

Magnetic and Crystal Structures of Tm₂CrS₄

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Y₂CrS₄ shows an antiferromagnetic transition at 65 K due to the ordering of Cr²⁺ ions. Its powder neutron diffraction patterns at both 90 K and 10 K could be refined by using the orthorhombic Er₂CrS₄-type structure (Pca2₁, No. 29) [1,2] while the magnetic structure was determined by using the pattern at 10 K. Recently we measured magnetic susceptibility of Tm₂CrS₄ and found magnetic anomalies at ca. 60 K and lower temperatures.

In this study, neutron diffraction measurements of Tm₂CrS₄ were performed at 80 K, 50 K, 40 K, 15 K, 10 K, and 3 K, on the high efficiency and resolution powder diffractometer, HERMES, of Institute for Materials Research, Tohoku University, installed at the JRR-3M Reactor in JAEA (Tokai). The wavelength of a neutron incident is 1.8265

Any distinct crystallographic phase transition was not observed between 80 K and 3 K. At 80 K, lattice parameters were determined to be $a = 12.4337(13)$ Å, $b = 7.4470(8)$ Å, and $c = 12.4082(13)$ Å, and decreased with decreasing temperature. Rietveld refinements confirmed that the crystal structure was isomorphous with Y₂CrS₄ at all measured temperatures.

Below 60 K, some magnetic peaks were observed and the peak intensities were gradually increased with decreasing temperature. This suggests that paramagnetic chromium and thulium ions were ordered together. These magnetic peaks could be indexed on the same crystallographic unit cell. In order to determine the magnetic structure, the magnetic peaks have been analyzed with the following assumptions. (1) Magnitudes of magnetic moments of chromium and thulium ions are the same

for respective kinds of ions. (2) Magnitudes of magnetic moments for chromium were fixed to be 3.27 Bohr magneton obtained by the refinement of neutron diffraction patterns at 10 K for Y₂CrS₄ [1,2]. (3) The directions of all magnetic moments are collinear. These assumptions have led to a magnetic structure as shown in Fig. 1. In this structure, magnetic moments of chromium and thulium ions order antiferromagnetically in each set of the 4a sites. The directions of all magnetic moments are parallel to the *c* axis. The refined magnetic moment of Tm is 4.57(4) Bohr magneton, which is smaller than 7 Bohr magneton expected as the trivalent free ions.

References

- [1] K. Tezuka et al., QuBS 2006, August 2006, Ricotti (Tokai, Japan), P-28-39.
- [2] K. Tezuka et al., Activity Report on Neutron Scattering Research: Experimental Reports, Vol. 13, nact06-33342.

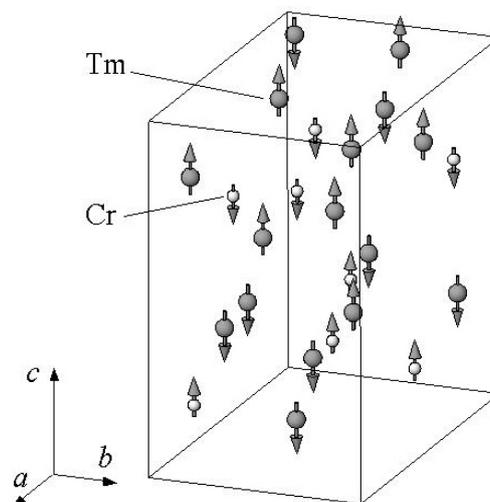


Fig. 1. Magnetic structure of Tm₂CrS₄.