Magnetic structure of the new iron arsenide $CaFe_4As_3$

Y. Nambu[1], H. Kimura[2], Y. Noda[2], and T.J. Sato[1]
[1]*ISSP–NSL, University of Tokyo,* [2]*IMRAM, Tohoku University*

The recent discovery of superconductivity (SC) in iron pnictides has opened a new chapter in SC research. A square iron chalgogenide/pnictide plane is a common theme in this family, which so far has been realized in the ZrCuSiAs (1111), $ThCr_2Si_2$ (122), anti-PbO (11) and Cu_2Sb (111) structures. Recently, chemically related $CaFe_4As_3$ has showed up to the stage. Similar to other parent compounds, $CaFe_4As_3$ is not superconducting down to 1.8 K. The novel framework structure is composed of shared FeAs tetrahedra with Ca atoms in the channels. Extending along the b-axis are FeAs strips where 4-fold As coordinated Fe occupy an approximately square lattice of finite width. Fe atoms that link strips (Fe4) on the other hand form $FeAs_5$ pyramids. Two phase transitions were detected through bulk properties. While only the upper transition at $T_N \sim 90$ K is marked by a significant specific heat anomaly, the lower one at $T_2 \sim 26$ K yields a strong reduction in resistivity. From previous experiments [1], we showed that the upper transition is to a longitudinal incommensurate (IC) spin density wave and the lower one is associated with the development of a transverse component and an apparent lock-in to commensurate order, which occurs in a 1st order fashion. Since the previous elucidation was based on only several data points obtained by a triple-axis spectrometer, detailed clarification of this complex magnetic structures with using e.g., a four-circle diffractometer is highly desired.

The measurements were performed at the four circle neutron di?ractometer T2-2 FONDER installed at JRR-3M. Both nuclear and magnetic reflections were collected at $T = 50$ and 10 K. Figure 1 depicts a comparison of observed and calculated squared nuclear structure factor taken at 10 K. Prior to the magnetic structure refinement, scale factor, atomic positions and Debye-Waller factors has been decided. We employed representation analysis to determine magnetic structures. Consistent with the previous result by the triple-axis experiments [1], magnetic structure at the IC phase is belonging to irreducible representation (irrep), τ_4 at 50 K. In the commensurate phase at 10 K, the system experiences the 1st order transition, leading the possibility of the magnetic structure belonging to irreps more than one. We assumed Fe4 (1+, 5-fold) is likely responsible for the 1st order transition and sort out all possibilities with keeping moments of Fe4 in any irreps. It turned out that the resultant magnetic structure with the best fit is involving the distinct irrep, τ_1 in Fe4.

[1] Y. Nambu *et al.*, Phys. Rev. Lett. **106**, 037201 (2011).

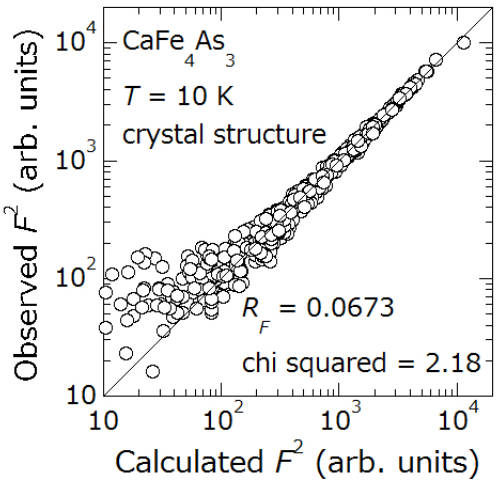

Fig. 1. Observed and calculated F^2 of $CaFe_4As_3$ at $T = 10$ K.