the diffraction data at 473 K where the compound is in paramagnetic phase (The ferromagnetic transition temperature of CrO₂ is about 390 K). Figure 1 shows the diffraction patterns at 473 K and the fitting results by using z-Rietveld.</p>

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

In the analysis, the reported tetragonal structure with a space group $P4_2/mnm$ which has a single Cr site is used. The calculated line almost reproduces the observed diffraction pattern, confirming that the averaged structure at 473 K is the tetragonal with $P4_2/mnm$. In Fig. 2, the atomic pair distribution function $G(r)$ obtained at 473 K is shown by open circles. The red line shows the fitting result using the tetragonal structure with $P4_2/mnm$ corresponding with the averaged structure. Clear discrepancy between the observed and calculated $G(r)$ is not observed, indicating that the local lattice distortion which can be detected in the present experimental accuracy is absent, at least, at 473 K. According to the NMR measurement, the inequivalent Cr sites have to exist in the ferromagnetic phase. Then we should perform the local structural analysis on the data obtained at 50 K although the PDF analysis in the ferromagnetic phase is difficult because of including magnetic scattering component.



References

- [1] Korotin et al. Phys. Rev. Lett. 80 (1998) 4305.
- [2] Shim et al. Phys. Rev. Lett. 99 (2007) 057209.