Investigation of magnetic structures of β -NaFeO₂ Single Crystal

The magnetization measurement on β -NaFeO₂ single crystal shows a transition at 120 K. Single crystal neutron diffraction reveals incommensurate peaks, suggesting an incommensurate spin structure. To investigate this structure, we attempted to grow more crystals for neutron experiment. However, further investigations into the low-temperature magnetic structures is challenging due to unstable growth parameters.

NaFeO₂ is crystallized in three different structures namely α , β , and γ -phase. a-NaFeO₂ is an antiferromagnet that has a rock-salt type crystal structure with R-3m space aroup similar to the multiferroic delafosite CuFeO₂. Systematic analyses by means of magnetization measurement and diffraction neutron revealed rich magneto-electric phase diagrams [1,2]. β -NaFeO₂ is also an antiferromagnet with $T_N \sim$ 720 K [3]. However, compared to the a--phase, the magnetic orderings in β -NaFeO₂ are still unexplored.

In our previous work, we obtained a single crystal of β -NaFeO₂ using the floating zone method. Careful characterizations on this crystal revealed a single-phase compound with an orthorhombic structure belonging to *Pna*2₁ space group.

Magnetization measurement on this crystal from 400 K to 3 K revealed several transitions, namely two kinks at around 120 K and 20 K which were observed along a and b-axes. The kink at 120 K is absent in c-axis. These anomalies hint at a magnetic transition that to our knowledge has not been reported yet.

In order to investigate these anomalies, we performed single crystal diffraction using AKANE facility in JRR-3 in collaboration with the group of Prof. M. Fujita. At room temperature, there are three magnetic reflections labeled as (100), (101), and (020). By scanning the momentum diagonally around (101) peak we revealed three incommensurate peaks as shown in Fig. 2 (a). These peaks were fitted using Gaussian function. We find that the position of the peak q2 and q3 remain unchanged with temperature. Interestingly, the position of q1 changes at around 140 K. This temperature is close to the observed high-temperature kink in magnetization data as shown in Fig. 2(b). Such feature indicates a an incommensurate spin structure.

To get more insight into this magnetic structure, we need to get information about the low-temperature magnetic structures of this compound. To do this we attempted to grow more single crystals in Institute Materials Research, Tohoku University, Sendai. The growth was performed using floating zone technique following the growth parameters we used before. We obtained several crystal boules with typical lengths of 20 mm and diameters of 5 mm. The XRD indicates a single-phase material. However, the Laue image taken for several crystal boules from different batches show an unclear reflection pattern. This indicates the quality of the crystal is still not so good compared to the one we used for neutron diffraction measurement. Possibly, this is due to the unstable growth parameters. These results make further investigation on the magnetic structure still inaccessible and thus further attempts at crystal growth are necessary in the future.



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