| MLF Experimental Report | 提出日 Date of Report |
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| 課題番号 Project No.<br>2017A0010<br>実験課題名 Title of experiment<br>Determination of dispersion relation of magnetic excitations in the antiferromagnetic alternating spin-3/2 chain compound $NdCrTiO_5$<br>実験責任者名 Name of principal investigator<br>Masashi Hase<br>所属 Affiliation<br>National Institute for Materials Science | 装置責任者 Name of responsible person<br>Shinichi Itoh<br>装置名 Name of Instrument/（BL No.）<br>HRC (BL12)<br>実施日 Date of Experiment<br>May 25 to 27, 2017 |

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.

$NdCrTiO_5$ powder

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.

It is expected that $Cr^{3+}$ spins form an antiferromagnetic (AF) alternating spin-3/2 chain in $NdCrTiO_5$. The ground state (GS) of the chain is a spin-singlet state. A spin gap exists between the GS and first excited triplet states. Both Cr and Nd moments, however, are ordered simultaneously at the transition temperature $T_N$ = 21 K. In previous HRC experiments (Project No.:2012B0009), we observed a large spin gap (20 meV) in the isostructural compound $NdCrGeO_5$. The transition temperature is low ($T_N$ = 2.5 K). It is not confirmed whether Cr moments are ordered or not. We infer that a probably small spin gap leads to the high $T_N$ in $NdCrTiO_5$ In order to investigate magnetic excitations in $NdCrTiO_5$, we performed inelastic neutron scattering (INS) experiments on $NdCrTiO_5$ powder using the HRC spectrometer.

Figure 1(a) shows an INS intensity map in the Q-ω plane at 3.5 K. The energy of incident neutrons (Ei) is 51.2 meV. We can see strong excitations around ω = 6.9 meV and Q = 1.2 $Å^{-1}$. The Q value is consistent with that of the zone center of the Cr spin-3/2 chain. As inferred, the spin gap of $NdCrTiO_5$ is small. Excitations around Q = 1.2 $Å^{-1}$ exist up to 20 meV. We will determine the dispersion relation of the magnetic excitations along the spin chain using the conversion method developed by Tomiyasu et al. Excitations around 20 meV and 28 meV remain up to high Q. Probably, these are crystal-field excitations of Nd. Similar excitations were observed in $NdCrGeO_5$.

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

Figure 1(b) shows an INS intensity map at 3.5 K obtained using neutrons of Ei = 11.5 meV. Excitations exist around 3.4 and 5.5 meV. These excitations were observed in the data obtained using neutrons of Ei = 8.2 meV. Therefore, these are excitations of $NdCrTiO_5$. The excitations around 3.4, 5.5, and 6.9 meV shows a similar Q dependence. Probably, the excitations around 3.4 and 5.5 meV originate from Cr spins. We will consider the origin of these excitations. Excitations around 2 meV remain up to high Q. Probably, these are also crystal-field excitations of Nd.

We also performed INS experiments at 10.4, 15.4, 21.0, 26.0, and 200 K. Figures. 1(c) and (d) show an INS intensity map at 15.4 K obtained using neutrons of Ei = 11.5 and 51.2 meV, respectively. As the temperature is raised, the excitations between 6 and 20 meV seem to be shifted to lower energies. Similar temperature dependence was observed in compounds having a spin gap and AF order. Examples are the spin 1/2 tetramer compound $Cu_2CdB_2O_6$ and the spin 3/2 dimer compound $CrVMoO_7$. We will consider the origin of the temperature dependence.

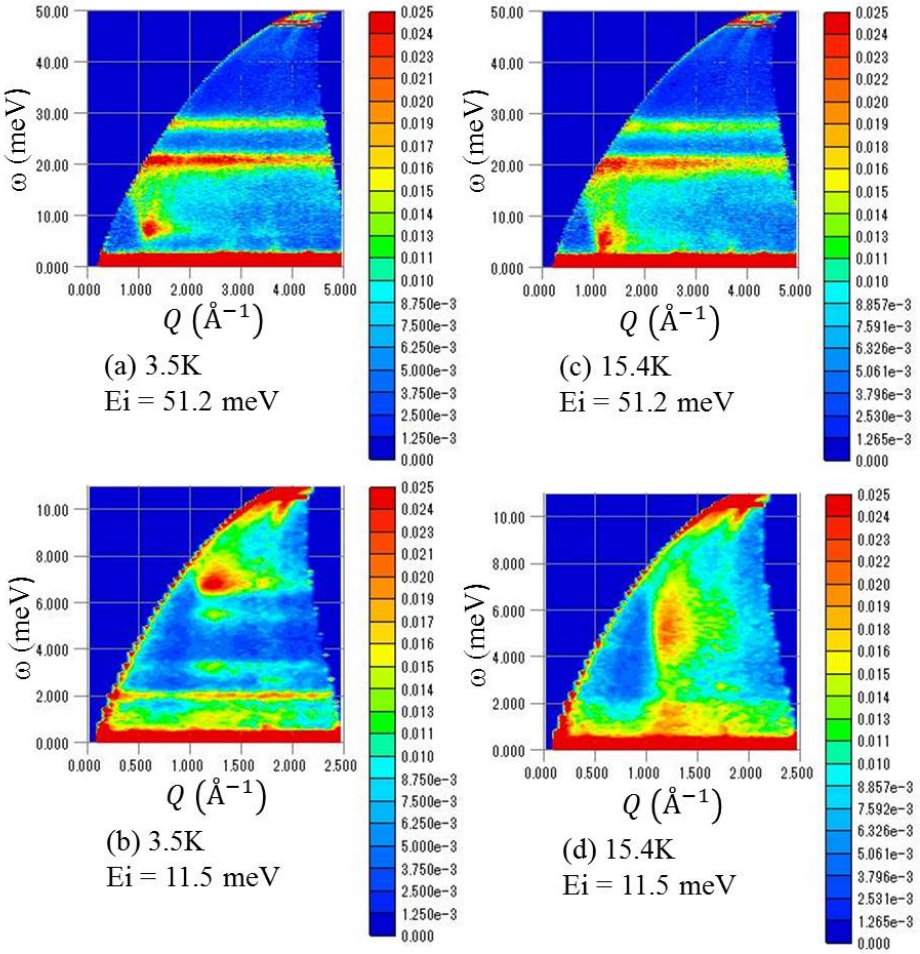


Fig 1　INS intensity maps of $NdCrTiO_5$ powder. The vertical and horizontal axes show the transfer energy and scattering vector magnitude, respectively.