Magnetic structural analysis of Pt_3Fe antiferromagnet by single crystal neutron diffraction

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Pt_3Fe exhibits antiferromagnetic ordering below T_{N1}~170K with a propagation wave vector $\mathbf{q}_1$=(1/2 1/2 0). However, when the chemical compostion slightly deviates from the stoichiometric Pt_3Fe towards Fe rich side, additional magnetic phase transition occurs at T_{N2}~110K and two types of magnetic ordering with $\mathbf{q}_1$ = (1/2 1/2 0) and $\mathbf{q}_2$ = (1/2 0 0) coexist [1]. So far, both magnetic domain model and noncollinear magnetic structural model were proposed [2]; however, the magnetic structure is still controversial. In this study, we performed a detailed magnetic structural analysis by a single crystal neutron diffraction to clarify the magnetic structure of non-stoichiometric Pt_3Fe.

We used the Pt_3Fe (Fe:25.6 at.%) single crystal with dimensions of 2.2×2.4×2.6mm^3. Neutron diffraction measurements were performed using four-circle off centered diffractometer (FONDER). We measured approximately 40 and 45 magnetic Bragg reflections for (1/2 1/2 0)-type and (1/2 0 0)-type magnetic structures, respectively, at T=10 K and 120 K.

Figure 1 shows the temperature dependence of the neutron scattering intensity. As the temperature decreases, the (1/2 1/2 0)-type magnetic reflections appear at T_{N1} and their intensities develop. At T=120 K just above T_{N2}, the neutron intensity at (0 1/2 1/2), (1/2 0 1/2) and (1/2 1/2 0) is almost the same, indicating that magnetic domains with $\mathbf{q}_1$ =(1/2 1/2 0), (1/2 0 1/2) or (0 1/2 1/2) coexist in a crystal with almost the same volume fraction. As the temperature is further reduced, (1/2 0 0)-type magnetic reflections start to develop below T_{N2}, associated with the sharp drop of the (1/2 1/2 0)-type ones. However, neutron intensity at (1/2 0 1/2) was not reduced at T_{N2} and very weakly temperature dependent below T_{N2}.

To determine the magnetic structure, observed neutron intensities (I_{obs}) were compared with calculated ones (I_{cal}) at T= 10 K assuming magnetic domain model. The I_{obs}- I_{cal} curve shows a good linearity for both types of magnetic structures. At T=120 K above T_{N2}, the domain model also well explains the observed results and the volume fraction of (0 1/2 1/2), (1/2 0 1/2), (1/2 1/2 0) magnetic structures was 30.4%, 36.8%, 32.8%, respectively. On the other hand, at T=10K, the volume fraction of (0 1/2 1/2), (1/2 0 1/2), (1/2 1/2 0), (1/2 0 0), (0 1/2 0), (1/2 0 0) magnetic structure was 11.8%, 21.2%, 13.9%, 18.2%, 19.0%, and 16.0%. Such difference indicates that large spin reorientation can occur at T_{N2} when the (1/2 0 0)-type domains are formed. Noncollinear magnetic structural model might be possible to explain the observed intensities, however, each domain should have different spin tilt angle.

[1] G.E. Bacon et al., Proc. R. Soc. A 272, 387, 1963.

[2] R. Matsui, Y. Tsunoda, J. Phys.: Condens. Matter vol. 21, 124209, 2009.

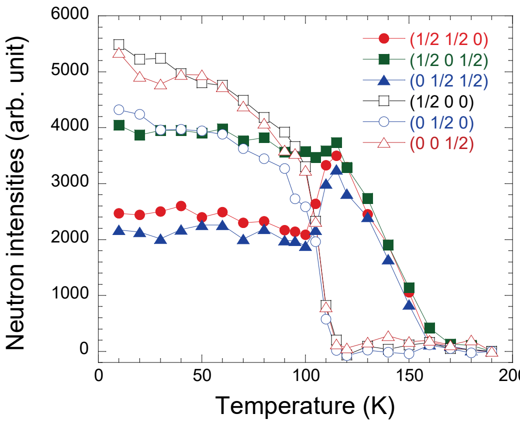

Fig. 1. Temperature dependence of magnetic neutron intensities at (1/2 1/2 0), (1/2 0 1/2), (0 1/2 1/2), (1/2 0 0), (0 1/2 0), (0 0 1/2) magnetic Bragg points.