実験報告書様式（一般利用課題・成果公開利用）

（ ※本報告書は英語で記述してください。ただし、産業利用課題として採択されている方は日本語で記述していただいても結構です。）

TOKAI CROSS **Experimental Report** J-PARC	提出日 Date of Report 27, August
課題番号 Project No. 2012A0001(U) 実験課題名 Title of experiment Analysis of spin dynamics in iron-based superconductor $LaFeAsO_{1-x}H_x$ 実験責任者名 Name of principal investigator Satoru Matsuishi 所属 Affiliation Materials and Structure Laboratory, Tokyo Institute of Technology	装置責任者 Name of responsible person Ryoichi Kajimoto 装置名 Name of Instrument/（BL No.） 4D Space Access Neutron Spectrometer (BL-01) 実施日時 Date and time of Experiment 21-26, June

試料、実験方法、利用の結果得られた主なデータ、考察、結論等を、記述して下さい。（適宜、図表添付のこと）
Please report your samples, experimental method and results, discussion and conclusions. Please add figures and tables for better explanation.

1. 試料 Name of sample(s) and chemical formula, or compositions including physical form.

[Sample]

Chemical formulas	Mass / g	Superconducting temperature / K
$LaFeAsO_{0.9}D_{0.1}$	30	27
$LaFeAsO_{0.8}D_{0.2}$	30	14
$LaFeAsO_{0.75}D_{0.35}$	30	34

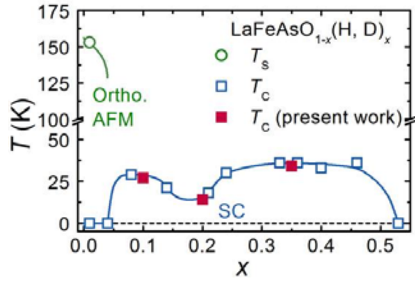

Figure 1: Phase diagram of $LaFeAsO_{1-x}(H, D)_x$

2. 実験方法及び結果（実験がうまくいかなかった場合、その理由を記述してください。）

Experimental method and results. If you failed to conduct experiment as planned, please describe reasons.

We performed inelastic neutron scattering (INS) measurements using the Fermi chopper spectrometer 4SEASONS at Materials and Life Science Experimental Facility (MLF) in Japan Proton Accelerator Research Complex (J-PARC) on $LaFeAsO_{1-x}D_x$ at temperature of 7 K. For the sample of $x = 0.35$, a high-temperature measurement at 150 K was also performed. To remove the background, INS from empty aluminum sample holder was measured at 7 K. We employed the multi-E_i method with incident neutron energies of $E_i = 151.4$, 45.5, 21.6, 12.6, and 8.2 meV. The measuring time of each sample and the sample holder were 27 hours and 18 hours, respectively, at the beam power of 210 kW.

Figure 2 shows INS intensity as a function of momentum transfer (Q) with several fixed energy transfers (E). For $x = 0.35$, phonon contributions were estimated from the data at 150 K and subtracted from data at 7 K to extract magnetic signals. The sample of $x = 0.1$ shows a peak centered at $(Q, E) = (1.1\ \text{Å}^{-1}, 15 \pm 0.5\ \text{meV})$ which has previously been observed in $LaFeAsO_{1-x}F_x$. However, the signal to noise ratio of the peak is smaller than that of $LaFeAsO_{1-x}F_x$ due to high background level arising from the strong incoherent scattering by impurity proton.

2. 実験方法及び結果（つづき） Experimental method and results (continued)

For x = 0.2 and 0.35, the peak disappears at E = 15 meV or less. Instead, for x = 0.35, another magnetic peak arises at the (Q, E) = (~1.3, 18 ± 0.5). By assuming that the observed signals are the superconducting resonant modes with resonance energy (E_r) of 15 and 18 meV, the E_r correspond to 6.4 and 6.1 k_BT_C, respectively, which are somewhat higher than that of other iron-based superconductors (4.3-5.4 k_BT_C).

