2014B0261: Determination of magnetic structures in frustrated spinel ACr_2O_4 (A = Cu, Ni)

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1. Introduction

Frustrated magnets are promising sources for exotic spin-orbit-lattice states, such as the underlying structures for multi-ferroics, orbital ordering, and spin-orbit molecule organization. Spinel materials have been the typical and colorful series. In $CuCr_2O_4$ and $NiCr_2O_4$, Cr^{3+} (d^3, spin S = 3/2, no orbital degree of freedom) forms a highly frustrated corner-sharing tetrahedral lattice called a pyrochlore lattice and is coupled with magnetic and Jahn-Teller active Cu^{2+} and Ni^{2+}. The magnetic structures were studied by angle-dispersive powder neutron diffractometry [e.g., E. Prince (1957), M. Reehuis *et al.* (2015)]. Recently, however, careful high-resolution powder synchrotron x-ray diffraction experiments have revealed the new slight orthorhombic lattice deformation in the *Fddd* space group below magnetic transition temperatures for these materials [e.g., H. Ishibashi *et al.* (2007), M. R. Suchomel *et al.* (2012)]. Furthermore, a new magnetic phase was discovered between 125 K and 155 K in $CuCr_2O_4$. This prompted us to determine the magnetic structures by combining SuperHPRD and irreducible representation analysis.

2. Experiment

Neutron diffraction experiments were performed on the Super-High-Resolution Powder Diffractometer (SuperHRPD) at the MLF of the J-PARC. Approximately 3 g of the sample was sealed in a 6-mm-diameter thin V cylinder with He exchange gas, which was positioned under the cold head in a He closed-cycle refrigerator. The crystal and magnetic structures were analyzed using the FullProf and SARAh software.

3. Results and Conclusions

The measured and resultant analyzed data for $CuCr_2O_4$ are summarized in Fig. 1 as the representative. Both the measurements and the analyses of crystal and magnetic structures were successfully completed. We submitted this result and is now under review.

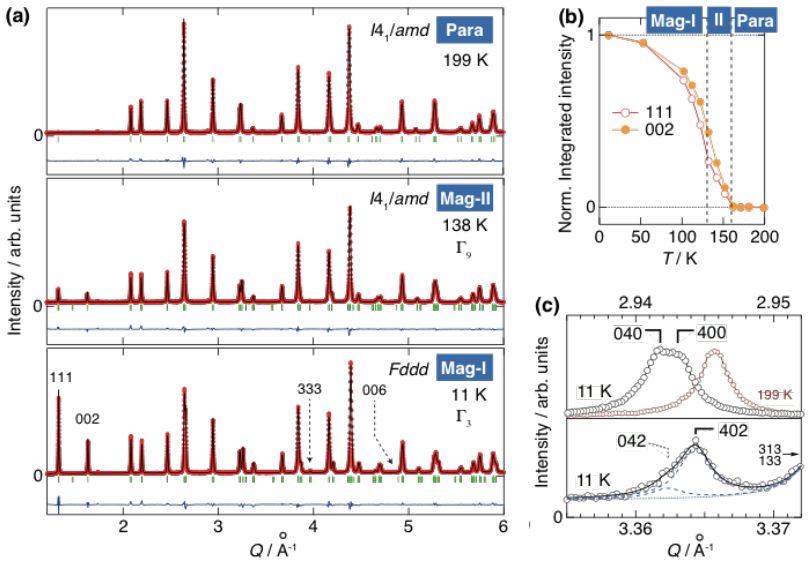

FIG. 1: (a) Powder neutron diffraction patterns measured in the middle bank in the three phases. The fitting curves were obtained for the crystal and magnetic structures described by the displayed symmetries. (b) Temperature dependence of the 111 and 002 integrated intensities normalized at 11 K. (c) Selected reflections recorded at 11 K in the backward bank. The curves in the lower panel are the fitting results obtained in the Γ_3 magnetic structure.