Investigation of magnetic structure of Fe-based superconductor Ca1-xLaxFeAs2

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For all of the Fe-based superconductors, the superconductivity appears with carrier-doping into a magnetic ordered state. Recently, it has been found in $LaFeAsO_{1-x}H_x$ that the superconductivity phase forms two-dome structure [1], which is sandwiched by two magnetic ordered phases as low-(SDW1) and high-electron-doped regime (SDW2) [2]. This suggests that the second dome of the superconductivity at higher doping region is associated with the SDW2. The superconducting transition temperature, T_c, in the second dome is higher than the first one, and the two superconducting phases seem to integrate in other 1111-type with different rare-earth element such as $SmFeAsO_{1-x}H_x$ with the maximum T_c of over 50 K [3]. Therefore, study of magnetism in the high doped region as well as low doped one is important to understand the mechanism of the Fe-based superconductivity with higher T_c.

Recently, new family of Fe-based superconductor of 112-type $Ca_{1-x}La_xFeAs_2$ has been discovered. In this family, T_c reaches 34 K with $x = 0.16$, decreases with electron doping through La^{3+}-substitution for Ca^{2+} and disappears toward $x \sim 0.25$. Intriguingly, a magnetism in high-doped region has been suggested from an anomaly in the resistivity observed at ~60 K with $x = 0.18$ – 0.25. This anomaly is probably caused by magnetic ordering. In fact, a nuclear magnetic resonance measurement suggests a sign of an antiferromagnetic ordering at T_{anom} [4]. Considering that the anomaly appears in rather-high-doped regime, the possible magnetism seems to be induced by the electron doping. Thus, the 112-type iron arsenides might be the second example of the novel magnetism of SDW2 which may hold the key to high T_c. Nevertheless, the magnetic structure has not been determined yet.

Therefore, we have conducted neutron diffraction measurements using HB2C (WAND) installed at HFIR, Oak Ridge National Laboratory. A single crystal of $Ca_{0.77}La_{0.23}FeAs_2$ was used for the measurement. The samples were prepared using the self-flux method, of which details are described in Ref. [5]. The sample is ~20 mg and the dimension is $1 \times 1 \times 0.1$ mm.

We first tried to decide the crystal orientation and scanned with the scattering plane as (HK0) reciprocal plane. Although we have found nuclear reflections of (2,0,0) and (0,2,0), some unexplainable problems prevented us from finding other peaks. For example, although the (2,0,0) reflection has observed at $\omega \sim 24.8^\circ$ in ω scans at around the detectors of $2\theta = 44^\circ$, the reflection disappeared unaccountably in tilt scans at $\omega = 24.8^\circ$. Another trouble is that the (2,0,0) peak is observed only with the specific step size. The (2,0,0) peak observed in the scan with the step size of 0.2° in ω scans disappears with smaller step sizes of 0.1 or 0.05° on the same condition for the rest. Causes for the troubles have not been clarified even now. To avoid consuming much time in fix the crystal orientation, we have changed the plan and switched to powder diffraction measurements.

Figure shows the powder diffraction pattern for $La_{0.77}La_{0.23}FeAs_2$ at 10 K and 100 K. The data of 100 K is shifted vertically for clarity. Calculated patterns for the 112 phase and FeAs phase as an impurity are also shown at the bottom of the figure. It is clear that the peaks from the impurity phase is as dominant as the main phase of the 112. This impurity is derived from the flux which was inevitably mixed with the sample when the powder sample is prepared on site. Even after collecting data for several days, any sign of magnetic reflections was not recognized in the difference

between the data of 10 K and 100 K. Considering the large dominance of the impurity as well as the large background, this result does not mean there is no magnetic reflections. Rather, possible magnetic reflections might be no higher than the ripples of background. To detect the magnetic reflection, a large amount of sample collected by picking many tiny fractions of single crystals buried in the flux is necessary.

References [1] S. Iimura et al. Nat Commun. 3, 943 (2012). [2] M. Hiraishi et al., Nat. Phys. 10, 300 (2014). [3] S. Matsuishi et al., Phys. Rev. B 89, 094510 (2014). [4] S. Kawasaki et al., Phys. Rev. B 92, 180508(R) (2015). [5] N. Katayama et al., J. Phys. Soc. Jpn. 82, 123702 (2013).

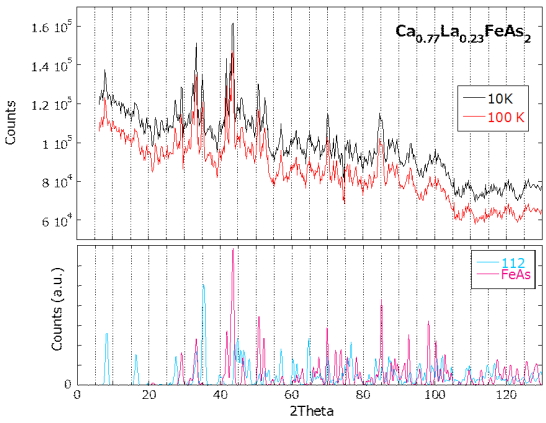

Fig. 1. Neutron diffraction pattern of the powder sample and calculated patterns of the 112 phase and FeAs.