To investigate the origin of magnetic scattering peaks, we performed the density functional theory (DFT) calculation for $LaFeAsO_{1-x}D_x$. **Figure 3** shows the calculated Fermi surface (FS) with orbital character ($d_{yz,xz}$ and d_{xy}). Based on the spin fluctuation theory, we focus on the only excitations between the states on FS with same orbital character.. Since the hole pockets around $\boldsymbol{k}$ = (0, 0) are almost same size as the electron pocket around $\boldsymbol{k}$ = (π, 0) at x = 0.1, the nesting between the hole and electron pockets is strong. The length of nesting vector $|\boldsymbol{Q}|$ ~ 1.1 $Å^{-1}$ is close to the momentum transfer of observed peak at x = 0.1, so that the INS with (Q, E) = (1.1, 15) would be derived from the FS nesting. As x increases, the nesting monotonically weakens because the hole pockets are gradually shrunken while the electron pockets are expanded. On the other hands, since the energy bands forming the hole pockets around $\boldsymbol{k}$ = (0, 0) are flattened and degenerated along the k_z direction, the hole pockets have large density of states (DOS) at x = 0.35 where the hole pockets are about to disappear (see a lower panels in **Fig. 3**). Therefore, the spin excitations along the $\boldsymbol{Q}$ ~ (π, 0.35π) whose length is about 1.2 $Å^{-1}$ would re-increase at x = 0.35. As a consequence, we suggest that the magnetic peak observed at x = 0.35 would be incommensurate spin fluctuations derived from the excitations between the hole and electron pockets.

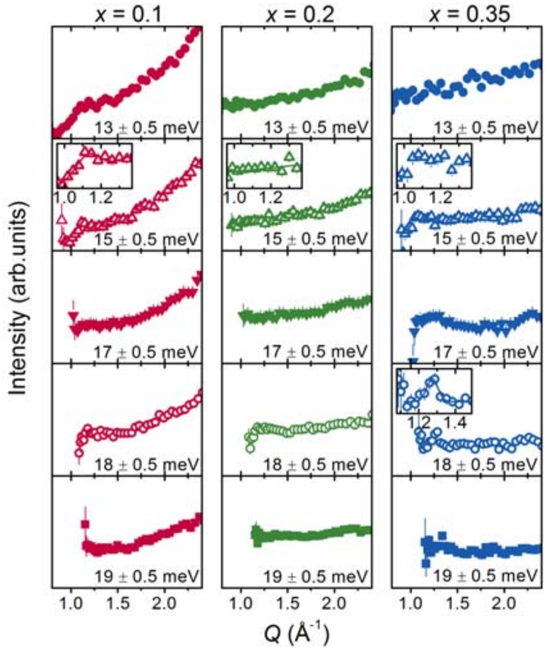

Figure 2: Neutron-scattering profiles scanned as a function of momentum transfer Q with fixed energy transfers. The incident energy is 45.5 meV.

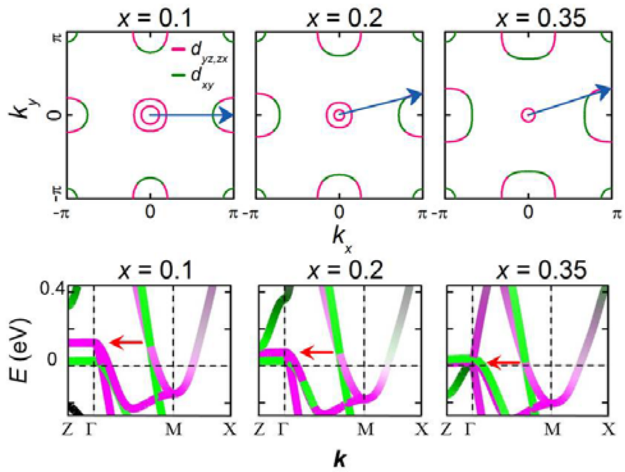

Figure 3: Upper: Unfolded 2D FS. The arrows are nesting vectors. Lower: Folded band structure. The arrows indicate the degenerate band.

We performed INS measurements on $LaFeAsO_{1-x}D_x$. The magnetic scattering with Q = 1.3 $Å^{-1}$ and E = 18 meV were newly observed at x = 0.35. The results of DFT calculations suggest that the scattering is originated in the excitations between electron pockets and hole pockets with large DOS. The present results imply that the high-T_C second dome may be induced by the incommensurate spin fluctuations with Q = 1.3 $Å^{-1}$.